
Supplementary Information

Unraveling the Mechanisms of Ketene Generation and Transformation in Syngas-to-Olefins Conversion over ZnCrO_x/SAPO-34 Catalysts

Zhuo-Yan Yao,¹ Sicong Ma^{2*} and Zhi-Pan Liu^{1,2*}

¹ State Key Laboratory of Porous Materials for Separation and Conversion, Collaborative Innovation Center of Chemistry for Energy Material, Shanghai Key Laboratory of Molecular Catalysis and Innovative Materials, Key Laboratory of Computational Physical Science, Department of Chemistry, Fudan University, Shanghai 200433, China

² State Key Laboratory of Metal Organic Chemistry, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, Shanghai 200032, China

Corresponding Author: *scma@mail.sioc.ac.cn; *zpliu@fudan.edu.cn

TOF evaluation of experimental CO conversion on the ZnCrO_x/SAPO-34 catalyst

The evaluation of Turnover Frequency (TOF) is defined as the number of reactant molecules converted per active site per unit time. For the CO conversion reaction, the TOF can be expressed as:

$$TOF = \frac{N_{CO}}{N_{Active\ Site} \cdot dt}$$

Where N_{CO} is the number of CO molecules converted, $N_{Active\ Site}$ is the number of active sites available on the catalyst surface, and dt is the time interval over which the reaction occurs.

To further elaborate, N_{CO} can be related to the molar quantity of CO (n_{CO}) using Avogadro's number, while $N_{Active\ Site}$ can be expressed in terms of the molar quantity of active sites ($n_{Active\ Site}$). Thus, the TOF can be rewritten as:

$$TOF = \frac{n_{CO}}{n_{Active\ Site} \cdot dt}$$

Here, n_{CO} is determined by the ideal gas law:

$$n_{CO} = \frac{pV}{RT} = \frac{p \cdot SV \cdot m_{zeo} \cdot dt}{RT}$$

where: p is the partial pressure of CO, V is the volume of the gas, R is the universal gas constant, T is the reaction temperature. The volume V can further be expressed according to the definition of space velocity (SV) by:

$$V = SV \cdot m_{zeo} \cdot dt$$

Similarly, $n_{Active\ Site}$ is related to the density of active sites H^* (ρ_H) and the mass of the zeolite catalyst (m_{zeo}) by:

$$n_{Active\ Site} = \rho_H \cdot m_{zeo}$$

Substituting these expressions into the TOF equation yields:

$$TOF = \frac{\frac{p \cdot SV \cdot m_{zeo} \cdot dt}{RT}}{\rho_H \cdot m_{zeo} \cdot dt} = \frac{p \cdot SV \cdot m_{zeo} \cdot dt}{\rho_H \cdot m_{zeo} \cdot RT \cdot dt} = \frac{p \cdot SV}{\rho_H \cdot RT}$$

Finally, by incorporating the total pressure (p_{CO}) and the conversion percentage (Cov%), the TOF can be expressed as:

$$TOF = \frac{p_{CO} \cdot Cov\% \cdot SV}{\rho_H \cdot RT}$$

Using the experimental conditions¹ of $p_{CO} = \frac{2.5 \times 10^6}{3.5}$ Pa, $Cov\% = 28\%$, $SV = 5143 \text{ mL } g_{cat}^{-1} h^{-1} = \frac{5143 \times 10^{-6}}{3600} \text{ m}^3 g_{cat}^{-1} s^{-1}$, $R = 8.314 \text{ J mol}^{-1} K^{-1}$, $T = 673 \text{ K}$. The density of active sites H^* (ρ_H) is estimated based on the molecular formula of H-SAPO-34, which is derived from the feed ratio in the zeolite synthesis process ($SiO_2:AlO_{1.5}:PO_{2.5} = 0.48:2:1.6$). The molecular formula of H-SAPO-34 can be

written by $\text{HSiAl}_5\text{P}_4\text{O}_{10} \cdot 0.2\text{SiO}_2$, with a relative molecular mass of $M_{zeo} = 459.91 \text{ g mol}^{-1}$. Thus, the density of active sites H^* (ρ_H) is given by:

$$\rho_H = \frac{1}{M_{zeo}} = \frac{1}{459.91} \text{ mol g}_{cat}^{-1}$$

The TOF was calculated to be:

$$TOF = \frac{\frac{2.5 \times 10^6}{3.5} \cdot 28 \% \cdot \frac{5143 \times 10^{-6}}{3600}}{\frac{1}{459.91} \cdot 8.314 \cdot 673} \approx 0.0235 \text{ s}^{-1}$$

This value indicates that each active site converts approximately 0.0235 CO molecules per second under the given reaction conditions.

CH₃OH and CH₂CO diffusion in the SAPO-34 catalyst

In order to evaluate how the diffusion of two key intermediates influence the reaction network, we have conducted umbrella sampling molecular dynamics with global neural network (G-NN) potential energy surface (PES) to extract the free energy barrier of diffusion across zeolite cages of CH₃OH and CH₂CO, as shown in Figure S9.

➤ Constrained Molecular Dynamics Sampling Method

In order to evaluate the diffusion of molecules across the zeolite cages, the traditional molecular dynamics (MD) method is quite inefficient due to most of the sampling locates within a specific zeolite cage. As a consequence, constrained MD utilizing umbrella sampling (US) method^{2,3} is adopted to mimic the diffusion process. The MD simulations were carried out in the canonical ensemble with a Nose-Hoover thermostat under 373 K/673 K with a time step of 1 fs interval. The total time is set to be 50 ps, with the first 5 ps to reach equilibrium and rest for production. For the US method, the reaction coordinate is defined as the molecules center along the z axis and is divided into 50 windows. The US method is achieved by imposing the harmonic bias potential to constrain a designated reaction coordinate ξ_i^{ref} for each window i .

$$\omega_i = \frac{K}{2}(\xi - \xi_i^{ref})^2$$

The resulting biased probability at each window $P_i^b(\xi)$ can be collected from MD simulation⁴:

$$P_i^b(\xi) = \frac{\exp \int \{-\beta[E(r) + \omega_i(\xi'(r))]\} \delta[\xi'(r) - \xi] d^N r}{\exp \int \{-\beta[E(r) + \omega_i(\xi'(r))]\} d^N r}$$

The derivative of free energy to the reaction coordinate ξ , $\frac{\partial G_i}{\partial \xi}$ can be derived from the following equation:

$$\frac{\partial G_i}{\partial \xi} = \frac{1}{\beta} \cdot \frac{\xi - \bar{\xi}_i^b}{(\sigma_i^b)^2} - K(\xi - \xi_i^{ref})$$

where $\bar{\xi}_i^b$ represents the mean value of ξ and σ_i^b represents the variance.

In this work, the force constant K for harmonic bias potential is set to 10.0 eV Å⁻² to keep the appropriate overlap of ξ between windows. The z coordinate varies from 3.0 Å to 15.0 Å during the US MD sampling process. For the CH₂CO diffusion, due to its highly reactive properties at high temperature, an additional harmonic bias potential was applied to C-C bond at its equilibrium bond length (1.31 Å). The force constant K of C-C binding potential is set as 100.0 eV Å⁻².

➤ Diffusion Free Energy Barrier of CH₃OH and CH₂CO

The diffusion free energy profile of CH₃OH and CH₂CO is plotted in Figure S9. In order to avoid potential influence of molecule interaction in the adjacent cages, we have adopted $2 \times 2 \times 2$ supercell of unit cell of AlPO-34 zeolite compared to the SAPO-34 cell reported in our work. Thus, we have conducted US MD sampling within the inner surface of AlPO-34 without acid site.

The diffusion behavior within the AlPO-34 zeolite framework was investigated to avoid the influence of acid site, as depicted in Figure S9. As illustrated in Figure S9 (red line), the CH₃OH diffusion profile in the acid-free system displays a diffusion free energy barrier of ~0.6 eV. For CH₂CO diffusion (see blue line in Figure S9), the acid-free system at 673 K exhibits a whole-molecule migration rather than dissociation. Notably, the diffusion of CH₂CO in the AlPO-34 zeolite with the absence of acid sites has a diffusion free barrier to ~0.4 eV.

In conclusion, the diffusion free energy of both two key intermediates, i.e. CH_3OH and CH_2CO , exhibits a barrier of no more than 0.6 eV. This indicates that their diffusion behavior is not the rate-determining step in the OX-ZEO catalytic system.

Reference

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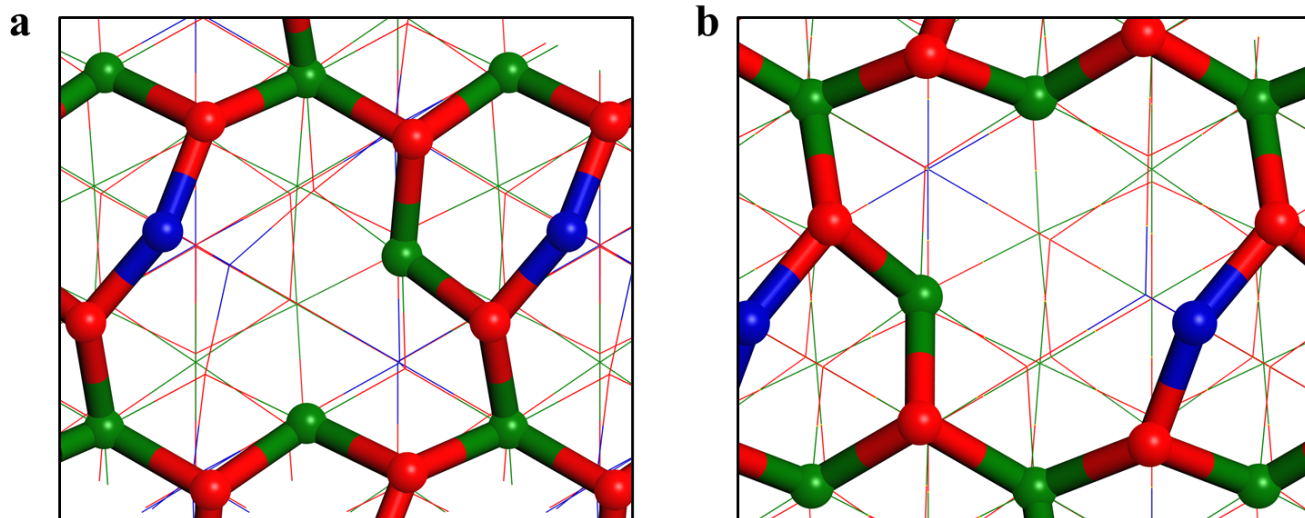


Figure S1 The structure of ZnCrO_x surface (a) $\text{Zn}_3\text{Cr}_3\text{O}_8$ (0001) surface; (b) ZnCr_2O_4 (111) surface.

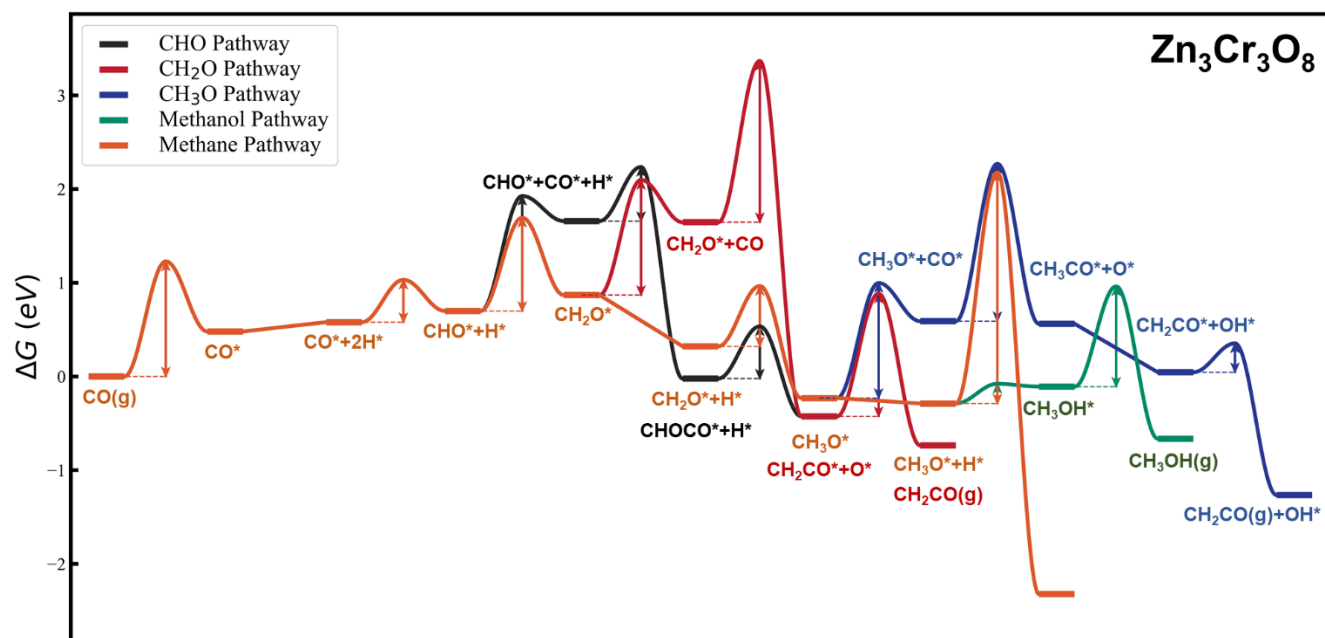


Figure S2 Gibbs free energy reaction profile of $\text{Zn}_3\text{Cr}_3\text{O}_8$ (0001) surface catalyzed ketene, methanol and methane formation pathway (Surface adsorbed species are denoted by the symbol *). Three ketene pathways are plotted in black, red and blue, with key C-C coupling with CO at CHO^* , CH_2O^* and CH_3O^* respectively. The methanol and methane pathway are plotted in green and orange lines.

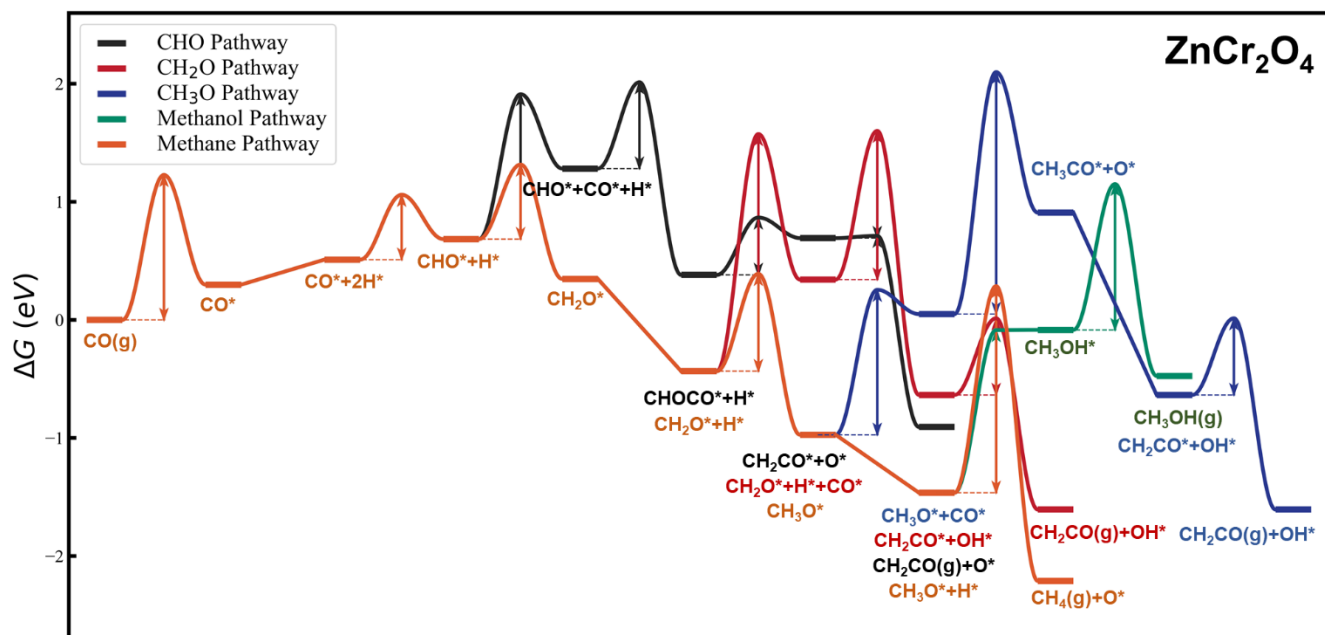


Figure S3 Gibbs free energy reaction profile of ZnCr₂O₄ (111) surface catalyzed ketene, methanol and methane formation pathways (Surface adsorbed species are denoted by the symbol *). Three ketene pathways are plotted in black, red and blue, with key C-C coupling with CO at CHO*, CH₂O*, CH₃O* respectively. The methanol and methane pathways are plotted in green and orange lines.

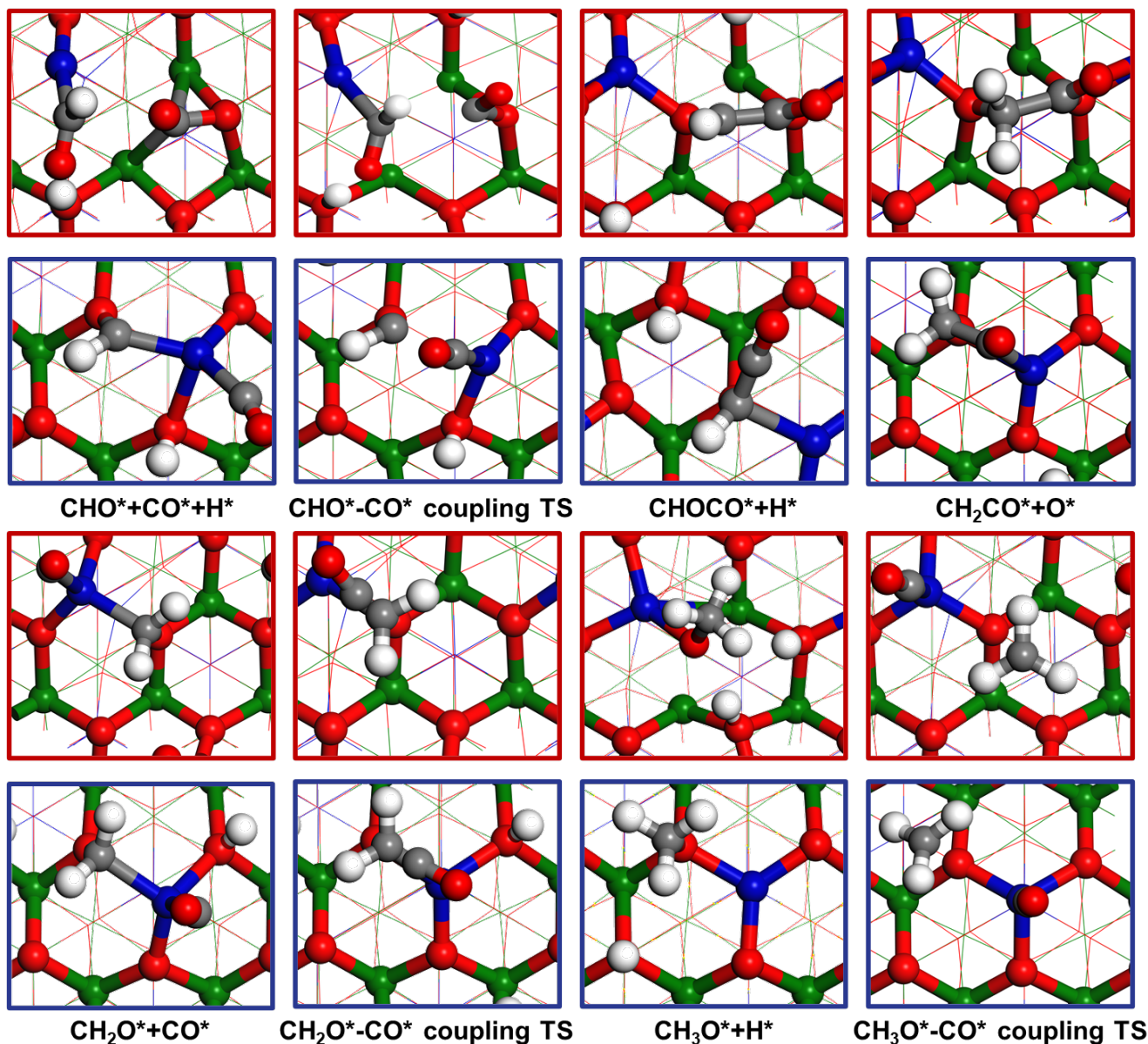


Figure S4 Surface structures of key intermediates and transition states in the C-C coupling pathway on the $\text{Zn}_3\text{Cr}_3\text{O}_8$ (0001) and ZnCr_2O_4 (111) surface (surface-adsorbed species and oxygen-containing adsorbed species are labeled with *). The frameworks on two surfaces are depicted in red and blue, respectively. Zn, Cr, O, C, and H atoms are represented by blue, green, red, gray, and white spheres.

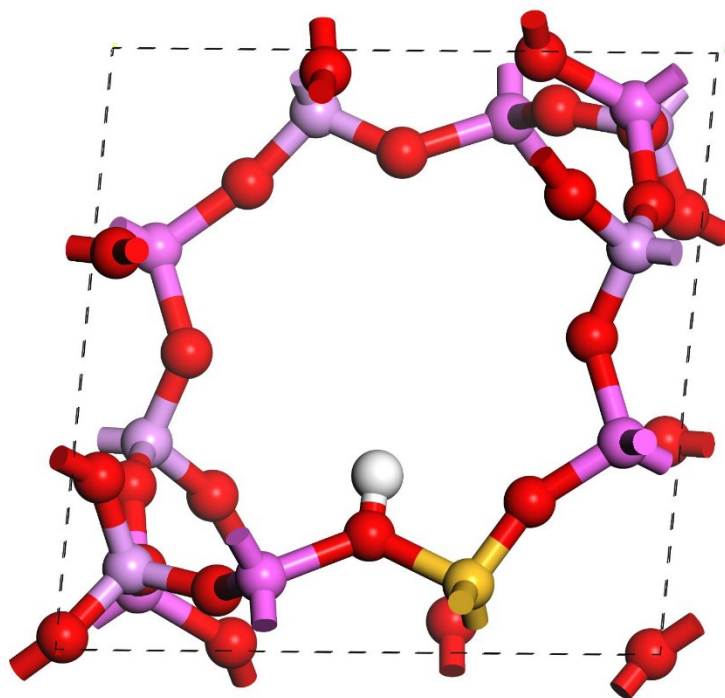


Figure S5 The active site of H site on the SAPO-34 surface.

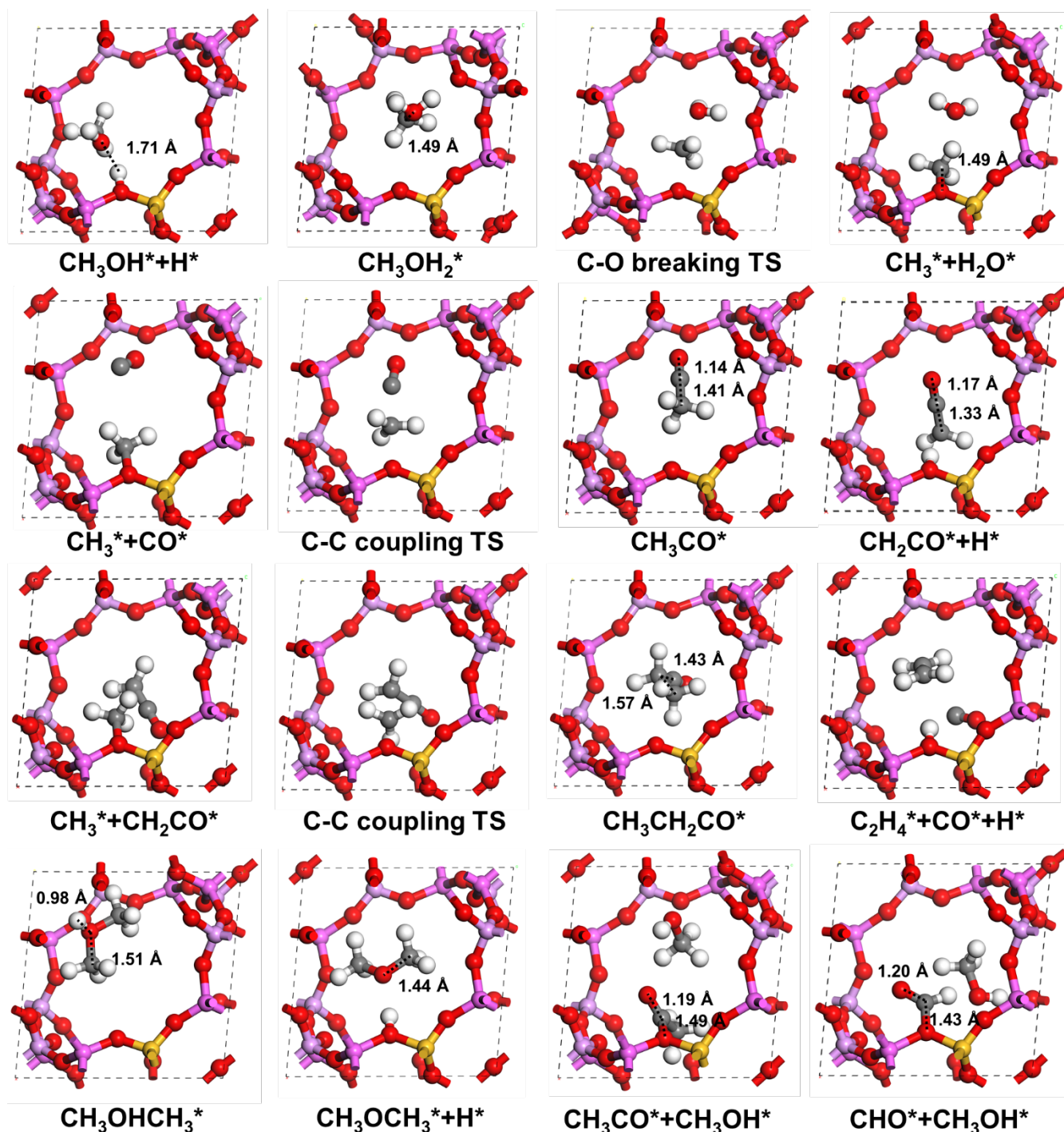


Figure S6 Surface structures of key intermediates and transition states in the C-C coupling pathway on the internal surface of SAPO-34 zeolite (surface-adsorbed species and oxygen-containing adsorbed species are labeled with *). Al, Si, P, O, C, and H atoms are represented by purple, yellow, pink, red, gray, and white spheres, respectively.

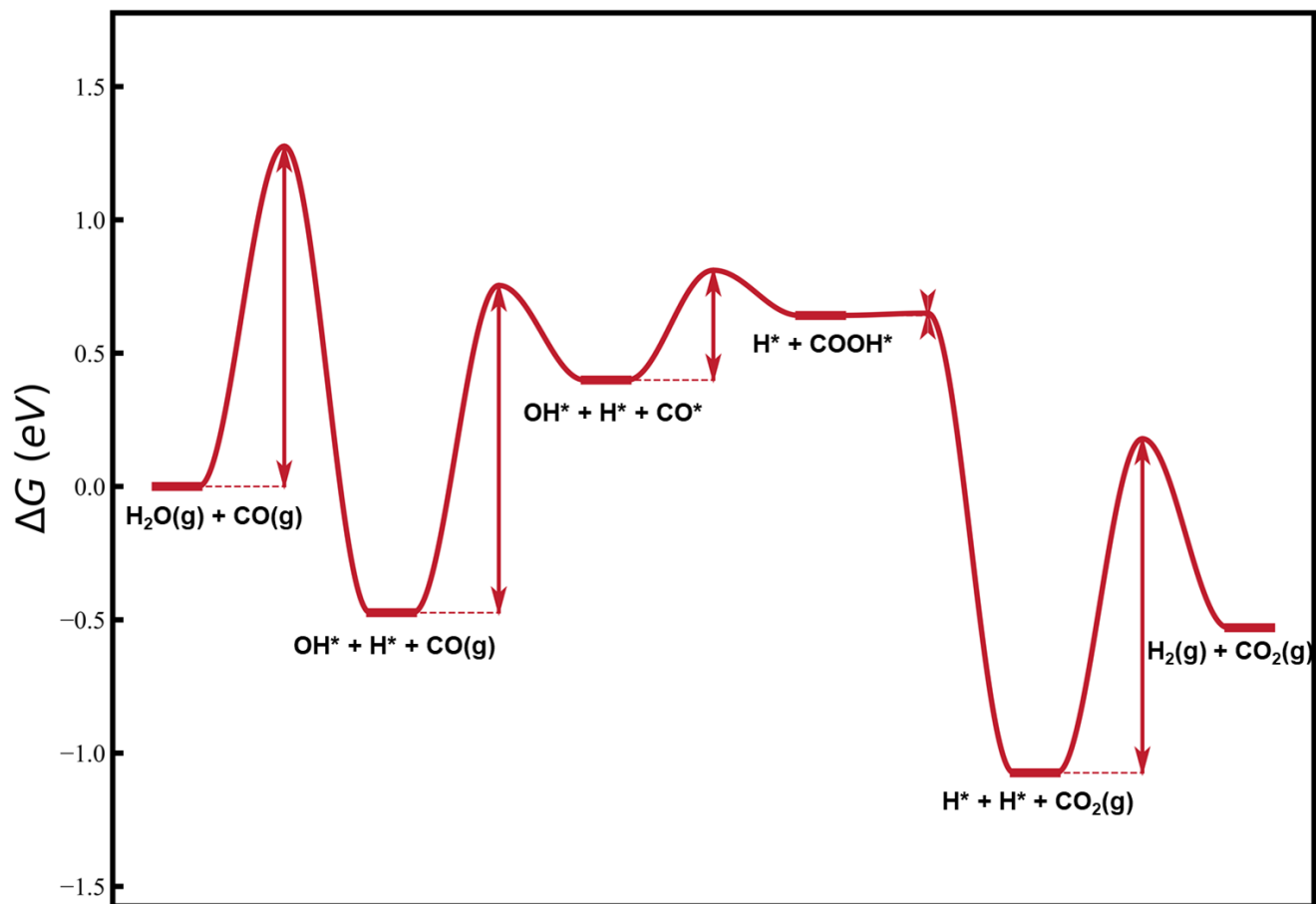


Figure S7 Gibbs free energy reaction profile of the water-gas shift (WGS) pathway catalyzed by $\text{Zn}_3\text{Cr}_3\text{O}_8$ (0001) surface (Surface adsorbed species are denoted by the symbol *).

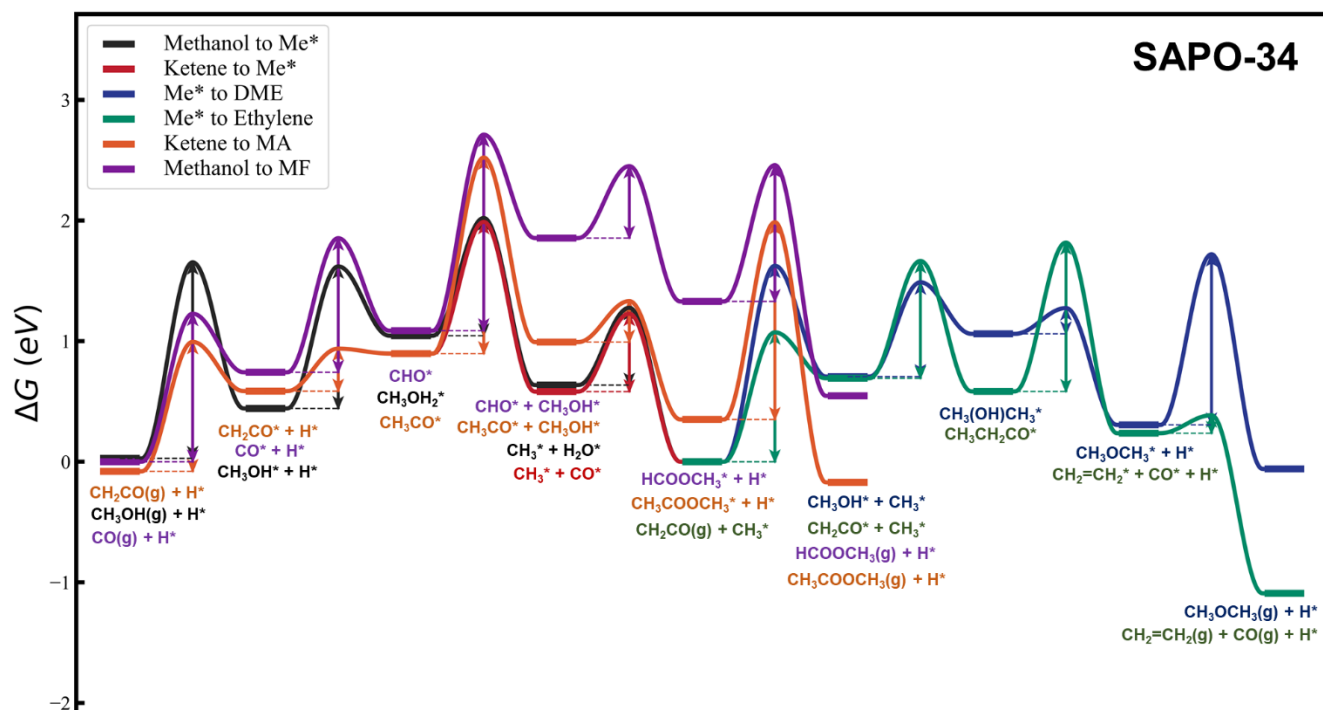


Figure S8 Gibbs free energy reaction profile of methanol and ketene reactions on SAPO-34 catalyst (Surface adsorbed species are denoted by the symbol *). Distinct colors represent different reaction pathways: methanol to CH_3^* (black), ketene to CH_3^* (red), CH_3^* to dimethyl ether (blue), CH_3^* to ethylene (green), ketene to methyl acetate (orange), and methanol to methyl formate (purple).

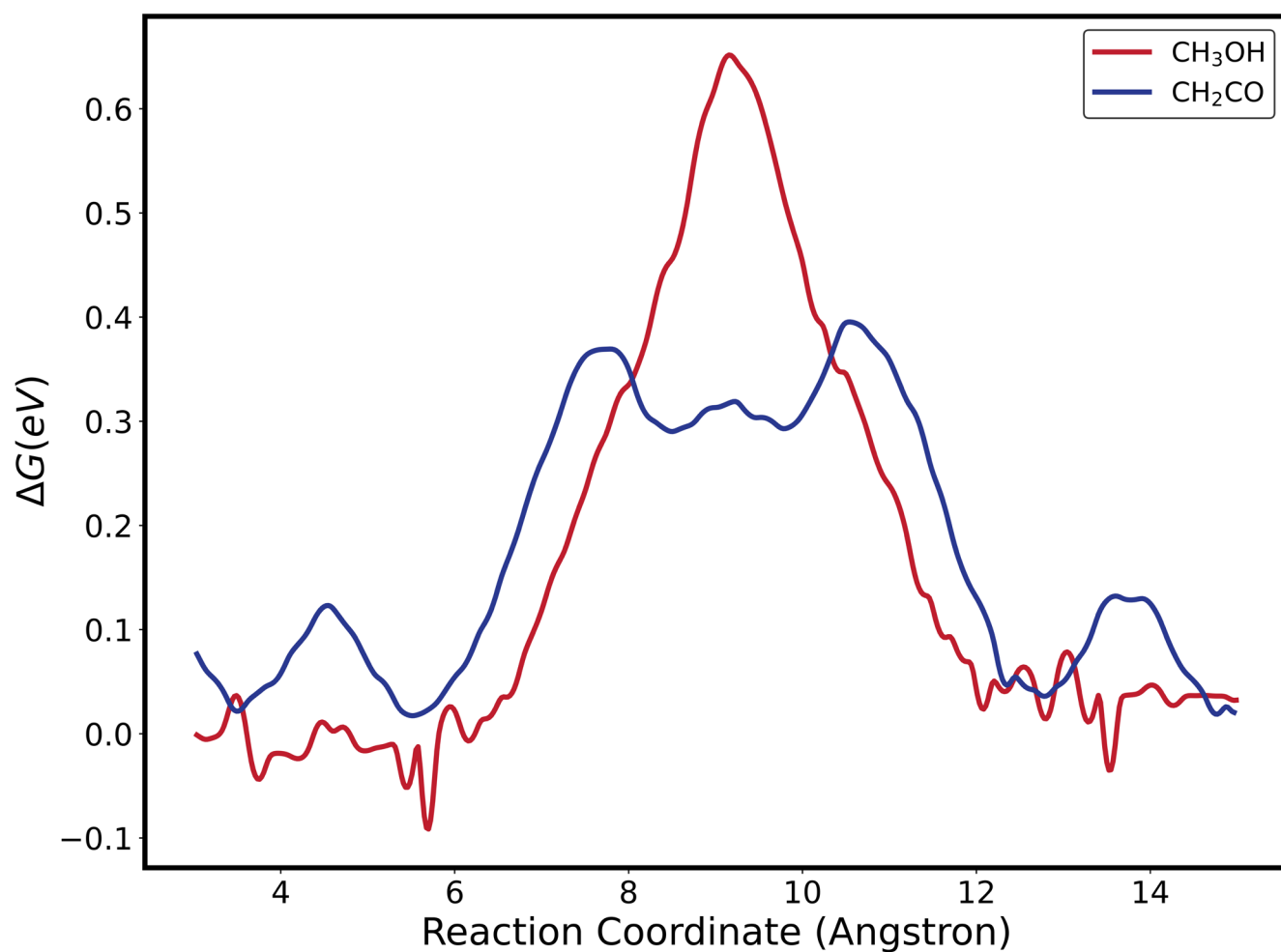


Figure S9 Diffusion free energy barriers of CH_3OH and CH_2CO in the AlPO-34 zeolite utilizing umbrella sampling molecular dynamics method. CH_3OH diffusion within the AlPO-34 is depicted in red line; CH_2CO diffusion in the AlPO-34 are depicted in blue line.

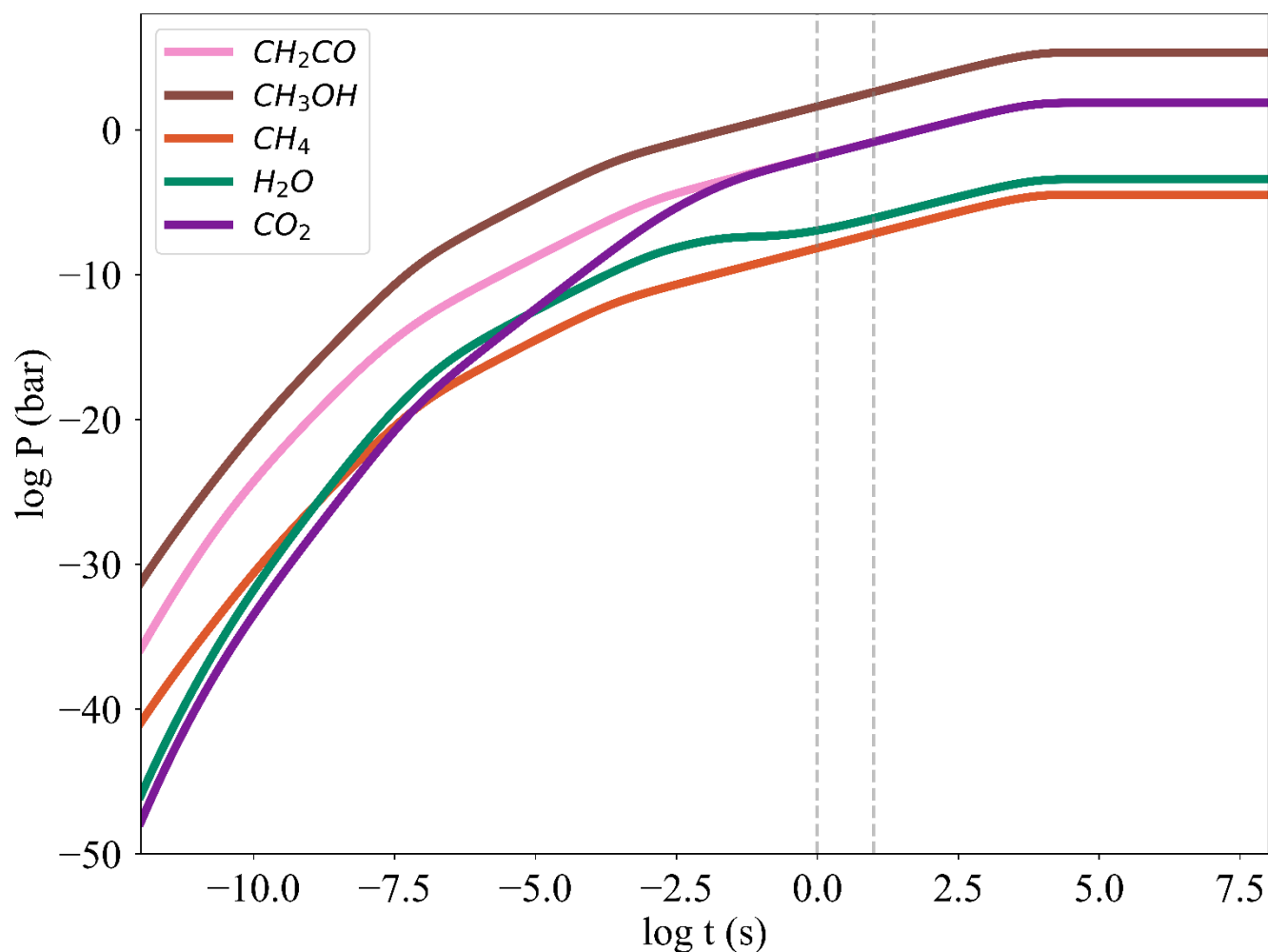


Figure S10 Microkinetic simulation results illustrating the partial pressures of CH_2CO (pink), CH_3OH (brown), CH_4 (orange), CO_2 (purple), and H_2O (green) as a function of time for the $\text{Zn}_3\text{Cr}_3\text{O}_8$ (0001) surface. Simulations were conducted under typical reaction conditions ($T = 673$ K, $P = 2.5$ MPa, $\text{H}_2:\text{CO} = 2.5$, space velocity = $5143 \text{ mL h}^{-1} \text{ g}^{-1}$). Approximate experimental contact times (1–10 s) are marked by gray dashed lines.

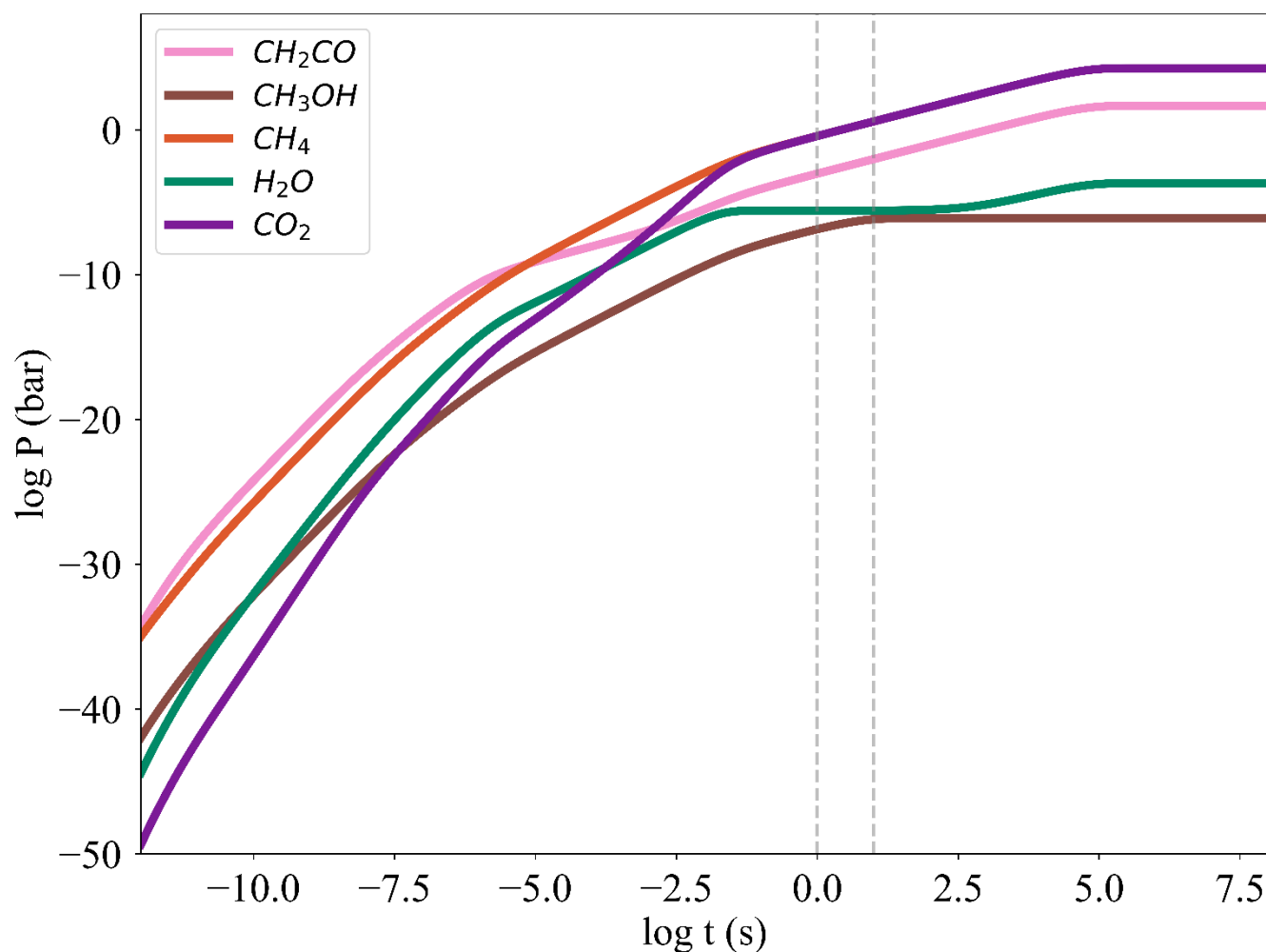


Figure S11 Microkinetic simulation results illustrating the partial pressures of CH_2CO (pink), CH_3OH (brown), CH_4 (orange), CO_2 (purple), and H_2O (green) as a function of time for the $ZnCr_2O_4$ (111) surface. Simulations were conducted under typical reaction conditions ($T = 673$ K, $P = 2.5$ MPa, $H_2:CO = 2.5$, space velocity = $5143 \text{ mL h}^{-1} \text{ g}^{-1}$). Approximate experimental contact times (1–10 s) are marked by gray dashed lines.

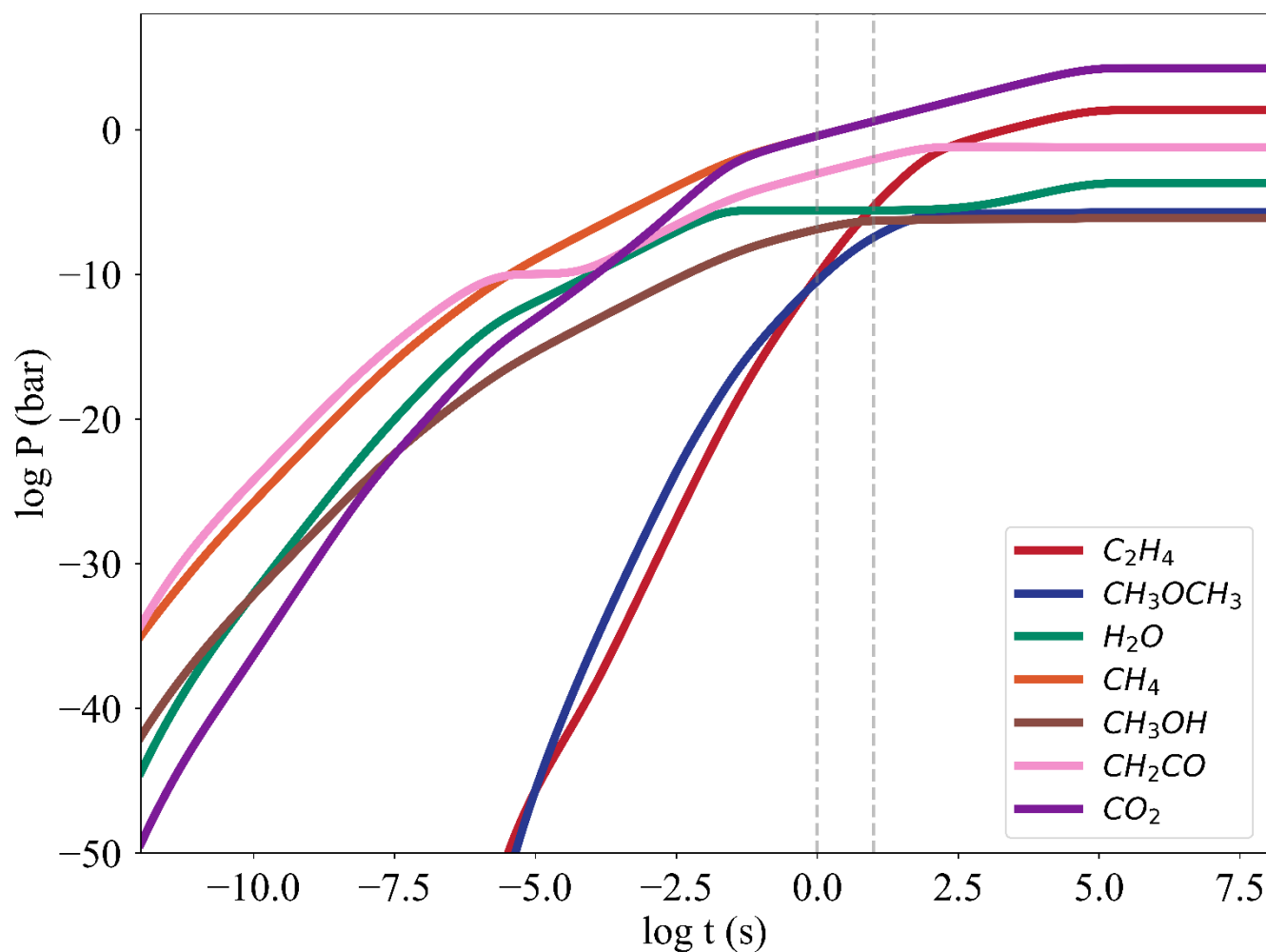


Figure S12 Microkinetic simulation results illustrating the partial pressures of C₂H₄ (red), CH₃OCH₃ (blue), H₂O (green), CH₄ (orange), CH₃OH (brown), CH₂CO (pink), and CO₂ (purple) as a function of time for the ZnCr₂O₄|SAPO-34 catalytic system. Simulations were conducted under typical reaction conditions (T = 673 K, P = 2.5 MPa, H₂:CO = 2.5, space velocity = 5143 mL h⁻¹ g⁻¹). Approximate experimental contact times (1–10 s) are marked by gray dashed lines.

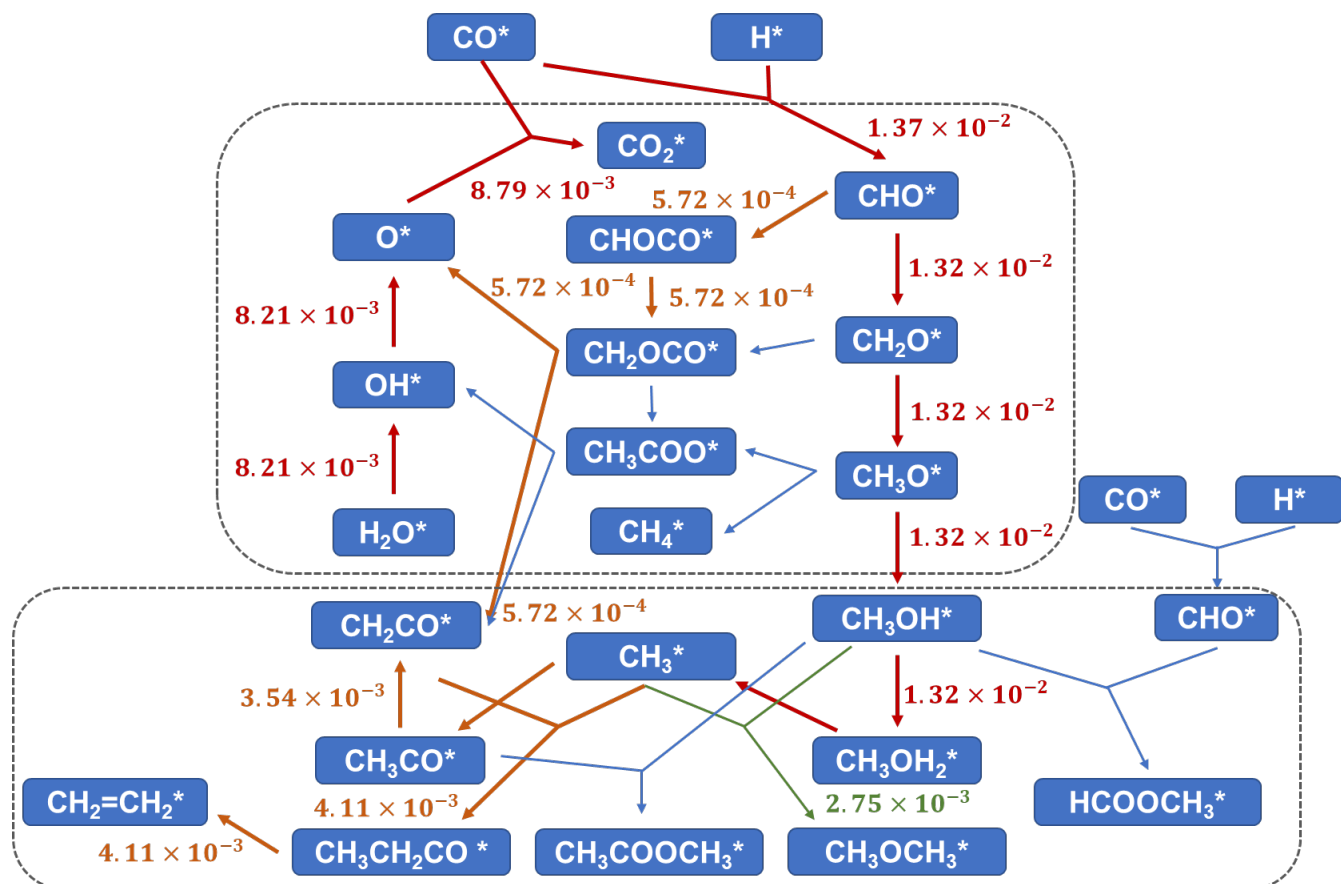


Figure S13 Reaction cycle on ZnCrO_x|SAPO-34 bifunctional catalyst surfaces at steady state under reaction conditions ($T = 673 \text{ K}$, $P_{H_2} = 17.9 \text{ bar}$, $P_{CO} = 7.1 \text{ bar}$, $V_{gt} = 5143 \text{ mL/h} \cdot g_{cat}$. on the Zn₃Cr₃O₈|SAPO-34 catalyst. The species on the surfaces of ZnCrO_x and SAPO-34 are enclosed in upper and lower frames, respectively.

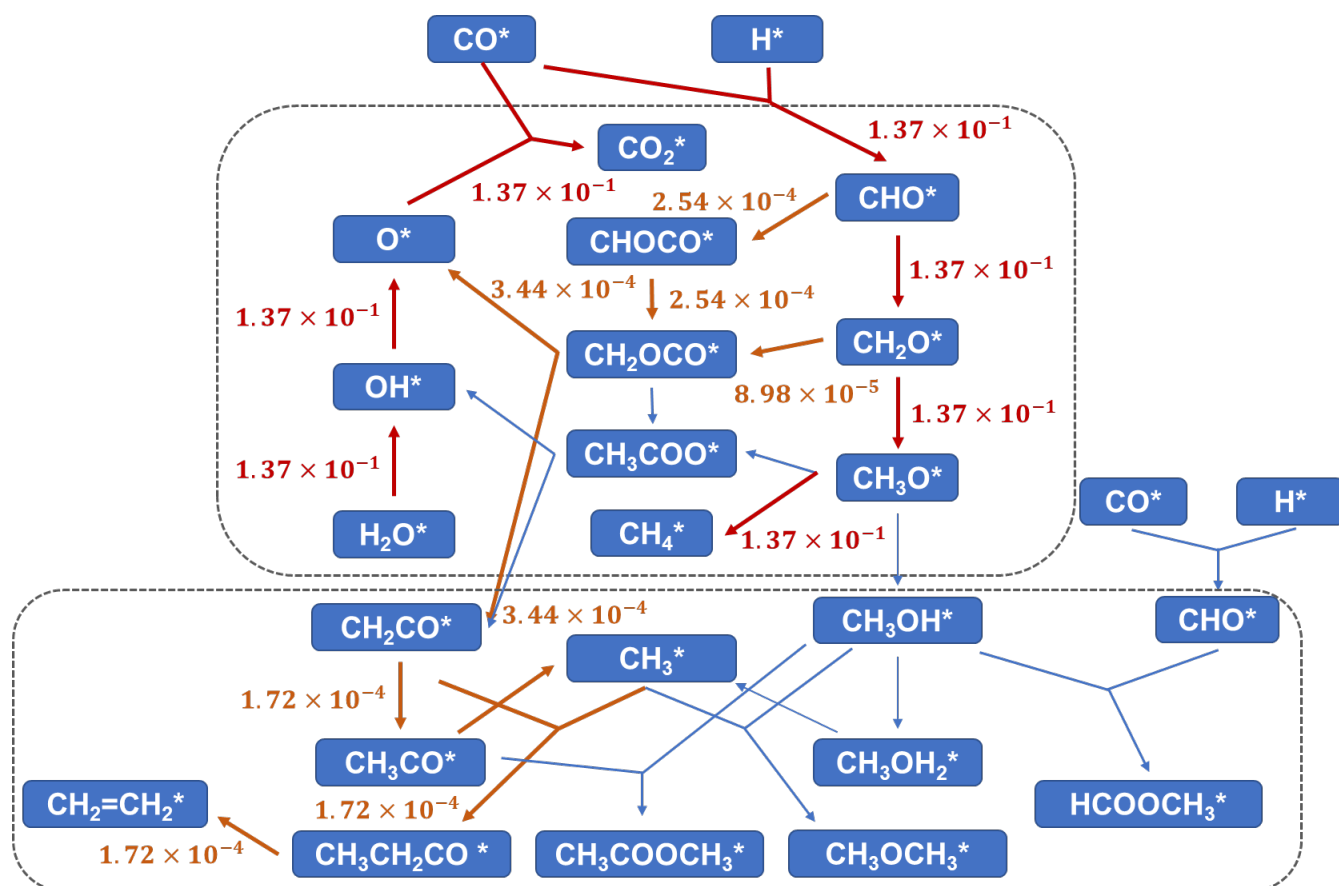


Figure S14 Reaction cycle on ZnCrO_x|SAPO-34 bifunctional catalyst surfaces at steady state under reaction conditions ($T = 673\text{ K}$, $P_{H_2} = 17.9\text{ bar}$, $P_{CO} = 7.1\text{ bar}$, $V_{gt} = 5143\text{ mL/h} \cdot g_{cat}$. on the ZnCr₂O₄|SAPO-34 catalyst. The species on the surfaces of ZnCrO_x and SAPO-34 are enclosed in upper and lower frames, respectively.

Table S1 Key kinetic data at steady state, including k_+ , K_{eq} , Z_i and r_i , for some important elementary reaction steps in the syngas conversion over the $Zn_3Cr_3O_8$ (0001) | SAPO-34 surface. (#1-#3 indicate three distinct sites on the $Zn_3Cr_3O_8$ (0001) surface: the Zn site, O site and Cr_2 bidentate site, respectively; #4 and #5 denote two types of adsorption modes in SAPO-34 zeolite, where #4 corresponds to the O atom of the SiO_4 tetrahedron and #5 represents the physical adsorption on the 8-MR inner surface).

	<i>step i</i>	k_+	K_{eq}	Z_i	r_i (s^{-1})
R1	#1 + CO <-> CO#1	9.00×10^3	3.54×10^{-5}	1.00	1.77×10^{-2}
R2	$H_2 + \#2 + \#2 <-> H\#2 + H\#2$	1.41×10^{11}	1.01×10^{-2}	1.00	1.73×10^{-2}
R3	$H\#2 + CO\#1 <-> CHO\#1 + \#2$	5.79×10^9	1.28×10^{-1}	1.00	8.92×10^{-3}
R4	$CO + \#3 <-> CO\#3$	9.00×10^3	9.16×10^{-9}	1.00	5.76×10^{-4}
R5	$CHO\#1 + CO\#3 <-> CHOCO\#3 + \#1$	6.60×10^8	5.26×10^7	1.85×10^{-10}	5.76×10^{-4}
R6	$H\#2 + CHOCO\#3 <-> CH_2OCO\#3 + \#2$	9.47×10^8	1.05×10^3	1.00	5.76×10^{-4}
R7	$CH_2OCO\#3 <-> O\#3 + CH_2CO$	2.21×10^3	2.10×10^2	0.04	5.76×10^{-4}
R8	$CHO\#1 + H\#2 <-> CH_2O\#1 + \#2$	4.98×10^5	5.30×10^{-2}	0.99	8.35×10^{-3}
R9	$CH_2O\#1 + CO\#3 <-> \#1 + CH_2COO\#3$	1.80	5.86×10^9	3.98×10^{-12}	3.52×10^{-14}
R10	$H\#2 + CH_2O\#1 <-> CH_3O\#1 + \#2$	2.10×10^8	1.36×10^4	1.00	8.35×10^{-3}
R11	$CO\#3 + CH_3O\#1 <-> CH_3COO\#3 + \#1$	3.70	1.61	1.45×10^{-10}	4.15×10^{-10}
R12	$CH_3COO\#3 + \#2 <-> H\#2 + CH_2COO\#3$	2.50×10^{12}	7.44×10^3	0.99	4.15×10^{-10}
R13	$CH_2COO\#3 <-> O\#3 + CH_2CO$	6.88×10^{10}	6.55×10^9	1.00	4.15×10^{-10}
R14	$H\#2 + CH_3O\#1 <-> CH_3OH\#1 + \#2$	7.53×10^{11}	3.01×10^{-1}	1.00	-8.21×10^{-3}
R15	$CH_3OH\#1 <-> \#1 + CH_3OH$	1.37×10^5	1.45×10^4	1.00	-8.21×10^{-3}
R16	$\#3 + H\#2 + CH_3O\#1 <-> \#2 + CH_4\#1 + O\#3$	4.78×10^{-6}	1.79×10^9	1.05×10^{-20}	8.35×10^{-3}
R17	$CH_4\#1 <-> \#1 + CH_4$	2.50×10^{12}	9.49×10^5	1.00	8.35×10^{-3}
R18	$OH\#3 + H\#2 <-> \#2 + H_2O\#3$	3.08×10^4	2.19×10^{-9}	1.00	2.44×10^{-9}
R19	$H_2O\#3 <-> \#3 + H_2O$	2.50×10^{12}	5.50×10^6	1.00	2.44×10^{-9}
R20	$H\#2 + OH\#3 <-> \#2 + H_2 + O\#3$	8.88×10^{11}	6.33×10^{-2}	1.00	8.79×10^{-3}
R21	$CO\#1 + O\#3 <-> CO_2\#1 + \#3$	1.16×10^{10}	1.53×10^{-2}	1.00	8.79×10^{-3}
R22	$CO_2\#1 <-> CO_2 + \#1$	2.50×10^{12}	7.05×10^{12}	1.00	8.21×10^{-3}
R23	$CH_3OH + \#4 <-> CH_3OH\#4$	9.48	7.95×10^{-4}	1.00	8.34×10^{-3}
R24	$H\#5 + CH_3OH\#4 <-> \#5 + CH_3OH_2\#4$	2.14×10^4	3.03×10^{-5}	1.00	8.21×10^{-3}
R25	$\#5 + CH_3OH_2\#4 <-> H_2O\#4 + CH_3\#5$	6.96×10^5	1.17×10^3	3.94×10^{-5}	8.21×10^{-3}
R26	$H_2O\#4 <-> H_2O + \#4$	2.24×10^8	5.79×10^4	0.97	8.21×10^{-3}
R27	$CH_2CO + \#4 <-> CH_2CO\#4$	1.47×10^9	1.05×10^{-5}	1.00	1.18×10^{-4}
R28	$H\#5 + CH_2CO\#4 <-> CH_3CO\#4 + \#5$	3.23×10^{10}	4.65×10^{-3}	1.00	1.18×10^{-4}
R29	$CH_3CO\#4 + \#5 <-> CO\#4 + CH_3\#5$	9.44×10^4	2.30×10^2	37.59	1.18×10^{-4}
R30	$CH_3\#5 + CH_3OH\#4 <-> \#5 + CH_3OHCH_3\#4$	1.99×10^7	2.23×10^{-3}	1.00	5.75×10^{-4}
R31	$\#5 + CH_3OHCH_3\#4 <-> CH_3OCH_3\#4 + H\#5$	3.56×10^{11}	4.49×10^5	1.00	-3.76×10^{-3}
R32	$CH_3OCH_3\#4 <-> CH_3OCH_3 + \#4$	2.50×10^{12}	5.42×10^2	1.00	-3.76×10^{-3}
R33	$CH_2CO\#4 + CH_3\#5 <-> \#5 + CH_3CH_2CO\#4$	7.36×10^5	6.58	0.96	5.68×10^{-4}
R34	$\#5 + CH_3CH_2CO\#4 + \#4 <-> CO\#4 + H\#5 + C_2H_4\#4$	8.02×10^3	3.93×10^2	7.65×10^{-4}	4.33×10^{-3}
R35	$CO\#4 <-> CO + \#4$	9.00×10^3	1.63×10^5	1.00	4.33×10^{-3}
R36	$C_2H_4\#4 <-> C_2H_4 + \#4$	1.08×10^{12}	2.43×10^4	1.00	4.33×10^{-3}
R37	$CH_3CO\#4 + \#5 + CH_3OH\#4 <-> H\#5 + CH_3COOCH_3\#4 + \#4$	4.04×10^{10}	6.40×10^4	1.00	2.21×10^{-9}
R38	$CH_3COOCH_3\#4 <-> CH_3COOCH_3 + \#4$	1.67×10^{-2}	8.05×10^3	0.12	2.21×10^{-9}
R39	$CO\#4 + H\#5 <-> CHO\#5 + \#4$	6.66×10^4	2.62×10^{-3}	1.00	7.03×10^{-6}
R40	$CHO\#5 + CH_3OH\#4 <-> H\#5 + HCOOCH_3\#4$	4.82×10^8	8.67×10^3	1.00	7.03×10^{-6}
R41	$HCOOCH_3\#4 <-> HCOOCH_3 + \#4$	4.83×10^4	7.24×10^5	1.00	7.03×10^{-6}

Table S2 Key kinetic data at steady state, including k_+ , K_{eq} , Z_i and r_i , for some important elementary reaction steps in the syngas conversion over the ZnCr_2O_4 (111) | SAPO-34 surface. (#1-#3 indicate three distinct sites on the ZnCr_2O_4 (111) surface: the Zn site, O site and Cr_2 bidentate site, respectively; #4 and #5 denote two types of adsorption modes in SAPO-34 zeolite, where #4 corresponds to the O atom of the SiO_4 tetrahedron and #5 represents the physical adsorption on the 8-MR inner surface).

	<i>step i</i>	k_+	K_{eq}	Z_i	r_i (s^{-1})
R1	#1 + CO $\leftrightarrow$ CO#1	9.48	8.14×10^{-4}	0.49	0.28
R2	H_2 + #2 $\leftrightarrow$ H#2 + H#2	2.04×10^{10}	1.45×10^{-3}	1.00	0.28
R3	H#2 + CO#1 $\leftrightarrow$ CHO#1 + #2	1.08×10^9	4.98×10^{-2}	1.00	0.14
R4	CO + #3 $\leftrightarrow$ CO#3	9.48	4.69×10^{-6}	1.00	3.44×10^{-4}
R5	CHO#1 + CO#3 $\leftrightarrow$ CHOCO#3 + #1	1.17×10^{20}	5.55×10^6	1.85×10^{-10}	2.54×10^{-4}
R6	H#2 + CHOCO#3 $\leftrightarrow$ $\text{CH}_2\text{COO}\#3$ + #2	3.22×10^9	4.60×10^{-3}	0.19	2.54×10^{-4}
R7	$\text{CH}_2\text{COO}\#3 \leftrightarrow \text{O}\#3 + \text{CH}_2\text{CO}$	2.50×10^{12}	9.56×10^{11}	7.13×10^{-6}	2.54×10^{-4}
R8	CHO#1 + H#2 $\leftrightarrow$ $\text{CH}_2\text{O}\#1$ + #2	2.50×10^{12}	1.98×10^4	1.00	0.14
R9	$\text{CH}_2\text{O}\#1 + \text{CO}\#3 \leftrightarrow \#1 + \text{CH}_2\text{COO}\#3$	5.19×10^3	2.07×10^7	1.02×10^{-14}	8.98×10^{-5}
R10	H#2 + $\text{CH}_2\text{O}\#1 \leftrightarrow \text{CH}_3\text{O}\#1$ + #2	9.49×10^6	1.08×10^4	1.00	0.14
R11	CO#3 + $\text{CH}_3\text{O}\#1 \leftrightarrow \text{CH}_3\text{COO}\#3$ + #1	6.33×10^{-3}	3.69×10^{-7}	6.30×10^{-11}	1.91×10^{-7}
R12	$\text{CH}_3\text{COO}\#3$ + #2 $\leftrightarrow$ H#2 + $\text{CH}_2\text{COO}\#3$	2.50×10^{12}	3.67×10^{11}	2.31×10^{-6}	1.91×10^{-7}
R13	OH#3 + H#2 $\leftrightarrow$ #2 + $\text{H}_2\text{O}\#3$	3.08×10^4	2.19×10^{-9}	1.00	2.71×10^{-7}
R14	$\text{H}_2\text{O}\#3 \leftrightarrow \#3 + \text{H}_2\text{O}$	2.50×10^{12}	5.50×10^6	1.00	2.71×10^{-7}
R15	$\text{CH}_3\text{O}\#1 + \text{H}\#2 \leftrightarrow \text{CH}_3\text{OH}\#1$ + #2	1.22×10^2	4.87×10^{-11}	1.00	5.89×10^{-8}
R16	$\text{CH}_3\text{OH}\#1 \leftrightarrow \text{CH}_3\text{OH} + \#1$	7.86×10^3	8.30×10^2	0.04	5.89×10^{-8}
R17	#3 + H#2 + $\text{CH}_3\text{O}\#1 \leftrightarrow \#1 + \text{CH}_4 + \text{O}\#3$ + #2	1.10	3.94×10^5	1.34×10^{-7}	0.14
R18	CO#1 + O#3 $\leftrightarrow$ $\text{CO}_2\#1$ + #3	1.16×10^{10}	1.53×10^{-2}	0.99	0.14
R19	$\text{CO}_2\#1 \leftrightarrow \text{CO}_2 + \#1$	2.50×10^{12}	7.05×10^{12}	1.00	0.14
R20	H#2 + OH#3 $\leftrightarrow$ #2 + $\text{H}_2 + \text{O}\#3$	8.88×10^{11}	6.33×10^{-2}	1.00	-2.71×10^{-7}
R21	$\text{CH}_3\text{OH} + \#4 \leftrightarrow \text{CH}_3\text{OH}\#4$	9.48	3.25×10^{-2}	0.79	5.89×10^{-8}
R22	H#5 + $\text{CH}_3\text{OH}\#4 \leftrightarrow \#5 + \text{CH}_3\text{OH}_2\#4$	3.12×10^4	3.01×10^{-3}	1.01	-2.69×10^{-7}
R23	#5 + $\text{CH}_3\text{OH}_2\#4 \leftrightarrow \text{H}_2\text{O}\#4 + \text{CH}_3\#5$	1.30×10^4	0.48	10.25	-2.69×10^{-7}
R24	$\text{H}_2\text{O}\#4 \leftrightarrow \text{H}_2\text{O} + \#4$	4.88×10^8	1.26×10^5	1.00	-2.69×10^{-7}
R25	$\text{CH}_3\#5 + \text{CH}_3\text{OH}\#4 \leftrightarrow \text{CH}_3\text{OHCH}_3\#4 + \#5$	1.05×10^7	9.94×10^{-1}	1.00	1.15×10^{-12}
R26	$\text{CH}_3\text{OHCH}_3\#4 + \#5 \leftrightarrow \text{CH}_3\text{OCH}_3\#4 + \text{H}\#5$	1.13×10^8	1.34×10^4	1.00	1.15×10^{-12}
R27	$\text{CH}_3\text{OCH}_3\#4 \leftrightarrow \#4 + \text{CH}_3\text{OCH}_3$	2.50×10^{12}	2.08	1.00	1.15×10^{-12}
R28	#4 + $\text{CH}_2\text{CO} \leftrightarrow \text{CH}_2\text{CO}\#4$	1.30×10^5	1.20	1.00	3.44×10^{-4}
R29	$\text{CH}_2\text{CO}\#4 + \text{H}\#5 \leftrightarrow \text{CH}_3\text{CO}\#4 + \#5$	1.46×10^{12}	4.45	1.00	1.72×10^{-4}
R30	$\text{CH}_3\text{CO}\#4 + \#5 \leftrightarrow \text{CH}_3\#5 + \text{CO}\#4$	25.3	8.93×10^{-3}	0.90	1.72×10^{-4}
R31	CO#4 $\leftrightarrow$ CO + #4	9.00×10^3	9.28×10^4	1.00	3.44×10^{-4}
R32	$\text{CH}_2\text{CO}\#4 + \text{CH}_3\#5 \leftrightarrow \#5 + \text{CH}_3\text{CH}_2\text{CO}\#4$	7.81×10^6	4.69	1.00	1.72×10^{-4}
R33	#5 + #4 + $\text{CH}_3\text{CH}_2\text{CO}\#4 \leftrightarrow \text{C}_2\text{H}_4\#4 + \text{CO}\#4 + \text{H}\#5$	1.29×10^6	1.18	1.00	1.72×10^{-4}
R34	$\text{C}_2\text{H}_4\#4 \leftrightarrow \text{C}_2\text{H}_4 + \#4$	9.22×10^{11}	2.84×10^3	1.00	1.72×10^{-4}
R35	$\text{CH}_3\text{CO}\#4 + \text{CH}_3\text{OH}\#4 + \#5 \leftrightarrow \text{CH}_3\text{COOCH}_3\#4 + \#4 + \text{H}\#5$	2.50×10^{12}	8.25×10^6	1.00	5.55×10^{-11}
R36	$\text{CH}_3\text{COOCH}_3\#4 \leftrightarrow \#4 + \text{CH}_3\text{COOCH}_3$	1.67×10^{-2}	16.9	0.99	5.55×10^{-11}
R37	CO#4 + H#5 $\leftrightarrow$ #4 + CHO#5	4.49×10^9	1.41×10^2	1.00	3.28×10^{-7}
R38	$\text{CH}_3\text{OH}\#4 + \text{CHO}\#5 \leftrightarrow \text{H}\#5 + \text{HCOOCH}_3\#4$	3.44×10^{10}	5.04×10^5	1.00	3.28×10^{-7}
R39	$\text{HCOOCH}_3\#4 \leftrightarrow \text{HCOOCH}_3 + \#4$	6.82×10^2	1.02×10^4	1.00	3.28×10^{-7}

Table S3 The energy difference between the G-NN and DFT PES results within the SAPO-34 zeolite surfaces.

name	N_{atom}	E_{G-NN}	E_{DFT}	ΔE (meV/atom)
TS-1	48	-284.29	-284.32	-0.68
TS-2	45	-268.45	-268.42	0.54
TS-3	46	-266.61	-266.57	0.85
TS-4	43	-284.05	-284.02	0.69
TS-5	47	-298.95	-298.87	1.54
TS-6	46	-281.22	-281.15	1.69
TS-7	44	-250.96	-250.95	0.19
TS-8	46	-266.94	-266.81	2.87
TS-9	43	-284.58	-284.39	4.23
TS-10	44	-297.16	-297.21	-1.02
TS-11	39	-267.42	-267.40	0.54
TS-12	47	-283.74	-283.78	-0.79
LM-1	48	-285.66	-285.42	5.37
LM-2	39	-298.94	-298.69	5.20
LM-3	45	-268.51	-268.49	0.50
LM-4	37	-267.61	-267.50	2.64
LM-5	41	-284.27	-284.17	2.30
LM-6	46	-299.30	-299.30	-0.06
LM-7	43	-281.76	-281.65	2.40
LM-8	44	-251.83	-251.69	3.70
LM-9	47	-285.73	-285.57	3.50
LM-10	38	-268.83	-268.86	-0.61
LM-11	46	-299.99	-299.90	1.76
LM-12	46	-251.92	-251.89	0.97
LM-13	43	-284.95	-284.92	0.75
LM-14	47	-282.39	-282.24	3.25
LM-15	44	-282.21	-282.20	0.16
LM-16	45	-268.13	-268.22	-1.90
LM-17	42	-237.81	-237.82	-0.31
LM-18	46	-285.55	-285.65	-2.27
LM-19	43	-268.71	-268.74	-0.59
LM-20	48	-281.63	-281.68	-1.26
LM-21	44	-267.79	-267.81	-0.44
LM-22	39	-284.58	-284.64	-1.34
LM-23	46	-254.59	-254.62	-0.72
Average	/	/	/	1.65

The coordinates of key configurations in arc format

➤ Zn₃Cr₂O₈ (0001) surface

CH₃CO* + O*

'BIOSYM archive 2

PBC=ON

```
Energy          0      -284      -284.820452
!DATE
PBC      5.9415   5.9415   25.2282   90.0000   90.0000   120.0000
Cr      0.156656152   3.397983290   1.657913820 CORE   1 Cr Cr   0.0000   1
Cr      3.130963189   3.398456174   1.658630356 CORE   2 Cr Cr   0.0000   2
Cr      4.614779765   0.826816860   1.683670079 CORE   3 Cr Cr   0.0000   3
Cr      -2.807655825   5.133964039   6.615086322 CORE   4 Cr Cr   0.0000   4
Cr      0.149101943   5.134941682   6.617609142 CORE   5 Cr Cr   0.0000   5
Cr      1.642319723   2.550567907   6.615086322 CORE   6 Cr Cr   0.0000   6
Cr      3.138653864   1.746312721   11.771197106 CORE   7 Cr Cr   0.0000   7
Cr      0.163755594   1.636423888   11.603055764 CORE   8 Cr Cr   0.0000   8
Cr      -1.415333648   4.153474955   11.779405684 CORE   9 Cr Cr   0.0000   9
Zn      1.646472779   0.847031220   0.363133415 CORE  10 Zn Zn   0.0000  10
Zn      1.643412764   0.818804873   3.554318843 CORE  11 Zn Zn   0.0000  11
Zn      1.641492493   4.268918738   4.183789225 CORE  12 Zn Zn   0.0000  12
Zn      -1.329171483   2.561163993   4.789620107 CORE  13 Zn Zn   0.0000  13
Zn      -1.307030745   2.540819198   8.425233167 CORE  14 Zn Zn   0.0000  14
Zn      1.593905778   0.853665740   9.077455015 CORE  15 Zn Zn   0.0000  15
Zn      2.146385982   3.942167805   9.503916117 CORE  16 Zn Zn   0.0000  16
Zn      1.564894511   4.237563251   13.251601925 CORE  17 Zn Zn   0.0000  17
O      0.061303495   1.798332401   0.682328896 CORE  18 O O   0.0000  18
O      3.228616518   1.800438362   0.681110184 CORE  19 O O   0.0000  19
O      -1.326944965   4.144399566   0.692021042 CORE  20 O O   0.0000  20
O      1.644093735   4.243856476   0.695574598 CORE  21 O O   0.0000  21
O      -1.326985044   2.552097774   2.774646592 CORE  22 O O   0.0000  22
O      0.252154021   5.021355178   2.788445554 CORE  23 O O   0.0000  23
O      1.643934912   2.674819099   2.782822643 CORE  24 O O   0.0000  24
O      3.033860368   5.019836651   2.790608293 CORE  25 O O   0.0000  25
O      3.028649918   3.472433884   5.534057952 CORE  26 O O   0.0000  26
O      0.253791173   3.472433884   5.535823926 CORE  27 O O   0.0000  27
O      4.611970545   0.730145022   5.535823926 CORE  28 O O   0.0000  28
O      1.642349430   0.842522522   5.550708564 CORE  29 O O   0.0000  29
O      1.644488370   4.271579926   7.688041668 CORE  30 O O   0.0000  30
O      0.288340995   1.624328263   7.797532056 CORE  31 O O   0.0000  31
O      -1.333926165   4.420799134   7.786683930 CORE  32 O O   0.0000  32
O      2.996417280   1.630708671   7.787188494 CORE  33 O O   0.0000  33
O      1.679041272   0.763834005   12.601594492 CORE  34 O O   0.0000  34
O      -2.585588817   5.095892362   10.468836724 CORE  35 O O   0.0000  35
O      1.730842476   2.330921109   10.482264414 CORE  36 O O   0.0000  36
O      -1.352242773   2.521445224   10.538945050 CORE  37 O O   0.0000  37
O      4.602144348   0.850655212   12.561977120 CORE  38 O O   0.0000  38
O      0.062525007   3.301491197   12.611032028 CORE  39 O O   0.0000  39
O      3.196480811   3.311602452   12.800933980 CORE  40 O O   0.0000  40
O      2.869325028   0.487016150   16.280364499 CORE  41 O O   0.0000  41
C      1.829060537   4.256292472   15.487197698 CORE  42 C C   0.0000  42
C      0.811927814   4.988595572   15.947856891 CORE  43 C C   0.0000  43
H      1.795333095   3.182944817   15.695551437 CORE  44 H H   0.0000  44
H      2.810671692   4.740479210   15.472829392 CORE  45 H H   0.0000  45
end
end
```

CH₃CO* + O*

'BIOSYM archive 2

PBC=ON

```
Energy          1      -277      -277.164336
!DATE
PBC      5.9415   5.9415   25.2282   90.0000   90.0000   120.0000
Cr      0.151005422   3.398957982   1.656057721 CORE   1 Cr Cr   0.0000   1
Cr      3.125477293   3.398852249   1.655984639 CORE   2 Cr Cr   0.0000   2
Cr      4.608938313   0.826896334   1.683016117 CORE   3 Cr Cr   0.0000   3
Cr      -2.807656000   5.133964000   6.615087000 CORE   4 Cr Cr   0.0000   4
Cr      0.149101900   5.134942000   6.617609000 CORE   5 Cr Cr   0.0000   5
Cr      1.642320000   2.550568000   6.615087000 CORE   6 Cr Cr   0.0000   6
Cr      3.200845361   1.565925267   11.568251956 CORE   7 Cr Cr   0.0000   7
Cr      0.133975789   1.601626165   11.612898286 CORE   8 Cr Cr   0.0000   8
Cr      -1.307702018   4.107197775   11.690663336 CORE   9 Cr Cr   0.0000   9
Zn      1.637832765   0.848435363   0.334186958 CORE  10 Zn Zn   0.0000  10
Zn      1.638540507   0.819731340   3.549929583 CORE  11 Zn Zn   0.0000  11
Zn      1.638861286   4.268891304   4.183617347 CORE  12 Zn Zn   0.0000  12
Zn      -1.329433230   2.561982509   4.785772820 CORE  13 Zn Zn   0.0000  13
Zn      -1.303510245   2.548639274   8.370066693 CORE  14 Zn Zn   0.0000  14
Zn      1.607216714   0.882532484   9.078678154 CORE  15 Zn Zn   0.0000  15
Zn      2.126753149   3.999088954   9.511772469 CORE  16 Zn Zn   0.0000  16
Zn      1.748000479   3.936648884   13.006904469 CORE  17 Zn Zn   0.0000  17
O      0.056973262   1.799580217   0.685303558 CORE  18 O O   0.0000  18
O      3.218989100   1.800169444   0.684971604 CORE  19 O O   0.0000  19
O      -1.333060696   4.148825055   0.695111270 CORE  20 O O   0.0000  20
O      1.638554812   4.244393994   0.696299063 CORE  21 O O   0.0000  21
O      -1.332279705   2.552726277   2.773042706 CORE  22 O O   0.0000  22
O      0.347841091   5.021297147   2.788062330 CORE  23 O O   0.0000  23
O      1.638474317   2.677198643   2.782392525 CORE  24 O O   0.0000  24
O      3.027983224   5.020577245   2.789664976 CORE  25 O O   0.0000  25
O      3.028650000   3.472434000   5.534058000 CORE  26 O O   0.0000  26
O      0.253791200   3.472434000   5.535824000 CORE  27 O O   0.0000  27
O      4.611970000   0.730145000   5.535824000 CORE  28 O O   0.0000  28
O      1.642349000   0.842522500   5.550709000 CORE  29 O O   0.0000  29
O      1.644488000   4.271580000   7.688042000 CORE  30 O O   0.0000  30
O      0.288341000   1.624328000   7.797532000 CORE  31 O O   0.0000  31
O      -1.333926000   4.420799000   7.786684000 CORE  32 O O   0.0000  32
O      2.996417000   1.630709000   7.787189000 CORE  33 O O   0.0000  33
O      -2.527302097   5.104928903   10.459407274 CORE  34 O O   0.0000  34
O      1.698393152   2.419472793   10.549166509 CORE  35 O O   0.0000  35
O      -1.304507963   2.467057071   10.513185308 CORE  36 O O   0.0000  36
O      4.636669829   0.608098036   12.511711529 CORE  37 O O   0.0000  37
O      -0.035490794   3.154963186   12.779431822 CORE  38 O O   0.0000  38
O      1.681480431   0.770756749   12.728050647 CORE  39 O O   0.0000  39
C      1.852677074   1.072386549   14.112679621 CORE  40 C C   0.0000  40
H      0.873786949   1.057498384   14.623657264 CORE  41 H H   0.0000  41
C      2.444197736   2.487204427   14.307883643 CORE  42 C C   0.0000  42
O      3.015188639   2.793818035   15.331917973 CORE  43 O O   0.0000  43
H      2.525022676   0.339236347   14.584965997 CORE  44 H H   0.0000  44
end
end
```

CH₃CO* + OH*

'BIOSYM archive 2

PBC=ON

```
Energy          2      -288      -288.856211
!DATE
PBC      5.9415   5.9415   25.2282   90.0000   90.0000   120.0000
Cr      0.155099362   3.396867534   1.656294071 CORE   1 Cr Cr   0.0000   1
```

Cr	3.129510233	3.397351572	1.656594717 CORE	2 Cr Cr	0.0000	2
Cr	4.613068085	0.825717912	1.681556187 CORE	3 Cr Cr	0.0000	3
Cr	-2.807656000	5.133964000	6.615087000 CORE	4 Cr Cr	0.0000	4
Cr	0.149101900	5.134942000	6.617609000 CORE	5 Cr Cr	0.0000	5
Cr	1.642320000	2.550568000	6.615087000 CORE	6 Cr Cr	0.0000	6
Cr	3.164521263	1.718016024	11.685786969 CORE	7 Cr Cr	0.0000	7
Cr	0.190574223	1.696666459	11.643667757 CORE	8 Cr Cr	0.0000	8
Cr	-1.318487635	4.252212089	11.677647107 CORE	9 Cr Cr	0.0000	9
Zn	1.644016695	0.846537761	0.366444349 CORE	10 Zn Zn	0.0000	10
Zn	1.641630305	0.817688155	3.553023286 CORE	11 Zn Zn	0.0000	11
Zn	1.640633510	4.269008083	4.182650759 CORE	12 Zn Zn	0.0000	12
Zn	-1.329073520	2.569721017	4.787710690 CORE	13 Zn Zn	0.0000	13
Zn	-1.307835173	2.543953030	8.418955858 CORE	14 Zn Zn	0.0000	14
Zn	1.588179054	0.869145993	9.083243245 CORE	15 Zn Zn	0.0000	15
Zn	2.117895042	3.998922418	9.505754981 CORE	16 Zn Zn	0.0000	16
Zn	1.561908786	4.358429423	13.285585723 CORE	17 Zn Zn	0.0000	17
O	0.058792909	1.797983788	0.679215414 CORE	18 O O	0.0000	18
O	3.227144857	1.799892900	0.677637593 CORE	19 O O	0.0000	19
O	-1.328741168	4.143172046	0.690151672 CORE	20 O O	0.0000	20
O	1.642684367	4.242653850	0.692890437 CORE	21 O O	0.0000	21
O	-1.328308786	2.550786651	2.772680223 CORE	22 O O	0.0000	22
O	0.250116673	5.020212770	2.786739238 CORE	23 O O	0.0000	23
O	1.642138403	2.673194252	2.780037179 CORE	24 O O	0.0000	24
O	3.032763487	5.019008254	2.788748739 CORE	25 O O	0.0000	25
O	3.028650000	3.472434000	5.534058000 CORE	26 O O	0.0000	26
O	0.253791200	3.472434000	5.535824000 CORE	27 O O	0.0000	27
O	4.611970000	0.730145000	5.535824000 CORE	28 O O	0.0000	28
O	1.642349000	0.842522500	5.550709000 CORE	29 O O	0.0000	29
O	1.644488000	4.271580000	7.688042000 CORE	30 O O	0.0000	30
O	0.288341000	1.624328000	7.797532000 CORE	31 O O	0.0000	31
O	-1.333926000	4.420799000	7.786684000 CORE	32 O O	0.0000	32
O	2.996417000	1.630709000	7.787189000 CORE	33 O O	0.0000	33
O	1.715947204	0.813047419	12.610739993 CORE	34 O O	0.0000	34
O	0.333697478	0.004906371	10.495648833 CORE	35 O O	0.0000	35
O	1.733117074	2.382292663	10.485399804 CORE	36 O O	0.0000	36
O	-1.317232818	2.559407562	10.538245917 CORE	37 O O	0.0000	37
O	4.645659385	0.999857458	12.750659629 CORE	38 O O	0.0000	38
O	0.081916044	3.360921758	12.692115719 CORE	39 O O	0.0000	39
O	3.299068962	3.335688183	12.911014326 CORE	40 O O	0.0000	40
C	1.541926483	3.754682272	15.545860713 CORE	41 C C	0.0000	41
H	2.417366583	4.226672714	15.998342985 CORE	42 H H	0.0000	42
H	3.918759957	2.959438519	13.579833837 CORE	43 H H	0.0000	43
H	1.589674159	2.692223164	15.284081039 CORE	44 H H	0.0000	44
O	-0.701277104	4.652803803	16.179423373 CORE	45 O O	0.0000	45
C	0.348383295	4.212124592	15.920516632 CORE	46 C C	0.0000	46

CH₂O*

!BIOSYM archive 2

PBC=ON

	Energy	3	-268	-268.324715		
!DATE						
PBC	5.9415	5.9415	25.2282	90.0000	90.0000	120.0000
Cr	0.150802152	3.390995920	1.657740471 CORE	1 Cr Cr	0.0000	1
Cr	3.124473009	3.390919789	1.657741510 CORE	2 Cr Cr	0.0000	2
Cr	4.608390682	0.819805797	1.682290578 CORE	3 Cr Cr	0.0000	3
Cr	-2.807655825	5.133964039	6.615086322 CORE	4 Cr Cr	0.0000	4
Cr	0.149101943	5.134941682	6.617609142 CORE	5 Cr Cr	0.0000	5
Cr	1.642319723	2.550567907	6.615086322 CORE	6 Cr Cr	0.0000	6
Cr	3.244697640	1.721799277	11.673921261 CORE	7 Cr Cr	0.0000	7
Cr	0.264560978	1.667225168	11.662868517 CORE	8 Cr Cr	0.0000	8
Cr	-1.256763848	4.205872027	11.661649774 CORE	9 Cr Cr	0.0000	9
Zn	1.637998462	0.838704405	0.365619757 CORE	10 Zn Zn	0.0000	10
Zn	1.638328231	0.812560297	3.553889027 CORE	11 Zn Zn	0.0000	11
Zn	1.639096697	4.266412515	4.183536316 CORE	12 Zn Zn	0.0000	12
Zn	-1.329784928	2.560385111	4.788145155 CORE	13 Zn Zn	0.0000	13
Zn	-1.305292383	2.543505768	8.400407549 CORE	14 Zn Zn	0.0000	14
Zn	1.585244682	0.870778264	9.093138623 CORE	15 Zn Zn	0.0000	15
Zn	2.125587348	3.997880367	9.499280529 CORE	16 Zn Zn	0.0000	16
Zn	1.453134870	4.449758916	13.101945715 CORE	17 Zn Zn	0.0000	17
O	0.054175958	1.791884938	0.680574007 CORE	18 O O	0.0000	18
O	3.221186958	1.792963551	0.680123672 CORE	19 O O	0.0000	19
O	-1.333601075	4.135895500	0.690443370 CORE	20 O O	0.0000	20
O	1.637984849	4.236796496	0.694510876 CORE	21 O O	0.0000	21
O	-1.332924187	2.545244009	2.773741822 CORE	22 O O	0.0000	22
O	0.246097889	5.014195809	2.787801450 CORE	23 O O	0.0000	23
O	1.637874000	2.668239875	2.782340302 CORE	24 O O	0.0000	24
O	3.028964672	5.013673986	2.789156529 CORE	25 O O	0.0000	25
O	3.028649918	3.472433884	5.534057952 CORE	26 O O	0.0000	26
O	0.253791173	3.472433884	5.535823926 CORE	27 O O	0.0000	27
O	4.611970545	0.730145022	5.535823926 CORE	28 O O	0.0000	28
O	1.642349430	0.842522522	5.550708564 CORE	29 O O	0.0000	29
O	1.644488370	4.271579926	7.688041668 CORE	30 O O	0.0000	30
O	0.288340995	1.624328263	7.797532056 CORE	31 O O	0.0000	31
O	-1.333926165	4.420799134	7.786683930 CORE	32 O O	0.0000	32
O	2.996417280	1.630708671	7.787188494 CORE	33 O O	0.0000	33
O	1.793996765	0.781216179	12.583951081 CORE	34 O O	0.0000	34
O	-2.631015039	5.121165090	10.526241317 CORE	35 O O	0.0000	35
O	1.766923927	2.387595645	10.496854611 CORE	36 O O	0.0000	36
O	-1.245060537	2.534601368	10.543003857 CORE	37 O O	0.0000	37
O	4.725910625	1.066143777	12.833175124 CORE	38 O O	0.0000	38
O	0.107741178	3.287246423	12.781353119 CORE	39 O O	0.0000	39
O	3.158755143	3.480609141	13.879291946 CORE	40 O O	0.0000	40
C	3.846204339	3.148296961	14.849215756 CORE	41 C C	0.0000	41
H	3.497359407	3.370862645	15.878089798 CORE	42 H H	0.0000	42
H	-1.134431562	2.635833163	14.661817754 CORE	43 H H	0.0000	43

CH₂O* + CO*

!BIOSYM archive 2

PBC=ON

	Energy	4	-285	-285.841467		
!DATE						
PBC	5.9415	5.9415	25.2282	90.0000	90.0000	120.0000
Cr	0.137499722	3.425659102	1.653923881 CORE	1 Cr Cr	0.0000	1
Cr	3.110539608	3.426566861	1.680307807 CORE	2 Cr Cr	0.0000	2
Cr	4.595587237	0.856090016	1.654088411 CORE	3 Cr Cr	0.0000	3
Cr	-2.807656000	5.133964000	6.615087000 CORE	4 Cr Cr	0.0000	4
Cr	0.149101900	5.134942000	6.617609000 CORE	5 Cr Cr	0.0000	5
Cr	1.642320000	2.550568000	6.615087000 CORE	6 Cr Cr	0.0000	6
Cr	3.136068041	1.698686075	11.791053230 CORE	7 Cr Cr	0.0000	7
Cr	0.159871651	1.569531119	11.584391527 CORE	8 Cr Cr	0.0000	8
Cr	-1.259292643	4.247535077	11.543129628 CORE	9 Cr Cr	0.0000	9
Zn	1.643133732	0.844602161	0.350886575 CORE	10 Zn Zn	0.0000	10
Zn	1.618838463	0.856867141	3.546060172 CORE	11 Zn Zn	0.0000	11
Zn	1.635976756	4.276918178	4.181400793 CORE	12 Zn Zn	0.0000	12
Zn	-1.326669592	2.557673303	4.782453618 CORE	13 Zn Zn	0.0000	13
Zn	-1.307216004	2.547304833	8.356142627 CORE	14 Zn Zn	0.0000	14
Zn	1.619169341	0.890723717	9.062377824 CORE	15 Zn Zn	0.0000	15
Zn	2.073501895	3.973733435	9.493928876 CORE	16 Zn Zn	0.0000	16
Zn	1.870359597	4.331417308	13.465577628 CORE	17 Zn Zn	0.0000	17

O	0.043137102	1.767408634	0.689610373	CORE	18	O	O	0.0000	18
O	3.260310019	1.737459032	0.679199440	CORE	19	O	O	0.0000	19
O	-1.293293780	4.142690011	0.680035245	CORE	20	O	O	0.0000	20
O	1.613020289	4.291056969	0.692203431	CORE	21	O	O	0.0000	21
O	-1.336031217	2.563384196	2.770575345	CORE	22	O	O	0.0000	22
O	0.254847916	5.075291927	2.778426135	CORE	23	O	O	0.0000	23
O	1.589402601	2.697014404	2.785762132	CORE	24	O	O	0.0000	24
O	2.981002379	5.108313483	2.786495610	CORE	25	O	O	0.0000	25
O	3.028650000	3.472434000	5.534058000	CORE	26	O	O	0.0000	26
O	0.253791200	3.472434000	5.535824000	CORE	27	O	O	0.0000	27
O	4.611970000	0.730145000	5.535824000	CORE	28	O	O	0.0000	28
O	1.642349000	0.842522500	5.550709000	CORE	29	O	O	0.0000	29
O	1.644488000	4.271580000	7.688042000	CORE	30	O	O	0.0000	30
O	0.288341000	1.624328000	7.797532000	CORE	31	O	O	0.0000	31
O	-1.333926000	4.420799000	7.786684000	CORE	32	O	O	0.0000	32
O	2.996417000	1.630709000	7.787189000	CORE	33	O	O	0.0000	33
O	1.653578323	0.746187271	12.620805029	CORE	34	O	O	0.0000	34
O	-2.608835482	5.144136902	10.420320586	CORE	35	O	O	0.0000	35
O	1.701250971	2.453211913	10.613230713	CORE	36	O	O	0.0000	36
O	-1.330693215	2.494540932	10.583427482	CORE	37	O	O	0.0000	37
O	4.650366626	0.812285867	12.652255487	CORE	38	O	O	0.0000	38
O	0.074882207	3.308823481	12.902802078	CORE	39	O	O	0.0000	39
O	3.371429759	3.158752223	13.319039473	CORE	40	O	O	0.0000	40
C	4.192602181	2.987626056	14.470840317	CORE	41	C	C	0.0000	41
H	3.852810697	3.612437731	15.312099351	CORE	42	H	H	0.0000	42
H	4.183420841	1.935959125	14.806606989	CORE	43	H	H	0.0000	43
O	0.494842775	3.758745890	15.023861386	CORE	44	O	O	0.0000	44
C	-0.321710651	3.364019218	14.163520288	CORE	45	C	C	0.0000	45

end
end

CH₃O* + CO*

'BIOSYM archive 2
PBC=ON

	Energy		5	-283	-283.481355				
'DATE									
PBC	5.9415	5.9415	25.2282	90.0000	90.0000	120.0000			
Cr	0.155362229	3.399676042	1.657803755	CORE	1	Cr Cr	0.0000	1	
Cr	3.129864067	3.400077537	1.658273797	CORE	2	Cr Cr	0.0000	2	
Cr	4.613607635	0.828200911	1.684161921	CORE	3	Cr Cr	0.0000	3	
Cr	-2.807655825	5.133964039	6.615086322	CORE	4	Cr Cr	0.0000	4	
Cr	0.149101943	5.134941682	6.617609142	CORE	5	Cr Cr	0.0000	5	
Cr	1.642319723	2.550567907	6.615086322	CORE	6	Cr Cr	0.0000	6	
Cr	3.190862397	1.728571860	11.733669170	CORE	7	Cr Cr	0.0000	7	
Cr	0.215115948	1.662289191	11.628932253	CORE	8	Cr Cr	0.0000	8	
Cr	-1.340821416	4.192489211	11.745663209	CORE	9	Cr Cr	0.0000	9	
Zn	1.644145567	0.849735549	0.352212303	CORE	10	Zn Zn	0.0000	10	
Zn	1.642092240	0.820000489	3.553066318	CORE	11	Zn Zn	0.0000	11	
Zn	1.641137991	4.269190215	4.184345932	CORE	12	Zn Zn	0.0000	12	
Zn	-1.329340892	2.561465941	4.789119805	CORE	13	Zn Zn	0.0000	13	
Zn	-1.305001864	2.544230772	8.415364045	CORE	14	Zn Zn	0.0000	14	
Zn	1.600018719	0.866496502	9.072658714	CORE	15	Zn Zn	0.0000	15	
Zn	2.154408298	3.976281991	9.517016116	CORE	16	Zn Zn	0.0000	16	
Zn	1.221004200	4.505329888	13.734644861	CORE	17	Zn Zn	0.0000	17	
O	0.060426231	1.800544609	0.684824218	CORE	18	O O	0.0000	18	
O	3.225929833	1.802191812	0.683767152	CORE	19	O O	0.0000	19	
O	-1.328522248	4.147985323	0.694724016	CORE	20	O O	0.0000	20	
O	1.642931763	4.245464836	0.697136736	CORE	21	O O	0.0000	21	
O	-1.328157829	2.553751481	2.774942709	CORE	22	O O	0.0000	22	
O	0.251266186	5.022646666	2.789153839	CORE	23	O O	0.0000	23	
O	1.642731330	2.676903011	2.783641643	CORE	24	O O	0.0000	24	
O	3.032248288	5.021353510	2.791319475	CORE	25	O O	0.0000	25	
O	3.028649918	3.472433884	5.534057952	CORE	26	O O	0.0000	26	
O	0.253791173	3.472433884	5.535823926	CORE	27	O O	0.0000	27	
O	4.611970545	0.730145022	5.535823926	CORE	28	O O	0.0000	28	
O	1.642349430	0.842522522	5.550708564	CORE	29	O O	0.0000	29	
O	1.644488370	4.271579926	7.688041668	CORE	30	O O	0.0000	30	
O	0.288340995	1.624328263	7.797532056	CORE	31	O O	0.0000	31	
O	-1.333926165	4.420799134	7.786683930	CORE	32	O O	0.0000	32	
O	2.996417280	1.630708671	7.787188494	CORE	33	O O	0.0000	33	
O	1.735633846	0.781865175	12.621119813	CORE	34	O O	0.0000	34	
O	-2.559833998	5.125782160	10.474913910	CORE	35	O O	0.0000	35	
O	1.768098465	2.340348321	10.476063776	CORE	36	O O	0.0000	36	
O	-1.310516113	2.542988069	10.553761403	CORE	37	O O	0.0000	37	
O	4.622400986	0.822264814	12.542965372	CORE	38	O O	0.0000	38	
O	0.156586678	3.401122975	12.562250307	CORE	39	O O	0.0000	39	
O	3.242746115	3.328717187	12.806098227	CORE	40	O O	0.0000	40	
O	3.470518090	0.037790787	16.703389685	CORE	41	O O	0.0000	41	
C	2.934269722	3.476353937	14.162145122	CORE	42	C C	0.0000	42	
C	0.422576990	5.106721198	15.558061134	CORE	43	C C	0.0000	43	
H	2.729022958	2.504103129	14.632638380	CORE	44	H H	0.0000	44	
H	-2.251261457	4.075365990	14.688964542	CORE	45	H H	0.0000	45	

end
end

CH₃O* + OH*

'BIOSYM archive 2
PBC=ON

	Energy		6	-272	-272.741229				
'DATE									
PBC	5.9415	5.9415	25.2282	90.0000	90.0000	120.0000			
Cr	0.155279076	3.398862370	1.656521684	CORE	1	Cr Cr	0.0000	1	
Cr	3.129320726	3.399073985	1.656664534	CORE	2	Cr Cr	0.0000	2	
Cr	4.613165119	0.827313031	1.682814759	CORE	3	Cr Cr	0.0000	3	
Cr	-2.807655825	5.133964039	6.615086322	CORE	4	Cr Cr	0.0000	4	
Cr	0.149101943	5.134941682	6.617609142	CORE	5	Cr Cr	0.0000	5	
Cr	1.642319723	2.550567907	6.615086322	CORE	6	Cr Cr	0.0000	6	
Cr	3.140299566	1.738848814	11.695541837	CORE	7	Cr Cr	0.0000	7	
Cr	0.177701265	1.648819784	11.597002894	CORE	8	Cr Cr	0.0000	8	
Cr	-1.356758168	4.247188802	11.697274370	CORE	9	Cr Cr	0.0000	9	
Zn	1.643130924	0.848654177	0.350878837	CORE	10	Zn Zn	0.0000	10	
Zn	1.641742941	0.819205873	3.549941317	CORE	11	Zn Zn	0.0000	11	
Zn	1.640966875	4.269534551	4.183543809	CORE	12	Zn Zn	0.0000	12	
Zn	-1.329188964	2.561329679	4.786174869	CORE	13	Zn Zn	0.0000	13	
Zn	-1.305633162	2.550110944	8.388743766	CORE	14	Zn Zn	0.0000	14	
Zn	1.606644158	0.878318693	9.065976666	CORE	15	Zn Zn	0.0000	15	
Zn	2.103770652	4.003071797	9.503295103	CORE	16	Zn Zn	0.0000	16	
Zn	1.540194092	4.565502914	13.726427776	CORE	17	Zn Zn	0.0000	17	
O	0.060035518	1.800298812	0.682954828	CORE	18	O O	0.0000	18	
O	3.225009535	1.801534531	0.682219309	CORE	19	O O	0.0000	19	
O	-1.328762093	4.147077005	0.692915531	CORE	20	O O	0.0000	20	
O	1.642518364	4.244344802	0.695058855	CORE	21	O O	0.0000	21	
O	-1.328437939	2.552991191	2.773068845	CORE	22	O O	0.0000	22	
O	0.250732089	5.021281703	2.787697689	CORE	23	O O	0.0000	23	
O	1.642412443	2.675902698	2.781674689	CORE	24	O O	0.0000	24	
O	3.032521036	5.020115701	2.789057446	CORE	25	O O	0.0000	25	
O	3.028649918	3.472433884	5.534057952	CORE	26	O O	0.0000	26	
O	0.253791173	3.472433884	5.535823926	CORE	27	O O	0.0000	27	
O	4.611970545	0.730145022	5.535823926	CORE	28	O O	0.0000	28	
O	1.642349430	0.842522522	5.550708564	CORE	29	O O	0.0000	29	
O	1.644488370	4.271579926	7.688041668	CORE	30	O O	0.0000	30	
O	0.288340995	1.624328263	7.797532056	CORE	31	O O	0.0000	31	
O	-1.333926165	4.420799134	7.786683930	CORE	32	O O	0.0000	32	

O 2.996417280 1.630708671 7.787188494 CORE 33 O O 0.0000 33
O 1.686598543 0.807685137 12.602112920 CORE 34 O O 0.0000 34
O 0.366680073 0.001808940 10.471702936 CORE 35 O O 0.0000 35
O 1.696047251 2.402793259 10.489030157 CORE 36 O O 0.0000 36
O -1.310758745 2.571011603 10.551982243 CORE 37 O O 0.0000 37
O 4.608825730 0.941264225 12.657872043 CORE 38 O O 0.0000 38
O 0.079498623 3.344679110 12.855332866 CORE 39 O O 0.0000 39
O 3.249810224 3.331070579 12.816071738 CORE 40 O O 0.0000 40
C 3.029802871 3.403434353 14.251878398 CORE 41 C C 0.0000 41
H 2.824917582 2.403984681 14.654866689 CORE 42 H H 0.0000 42
H -2.059032124 3.878512695 14.759450860 CORE 43 H H 0.0000 43
H -0.414681691 2.891181398 13.571817897 CORE 44 H H 0.0000 44
end
end

CH₃CO* + O*

'BIOSYM archive 2
PBC=ON

Energy 7 -288 -288.403983
!DATE
PBC 5.9415 5.9415 25.2282 90.0000 90.0000 120.0000
Cr 0.152583513 3.400114364 1.657193636 CORE 1 Cr Cr 0.0000 1
Cr 3.127188844 3.400025382 1.657229513 CORE 2 Cr Cr 0.0000 2
Cr 4.610674205 0.828186349 1.683692121 CORE 3 Cr Cr 0.0000 3
Cr -2.807656000 5.133964000 6.615087000 CORE 4 Cr Cr 0.0000 4
Cr 0.149101900 5.134942000 6.617609000 CORE 5 Cr Cr 0.0000 5
Cr 1.642320000 2.550568000 6.615087000 CORE 6 Cr Cr 0.0000 6
Cr 3.100276028 1.939875131 11.837094855 CORE 7 Cr Cr 0.0000 7
Cr 0.145330730 1.753939376 11.581286139 CORE 8 Cr Cr 0.0000 8
Cr -1.388775369 4.301485093 11.767955057 CORE 9 Cr Cr 0.0000 9
Zn 1.640203610 0.849930814 0.341194023 CORE 10 Zn Zn 0.0000 10
Zn 1.639738832 0.820200065 3.551288048 CORE 11 Zn Zn 0.0000 11
Zn 1.639673072 4.269357941 4.184228934 CORE 12 Zn Zn 0.0000 12
Zn -1.329403303 2.561628469 4.788493921 CORE 13 Zn Zn 0.0000 13
Zn -1.308637320 2.546422358 8.412533924 CORE 14 Zn Zn 0.0000 14
Zn 1.606619830 0.859696326 9.067919600 CORE 15 Zn Zn 0.0000 15
Zn 2.181863895 4.005506730 9.502735337 CORE 16 Zn Zn 0.0000 16
Zn 1.474203441 4.420581636 13.504854730 CORE 17 Zn Zn 0.0000 17
O 0.057815702 1.800785171 0.684955916 CORE 18 O O 0.0000 18
O 3.221649247 1.801530113 0.684401049 CORE 19 O O 0.0000 19
O -1.331329592 4.149689071 0.695281861 CORE 20 O O 0.0000 20
O 1.640200295 4.245522794 0.696521001 CORE 21 O O 0.0000 21
O -1.330731001 2.553685700 2.773877075 CORE 22 O O 0.0000 22
O 0.249176842 5.022647277 2.788567142 CORE 23 O O 0.0000 23
O 1.640064346 2.677457454 2.783040533 CORE 24 O O 0.0000 24
O 3.029389459 5.021641745 2.790424171 CORE 25 O O 0.0000 25
O 3.028650000 3.472434000 5.534058000 CORE 26 O O 0.0000 26
O 0.253791200 3.472434000 5.535824000 CORE 27 O O 0.0000 27
O 4.611970000 0.730145000 5.535824000 CORE 28 O O 0.0000 28
O 1.642349000 0.842522500 5.550709000 CORE 29 O O 0.0000 29
O 1.644488000 4.271580000 7.688042000 CORE 30 O O 0.0000 30
O 0.288341000 1.624328000 7.797532000 CORE 31 O O 0.0000 31
O -1.333926000 4.420799000 7.786684000 CORE 32 O O 0.0000 32
O 2.996417000 1.630709000 7.787189000 CORE 33 O O 0.0000 33
O 1.664570038 0.926827531 12.617878182 CORE 34 O O 0.0000 34
O 0.356753764 0.063034503 10.468316538 CORE 35 O O 0.0000 35
O 1.800803250 2.353138795 10.477925548 CORE 36 O O 0.0000 36
O -1.370948747 2.650995164 10.548244183 CORE 37 O O 0.0000 37
O 4.501461301 0.949316245 12.467087831 CORE 38 O O 0.0000 38
O 0.136119584 3.481506569 12.510486965 CORE 39 O O 0.0000 39
O 3.149168216 3.478340807 12.764936296 CORE 40 O O 0.0000 40
C 2.699271637 3.476264269 16.121850907 CORE 41 C C 0.0000 41
H 2.735615222 3.542275814 17.218449029 CORE 42 H H 0.0000 42
H 3.683250449 3.696850598 15.677931548 CORE 43 H H 0.0000 43
H 2.445918013 2.455249361 15.794796563 CORE 44 H H 0.0000 44
O 3.993857561 0.055187696 16.217472212 CORE 45 O O 0.0000 45
C 1.692461058 4.440723886 15.547536533 CORE 46 C C 0.0000 46
end
end

CH₃O*

'BIOSYM archive 2
PBC=ON

Energy 8 -273 -273.287658
!DATE
PBC 5.9415 5.9415 25.2282 90.0000 90.0000 120.0000
Cr 0.154200352 3.400612620 1.656915527 CORE 1 Cr Cr 0.0000 1
Cr 3.128561180 3.400678385 1.656987932 CORE 2 Cr Cr 0.0000 2
Cr 4.612291936 0.828834328 1.683339376 CORE 3 Cr Cr 0.0000 3
Cr -2.807655825 5.133964039 6.615086322 CORE 4 Cr Cr 0.0000 4
Cr 0.149101943 5.134941682 6.617609142 CORE 5 Cr Cr 0.0000 5
Cr 1.642319723 2.550567907 6.615086322 CORE 6 Cr Cr 0.0000 6
Cr 3.223276146 1.695674322 11.717448300 CORE 7 Cr Cr 0.0000 7
Cr 0.250922512 1.637090730 11.615942587 CORE 8 Cr Cr 0.0000 8
Cr -1.284633151 4.179314285 11.719875716 CORE 9 Cr Cr 0.0000 9
Zn 1.642126610 0.850140460 0.348491640 CORE 10 Zn Zn 0.0000 10
Zn 1.641139254 0.820837795 3.550947246 CORE 11 Zn Zn 0.0000 11
Zn 1.640683460 4.269828208 4.183576369 CORE 12 Zn Zn 0.0000 12
Zn -1.329321782 2.561704680 4.788383232 CORE 13 Zn Zn 0.0000 13
Zn -1.301944707 2.542032584 8.415349119 CORE 14 Zn Zn 0.0000 14
Zn 1.604797794 0.863128177 9.078220853 CORE 15 Zn Zn 0.0000 15
Zn 2.174411876 3.960723699 9.473854686 CORE 16 Zn Zn 0.0000 16
Zn 1.605111419 4.280352110 12.841648473 CORE 17 Zn Zn 0.0000 17
O 0.059292651 1.801496156 0.683475204 CORE 18 O O 0.0000 18
O 3.224026755 1.802744401 0.682601962 CORE 19 O O 0.0000 19
O -1.329742141 4.148850289 0.693263556 CORE 20 O O 0.0000 20
O 1.641723101 4.246042266 0.695538079 CORE 21 O O 0.0000 21
O -1.329334716 2.554414937 2.773608513 CORE 22 O O 0.0000 22
O 0.250259752 5.022978413 2.788017777 CORE 23 O O 0.0000 23
O 1.641660551 2.677525867 2.782198215 CORE 24 O O 0.0000 24
O 3.031402903 5.021878996 2.789588829 CORE 25 O O 0.0000 25
O 3.028649918 3.472433884 5.534057952 CORE 26 O O 0.0000 26
O 0.253791173 3.472433884 5.535823926 CORE 27 O O 0.0000 27
O 4.611970545 0.730145022 5.535823926 CORE 28 O O 0.0000 28
O 1.642349430 0.842522522 5.550708564 CORE 29 O O 0.0000 29
O 1.644488370 4.271579926 7.688041668 CORE 30 O O 0.0000 30
O 0.288340995 1.624328263 7.797532056 CORE 31 O O 0.0000 31
O -1.333926165 4.420799134 7.786683930 CORE 32 O O 0.0000 32
O 2.996417280 1.630708671 7.787188494 CORE 33 O O 0.0000 33
O 1.774449238 0.758065904 12.596107724 CORE 34 O O 0.0000 34
O -2.573780692 5.083723281 10.497632988 CORE 35 O O 0.0000 35
O 1.794258324 2.370045397 10.501768738 CORE 36 O O 0.0000 36
O -1.270590935 2.516708690 10.538215479 CORE 37 O O 0.0000 37
O 4.720597734 0.941158152 12.696087878 CORE 38 O O 0.0000 38
O 0.110849739 3.254433651 12.703335553 CORE 39 O O 0.0000 39
O 3.327464160 3.290102833 13.002081699 CORE 40 O O 0.0000 40
C 3.680301848 3.084646186 14.406804987 CORE 41 C C 0.0000 41
H 2.893170555 3.525705588 15.037164616 CORE 42 H H 0.0000 42
H -1.298573565 3.568585248 14.602911333 CORE 43 H H 0.0000 43
H 3.763522238 2.009234355 14.595884315 CORE 44 H H 0.0000 44
end
end

CH₃OH* + H*

!BIOSYM archive 2

PBC=ON

Energy		9	-280	-280.803162				
!DATE								
PBC	5.9415	5.9415	25.2282	90.0000	90.0000	120.0000		
Cr	0.158756690	3.388541127	1.648967445	CORE	1	Cr Cr	0.0000	1
Cr	3.132599391	3.389658249	1.649991759	CORE	2	Cr Cr	0.0000	2
Cr	4.617153039	0.818006277	1.674657833	CORE	3	Cr Cr	0.0000	3
Cr	-2.807655825	5.133964039	6.615086322	CORE	4	Cr Cr	0.0000	4
Cr	1.642319723	2.550567907	6.615086322	CORE	5	Cr Cr	0.0000	5
Cr	0.149101943	5.134941682	6.617609142	CORE	6	Cr Cr	0.0000	6
Cr	3.081412875	1.684868601	11.644921934	CORE	7	Cr Cr	0.0000	7
Cr	-1.378791100	4.280591751	11.601154266	CORE	8	Cr Cr	0.0000	8
Cr	0.092193400	1.688158467	11.648472244	CORE	9	Cr Cr	0.0000	9
Zn	1.648060637	0.838035230	0.361039709	CORE	10	Zn Zn	0.0000	10
Zn	1.645085033	0.811587651	3.533556056	CORE	11	Zn Zn	0.0000	11
Zn	1.642725522	4.267937409	4.172494626	CORE	12	Zn Zn	0.0000	12
Zn	-1.328724096	2.560360721	4.772810937	CORE	13	Zn Zn	0.0000	13
Zn	-1.313731404	2.527706843	8.374544312	CORE	14	Zn Zn	0.0000	14
Zn	1.636196562	0.830655484	9.006065990	CORE	15	Zn Zn	0.0000	15
Zn	1.950424055	3.917180393	9.503989521	CORE	16	Zn Zn	0.0000	16
Zn	1.923785423	4.616509024	12.912739513	CORE	17	Zn Zn	0.0000	17
O	3.229256912	1.793705002	0.670964113	CORE	18	O O	0.0000	18
O	0.064106305	1.791932269	0.672481677	CORE	19	O O	0.0000	19
O	-1.324686678	4.134724964	0.683561381	CORE	20	O O	0.0000	20
O	1.645891558	4.234043697	0.686362953	CORE	21	O O	0.0000	21
O	-1.325243619	2.543282768	2.768033592	CORE	22	O O	0.0000	22
O	1.645701601	2.665890597	2.776024102	CORE	23	O O	0.0000	23
O	0.252154544	5.011677075	2.783396196	CORE	24	O O	0.0000	24
O	3.038265417	5.010094635	2.783958930	CORE	25	O O	0.0000	25
O	3.028649918	3.472433884	5.534057952	CORE	26	O O	0.0000	26
O	0.253791173	3.472433884	5.535823926	CORE	27	O O	0.0000	27
O	4.611970545	0.730145022	5.535823926	CORE	28	O O	0.0000	28
O	1.642349430	0.842522522	5.550708564	CORE	29	O O	0.0000	29
O	1.644488770	4.271579926	7.688041668	CORE	30	O O	0.0000	30
O	-1.333926165	4.420799134	7.786683930	CORE	31	O O	0.0000	31
O	2.996417280	1.630708671	7.787188494	CORE	32	O O	0.0000	32
O	0.288340995	1.624328263	7.797532056	CORE	33	O O	0.0000	33
O	1.582638852	2.197296409	10.401771256	CORE	34	O O	0.0000	34
O	-1.368947401	2.562299381	10.540838583	CORE	35	O O	0.0000	35
O	2.727378531	4.905472064	11.004010818	CORE	36	O O	0.0000	36
O	1.573862439	0.815676111	12.641670209	CORE	37	O O	0.0000	37
O	0.291937023	3.498135058	12.654369214	CORE	38	O O	0.0000	38
O	4.551381489	1.372655628	13.029627102	CORE	39	O O	0.0000	39
O	3.048129095	3.408565361	14.231907810	CORE	40	O O	0.0000	40
C	-2.107312462	4.048396835	15.273351099	CORE	41	C C	0.0000	41
H	-0.037582105	3.170961978	13.516546170	CORE	42	H H	0.0000	42
H	3.556390536	2.603204251	13.873430752	CORE	43	H H	0.0000	43
H	-1.468459436	4.833679299	14.838382069	CORE	44	H H	0.0000	44
H	-1.510461009	3.283879211	15.790680701	CORE	45	H H	0.0000	45
H	3.135778672	4.496723223	15.990650820	CORE	46	H H	0.0000	46
end								
end								

CH₃O* + CO*

!BIOSYM archive 2

PBC=ON

Energy		10	-288	-288.311229				
!DATE								
PBC	5.9415	5.9415	25.2282	90.0000	90.0000	120.0000		
Cr	0.154792752	3.400966255	1.656779452	CORE	1	Cr Cr	0.0000	1
Cr	3.129214986	3.401002303	1.656837407	CORE	2	Cr Cr	0.0000	2
Cr	4.612718020	0.829353780	1.682612160	CORE	3	Cr Cr	0.0000	3
Cr	-2.807656000	5.133964000	6.615087000	CORE	4	Cr Cr	0.0000	4
Cr	0.149101900	5.134942000	6.617609000	CORE	5	Cr Cr	0.0000	5
Cr	1.642320000	2.550568000	6.615087000	CORE	6	Cr Cr	0.0000	6
Cr	3.136075040	1.703070731	11.717692776	CORE	7	Cr Cr	0.0000	7
Cr	0.172237273	1.644885420	11.605181910	CORE	8	Cr Cr	0.0000	8
Cr	-1.371946212	4.190808186	11.738012632	CORE	9	Cr Cr	0.0000	9
Zn	1.642792009	0.850698052	0.358167446	CORE	10	Zn Zn	0.0000	10
Zn	1.641575229	0.820703038	3.551982618	CORE	11	Zn Zn	0.0000	11
Zn	1.640556601	4.269753323	4.183469384	CORE	12	Zn Zn	0.0000	12
Zn	-1.329087316	2.561403218	4.787837035	CORE	13	Zn Zn	0.0000	13
Zn	-1.309179387	2.545035138	8.409486107	CORE	14	Zn Zn	0.0000	14
Zn	1.595389135	0.862600288	9.078995531	CORE	15	Zn Zn	0.0000	15
Zn	2.124623205	3.971720570	9.494426238	CORE	16	Zn Zn	0.0000	16
Zn	1.504369391	4.278959363	13.191336978	CORE	17	Zn Zn	0.0000	17
O	0.058925121	1.801735903	0.680949882	CORE	18	O O	0.0000	18
O	3.225773577	1.803452261	0.680447511	CORE	19	O O	0.0000	19
O	-1.329277618	4.148312619	0.691285937	CORE	20	O O	0.0000	20
O	1.642292404	4.246292766	0.694265779	CORE	21	O O	0.0000	21
O	-1.328749788	2.554628046	2.773314962	CORE	22	O O	0.0000	22
O	0.250409831	5.023365713	2.787443955	CORE	23	O O	0.0000	23
O	1.642064110	2.676840719	2.781318784	CORE	24	O O	0.0000	24
O	3.032124398	5.022130303	2.789326568	CORE	25	O O	0.0000	25
O	3.028650000	3.472434000	5.540580000	CORE	26	O O	0.0000	26
O	0.253791200	3.472434000	5.535824000	CORE	27	O O	0.0000	27
O	4.611970000	0.730145000	5.535824000	CORE	28	O O	0.0000	28
O	1.642349000	0.842522500	5.550709000	CORE	29	O O	0.0000	29
O	1.644488000	4.271580000	7.688042000	CORE	30	O O	0.0000	30
O	0.288341000	1.624328000	7.797532000	CORE	31	O O	0.0000	31
O	-1.333926000	4.420799000	7.786684000	CORE	32	O O	0.0000	32
O	2.996417000	1.630709000	7.787189000	CORE	33	O O	0.0000	33
O	1.687852314	0.772994486	12.619496400	CORE	34	O O	0.0000	34
O	-2.608054732	5.102776706	10.486301534	CORE	35	O O	0.0000	35
O	1.719671194	2.377446754	10.501719237	CORE	36	O O	0.0000	36
O	-1.352148647	2.531864918	10.548302309	CORE	37	O O	0.0000	37
O	4.629421137	0.884174059	12.625880772	CORE	38	O O	0.0000	38
O	0.037447120	3.270234184	12.690643426	CORE	39	O O	0.0000	39
O	3.253610798	3.269811494	13.060736384	CORE	40	O O	0.0000	40
C	3.700725991	2.951475845	14.403960518	CORE	41	C C	0.0000	41
H	-2.120335676	3.892813087	14.961930991	CORE	42	H H	0.0000	42
H	-1.286898339	2.417709564	14.348403519	CORE	43	H H	0.0000	43
H	2.933141213	2.322042049	14.881072530	CORE	44	H H	0.0000	44
O	0.407392303	4.759221844	16.252255017	CORE	45	O O	0.0000	45
C	1.064996060	4.475757668	15.361232240	CORE	46	C C	0.0000	46
end								
end								

CH₃O* + H* + H*

!BIOSYM archive 2

PBC=ON

Energy		11	-280	-280.985270				
!DATE								
PBC	5.9415	5.9415	25.2282	90.0000	90.0000	120.0000		
Cr	0.156276378	3.391215276	1.646982190	CORE	1	Cr Cr	0.0000	1
Cr	3.129776503	3.391796589	1.647385977	CORE	2	Cr Cr	0.0000	2
Cr	4.614042520	0.820237001	1.673312933	CORE	3	Cr Cr	0.0000	3
Cr	-2.807655825	5.133964039	6.615086322	CORE	4	Cr Cr	0.0000	4
Cr	1.642319723	2.550567907	6.615086322	CORE	5	Cr Cr	0.0000	5
Cr	0.149101943	5.134941682	6.617609142	CORE	6	Cr Cr	0.0000	6

Cr	0.100452764	1.702705895	11.641659386	CORE	7	Cr	Cr	0.0000	7
Cr	3.057125710	1.693962623	11.613184081	CORE	8	Cr	Cr	0.0000	8
Zn	-1.390595315	4.296399636	11.604763222	CORE	9	Cr	Cr	0.0000	9
Cr	1.644027385	0.841711013	0.351541624	CORE	10	Zn	Zn	0.0000	10
Zn	1.642497496	0.813617856	3.528836720	CORE	11	Zn	Zn	0.0000	11
Zn	1.642153421	4.268575966	4.169493770	CORE	12	Zn	Zn	0.0000	12
Zn	-1.328839906	2.560512001	4.768709127	CORE	13	Zn	Zn	0.0000	13
Zn	-1.314937463	2.531634173	8.364541543	CORE	14	Zn	Zn	0.0000	14
Zn	1.637949489	0.843154201	9.007616577	CORE	15	Zn	Zn	0.0000	15
Zn	1.930890184	3.976722211	9.510330300	CORE	16	Zn	Zn	0.0000	16
Zn	2.058737919	4.387559824	12.956834111	CORE	17	Zn	Zn	0.0000	17
O	3.225767651	1.796377605	0.670982045	CORE	18	O	O	0.0000	18
O	0.061284506	1.794922687	0.671658531	CORE	19	O	O	0.0000	19
O	-1.327621013	4.139572571	0.683806982	CORE	20	O	O	0.0000	20
O	1.643267351	4.236586686	0.685431392	CORE	21	O	O	0.0000	21
O	-1.327757399	2.545740055	2.766544961	CORE	22	O	O	0.0000	22
O	1.643148507	2.668479138	2.775195702	CORE	23	O	O	0.0000	23
O	0.250490616	5.013348230	2.783649444	CORE	24	O	O	0.0000	24
O	3.035435472	5.012299219	2.783484881	CORE	25	O	O	0.0000	25
O	3.028649918	3.472433884	5.534057952	CORE	26	O	O	0.0000	26
O	0.253791173	3.472433884	5.535823926	CORE	27	O	O	0.0000	27
O	4.611970545	0.730145022	5.535823926	CORE	28	O	O	0.0000	28
O	1.642349430	0.842522522	5.550708564	CORE	29	O	O	0.0000	29
O	1.644488370	4.271579926	7.688041668	CORE	30	O	O	0.0000	30
O	-1.333926165	4.420799134	7.786683930	CORE	31	O	O	0.0000	31
O	2.996417280	1.630708671	7.787188494	CORE	32	O	O	0.0000	32
O	0.288340995	1.624328263	7.797532056	CORE	33	O	O	0.0000	33
O	1.558150182	2.241766311	10.400330636	CORE	34	O	O	0.0000	34
O	-1.376076857	2.564667289	10.554815415	CORE	35	O	O	0.0000	35
O	2.712259481	4.933045685	11.008948510	CORE	36	O	O	0.0000	36
O	0.266860017	3.517103557	12.647222713	CORE	37	O	O	0.0000	37
O	1.573363641	0.851068079	12.613012762	CORE	38	O	O	0.0000	38
O	4.537476938	1.186234084	12.997074954	CORE	39	O	O	0.0000	39
O	3.356450154	3.433385382	14.015805346	CORE	40	O	O	0.0000	40
C	-2.192180811	4.087137594	15.231865943	CORE	41	C	C	0.0000	41
H	-0.150722000	3.396750053	13.524555688	CORE	42	H	H	0.0000	42
H	4.210073681	1.905681634	13.706502242	CORE	43	H	H	0.0000	43
H	-1.451548988	3.459219126	15.761422740	CORE	44	H	H	0.0000	44
H	-1.738914434	5.074894001	15.033510553	CORE	45	H	H	0.0000	45
H	2.896148871	4.221284796	15.921107343	CORE	46	H	H	0.0000	46

end

end

CH₄* + OH*

!BIOSYM archive 2

PBC=ON

	Energy	12	-281	-281.892116					
!DATE									
PBC	5.9415	5.9415	25.2282	90.0000	90.0000	120.0000			
Cr	0.156439676	3.397162545	1.654130569	CORE	1	Cr	Cr	0.0000	1
Cr	3.130474880	3.397278625	1.654195983	CORE	2	Cr	Cr	0.0000	2
Cr	4.614316790	0.825396392	1.680304477	CORE	3	Cr	Cr	0.0000	3
Cr	-2.807655825	5.133964039	6.615086322	CORE	4	Cr	Cr	0.0000	4
Cr	1.642319723	2.550567907	6.615086322	CORE	5	Cr	Cr	0.0000	5
Cr	0.149101943	5.134941682	6.617609142	CORE	6	Cr	Cr	0.0000	6
Cr	0.289565931	1.733425425	11.600387243	CORE	7	Cr	Cr	0.0000	7
Cr	3.207469044	1.793168236	11.719524491	CORE	8	Cr	Cr	0.0000	8
Cr	-1.307290168	4.238963650	11.759256374	CORE	9	Cr	Cr	0.0000	9
Zn	1.644484577	0.846377203	0.349200570	CORE	10	Zn	Zn	0.0000	10
Zn	1.642755066	0.817528743	3.545067262	CORE	11	Zn	Zn	0.0000	11
Zn	1.641634532	4.269635502	4.181676475	CORE	12	Zn	Zn	0.0000	12
Zn	-1.329200180	2.561380801	4.782374430	CORE	13	Zn	Zn	0.0000	13
Zn	-1.305906406	2.542353052	8.367410950	CORE	14	Zn	Zn	0.0000	14
Zn	1.597745387	0.857207684	9.064637199	CORE	15	Zn	Zn	0.0000	15
Zn	2.181816274	4.011716114	9.472361649	CORE	16	Zn	Zn	0.0000	16
Zn	1.769239550	4.201061393	13.074435860	CORE	17	Zn	Zn	0.0000	17
O	3.226216146	1.800534022	0.679785975	CORE	18	O	O	0.0000	18
O	0.061874150	1.798937204	0.680892121	CORE	19	O	O	0.0000	19
O	-1.327413402	4.145168153	0.690901817	CORE	20	O	O	0.0000	20
O	1.643708626	4.242084956	0.692591724	CORE	21	O	O	0.0000	21
O	-1.327403022	2.551194031	2.770967950	CORE	22	O	O	0.0000	22
O	1.643532796	2.674115151	2.779446920	CORE	23	O	O	0.0000	23
O	0.251474328	5.019120925	2.785665828	CORE	24	O	O	0.0000	24
O	3.034213616	5.017733552	2.786581202	CORE	25	O	O	0.0000	25
O	3.028649918	3.472433884	5.534057952	CORE	26	O	O	0.0000	26
O	0.253791173	3.472433884	5.535823926	CORE	27	O	O	0.0000	27
O	4.611970545	0.730145022	5.535823926	CORE	28	O	O	0.0000	28
O	1.642349430	0.842522522	5.550708564	CORE	29	O	O	0.0000	29
O	1.644488370	4.271579926	7.688041668	CORE	30	O	O	0.0000	30
O	-1.333926165	4.420799134	7.786683930	CORE	31	O	O	0.0000	31
O	2.996417280	1.630708671	7.787188494	CORE	32	O	O	0.0000	32
O	0.288340995	1.624328263	7.797532056	CORE	33	O	O	0.0000	33
O	1.812087979	2.376851248	10.473537694	CORE	34	O	O	0.0000	34
O	-1.258911941	2.555470035	10.567637865	CORE	35	O	O	0.0000	35
O	-2.624911195	5.143081244	10.545744144	CORE	36	O	O	0.0000	36
O	0.178968988	3.376562854	12.670154826	CORE	37	O	O	0.0000	37
O	1.768503634	0.846498731	12.599455930	CORE	38	O	O	0.0000	38
O	4.750572885	0.998375598	12.878255094	CORE	39	O	O	0.0000	39
O	3.399369916	3.306874197	12.905533076	CORE	40	O	O	0.0000	40
C	-1.043183066	3.617557654	16.562538409	CORE	41	C	C	0.0000	41
H	-0.937185880	3.424973275	15.486541807	CORE	42	H	H	0.0000	42
H	4.775630845	1.592052225	13.658226422	CORE	43	H	H	0.0000	43
H	-0.178264329	3.214869715	17.104589435	CORE	44	H	H	0.0000	44
H	-1.104733923	4.700604333	16.727764461	CORE	45	H	H	0.0000	45
H	3.983485813	3.140814220	16.936876289	CORE	46	H	H	0.0000	46

CHOCO* + H*

!BIOSYM archive 2

PBC=ON

	Energy	13	-276	-276.572643					
!DATE									
PBC	5.9415	5.9415	25.2282	90.0000	90.0000	120.0000			
Cr	0.153745153	3.396675527	1.652327735	CORE	1	Cr	Cr	0.0000	1
Cr	3.127619637	3.397055961	1.652491874	CORE	2	Cr	Cr	0.0000	2
Cr	4.611381397	0.824719622	1.679430038	CORE	3	Cr	Cr	0.0000	3
Cr	-2.807656000	5.133964000	6.615087000	CORE	4	Cr	Cr	0.0000	4
Cr	0.149101900	5.134942000	6.617609000	CORE	5	Cr	Cr	0.0000	5
Cr	1.642320000	2.550568000	6.615087000	CORE	6	Cr	Cr	0.0000	6
Cr	3.259935664	1.705354216	11.631841532	CORE	7	Cr	Cr	0.0000	7
Cr	0.240974701	1.771170040	11.592786891	CORE	8	Cr	Cr	0.0000	8
Cr	-1.300544995	4.233338998	11.724895177	CORE	9	Cr	Cr	0.0000	9
Zn	1.640361152	0.845998232	0.330540558	CORE	10	Zn	Zn	0.0000	10
Zn	1.641150682	0.817922413	3.541989688	CORE	11	Zn	Zn	0.0000	11
Zn	1.640715314	4.269582241	4.180250557	CORE	12	Zn	Zn	0.0000	12
Zn	-1.329452834	2.561483263	4.778056316	CORE	13	Zn	Zn	0.0000	13
Zn	-1.307213235	2.545584196	8.305087004	CORE	14	Zn	Zn	0.0000	14
Zn	1.599425420	0.864570504	9.069990349	CORE	15	Zn	Zn	0.0000	15
Zn	2.164563856	4.036301824	9.487469113	CORE	16	Zn	Zn	0.0000	16
Zn	1.920002723	3.928466719	13.101118480	CORE	17	Zn	Zn	0.0000	17
O	0.060148911	1.798556203	0.681844034	CORE	18	O	O	0.0000	18
O	3.220362949	1.799382429	0.681887274	CORE	19	O	O	0.0000	19

O	-1.330320436	4.146517770	0.691509130 CORE	20	O	O	0.0000	20
O	1.640780008	4.241764178	0.692549114 CORE	21	O	O	0.0000	21
O	-1.330106734	2.550884051	2.769482250 CORE	22	O	O	0.0000	22
O	0.249368257	5.018189582	2.785258183 CORE	23	O	O	0.0000	23
O	1.640716090	2.675090224	2.779273650 CORE	24	O	O	0.0000	24
O	3.031666275	5.017638155	2.785758031 CORE	25	O	O	0.0000	25
O	3.028650000	3.472434000	5.534058000 CORE	26	O	O	0.0000	26
O	0.253791200	3.472434000	5.535824000 CORE	27	O	O	0.0000	27
O	4.611970000	0.730145000	5.535824000 CORE	28	O	O	0.0000	28
O	1.642349000	0.842522500	5.550709000 CORE	29	O	O	0.0000	29
O	1.644488000	4.271580000	7.688042000 CORE	30	O	O	0.0000	30
O	0.288341000	1.624328000	7.797532000 CORE	31	O	O	0.0000	31
O	-1.333926000	4.420799000	7.786684000 CORE	32	O	O	0.0000	32
O	2.996417000	1.630709000	7.787189000 CORE	33	O	O	0.0000	33
O	0.345416798	0.037625929	10.549338442 CORE	34	O	O	0.0000	34
O	1.787072436	2.399536631	10.496628464 CORE	35	O	O	0.0000	35
O	-1.253414929	2.564811526	10.562002085 CORE	36	O	O	0.0000	36
O	4.785967923	0.826397536	12.809433746 CORE	37	O	O	0.0000	37
O	0.132318074	3.361531082	12.697200765 CORE	38	O	O	0.0000	38
O	1.761188512	0.902987804	12.788662090 CORE	39	O	O	0.0000	39
C	2.141524591	1.210512696	14.082259776 CORE	40	C	C	0.0000	40
H	1.888067962	0.476342754	14.854747616 CORE	41	H	H	0.0000	41
C	2.700693534	2.461360973	14.380168239 CORE	42	C	C	0.0000	42
O	3.305138172	2.882025113	15.377654039 CORE	43	O	O	0.0000	43
H	4.779019305	1.296744706	13.670228877 CORE	44	H	H	0.0000	44
end								
end								

CHOCO* + OH*

'BIOSYM archive 2
PBC=ON

	Energy		14	-284	-284.723967			
IDATE								
PBC	5.9415	5.9415	25.2282	90.0000	90.0000	120.0000		
Cr	0.138484179	3.422941671	1.654533266 CORE	1	Cr Cr	0.0000	1	
Cr	3.114411260	3.426305022	1.685115494 CORE	2	Cr Cr	0.0000	2	
Cr	4.598776858	0.856591591	1.643489425 CORE	3	Cr Cr	0.0000	3	
Cr	-2.807656000	5.133964000	6.615087000 CORE	4	Cr Cr	0.0000	4	
Cr	0.149101900	5.134942000	6.617609000 CORE	5	Cr Cr	0.0000	5	
Cr	1.642320000	2.550568000	6.615087000 CORE	6	Cr Cr	0.0000	6	
Cr	3.171019223	1.669449229	11.736180387 CORE	7	Cr Cr	0.0000	7	
Cr	0.107506255	1.563334926	11.577032266 CORE	8	Cr Cr	0.0000	8	
Cr	-1.295629541	4.159188301	11.543976945 CORE	9	Cr Cr	0.0000	9	
Zn	1.654071262	0.833597750	0.346667051 CORE	10	Zn Zn	0.0000	10	
Zn	1.618819275	0.861774206	3.547875908 CORE	11	Zn Zn	0.0000	11	
Zn	1.640419538	4.280279458	4.182371916 CORE	12	Zn Zn	0.0000	12	
Zn	-1.327469281	2.555473908	4.784668569 CORE	13	Zn Zn	0.0000	13	
Zn	-1.309533723	2.544833076	8.305164568 CORE	14	Zn Zn	0.0000	14	
Zn	1.609594161	0.881527318	9.065533568 CORE	15	Zn Zn	0.0000	15	
Zn	2.057944282	3.953639207	9.502440199 CORE	16	Zn Zn	0.0000	16	
Zn	1.756813034	4.272382284	13.569854339 CORE	17	Zn Zn	0.0000	17	
O	0.047437355	1.748422687	0.692775445 CORE	18	O O	0.0000	18	
O	3.277436584	1.714608648	0.672629552 CORE	19	O O	0.0000	19	
O	-1.283773529	4.128925982	0.681576341 CORE	20	O O	0.0000	20	
O	1.615711060	4.302777862	0.695004023 CORE	21	O O	0.0000	21	
O	-1.330729073	2.555675299	2.771326889 CORE	22	O O	0.0000	22	
O	0.262773619	5.081900376	2.769551296 CORE	23	O O	0.0000	23	
O	1.588072326	2.701011878	2.782922558 CORE	24	O O	0.0000	24	
O	2.974827593	5.124308645	2.783099225 CORE	25	O O	0.0000	25	
O	3.028650000	3.472434000	5.534058000 CORE	26	O O	0.0000	26	
O	0.253791200	3.472434000	5.535824000 CORE	27	O O	0.0000	27	
O	4.611970000	0.730145000	5.535824000 CORE	28	O O	0.0000	28	
O	1.642349000	0.842522500	5.550709000 CORE	29	O O	0.0000	29	
O	1.644488000	4.271580000	7.688042000 CORE	30	O O	0.0000	30	
O	0.288341000	1.624328000	7.797532000 CORE	31	O O	0.0000	31	
O	-1.333926000	4.420799000	7.786684000 CORE	32	O O	0.0000	32	
O	2.996417000	1.630709000	7.787189000 CORE	33	O O	0.0000	33	
O	1.636100660	0.723459827	12.692927094 CORE	34	O O	0.0000	34	
O	-2.612800723	5.123121418	10.427905795 CORE	35	O O	0.0000	35	
O	1.682357104	2.403114070	10.602115711 CORE	36	O O	0.0000	36	
O	-1.330455882	2.441057219	10.538915505 CORE	37	O O	0.0000	37	
O	4.651006163	0.729787057	12.637953722 CORE	38	O O	0.0000	38	
O	0.022936109	3.252330399	12.828040241 CORE	39	O O	0.0000	39	
O	3.342740273	3.131395614	13.338802423 CORE	40	O O	0.0000	40	
C	-1.739825846	3.119216557	14.405247953 CORE	41	C C	0.0000	41	
H	1.619376674	0.660765587	13.665196606 CORE	42	H H	0.0000	42	
H	3.801041197	2.993786285	15.412828660 CORE	43	H H	0.0000	43	
O	0.578649670	3.457327486	14.995715358 CORE	44	O O	0.0000	44	
C	-0.386424725	3.241476473	14.156525150 CORE	45	C C	0.0000	45	
end								
end								

CHOCO* + OH*

'BIOSYM archive 2
PBC=ON

Energy		15	-285	-285.371745				
IDate								
PBC	5.9415	5.9415	25.2282	90.0000	90.0000	120.0000		
Cr	0.142146988	3.422872504	1.652441846 CORE	1	Cr Cr	0.0000	1	
Cr	3.114463007	3.424191323	1.679979723 CORE	2	Cr Cr	0.0000	2	
Cr	4.600052329	0.853032375	1.653686139 CORE	3	Cr Cr	0.0000	3	
Cr	-2.807656000	5.133964000	6.615087000 CORE	4	Cr Cr	0.0000	4	
Cr	0.149101900	5.134942000	6.617609000 CORE	5	Cr Cr	0.0000	5	
Cr	1.642320000	2.550568000	6.615087000 CORE	6	Cr Cr	0.0000	6	
Cr	3.171877254	1.667111585	11.734823685 CORE	7	Cr Cr	0.0000	7	
Cr	0.109201441	1.563804456	11.578231474 CORE	8	Cr Cr	0.0000	8	
Cr	-1.296997831	4.158048068	11.547379175 CORE	9	Cr Cr	0.0000	9	
Zn	1.649269748	0.840676807	0.345007307 CORE	10	Zn Zn	0.0000	10	
Zn	1.621081198	0.854335691	3.545274273 CORE	11	Zn Zn	0.0000	11	
Zn	1.636290462	4.276104503	4.181013230 CORE	12	Zn Zn	0.0000	12	
Zn	-1.326089460	2.558185846	4.779329869 CORE	13	Zn Zn	0.0000	13	
Zn	-1.309804664	2.544370495	8.309504848 CORE	14	Zn Zn	0.0000	14	
Zn	1.611035118	0.881180609	9.066845716 CORE	15	Zn Zn	0.0000	15	
Zn	2.054979198	3.956996204	9.505446067 CORE	16	Zn Zn	0.0000	16	
Zn	1.757268465	4.275655737	13.572767461 CORE	17	Zn Zn	0.0000	17	
O	0.050261130	1.763663995	0.692082095 CORE	18	O O	0.0000	18	
O	3.264553849	1.734794492	0.680391197 CORE	19	O O	0.0000	19	
O	-1.288610275	4.139513175	0.678758314 CORE	20	O O	0.0000	20	
O	1.616981300	4.288566453	0.692360072 CORE	21	O O	0.0000	21	
O	-1.331410336	2.561052936	2.769708587 CORE	22	O O	0.0000	22	
O	0.258100051	5.072313323	2.777251126 CORE	23	O O	0.0000	23	
O	1.593797180	2.695783863	2.786836641 CORE	24	O O	0.0000	24	
O	2.984971380	5.104255057	2.785750848 CORE	25	O O	0.0000	25	
O	3.028650000	3.472434000	5.534058000 CORE	26	O O	0.0000	26	
O	0.253791200	3.472434000	5.535824000 CORE	27	O O	0.0000	27	
O	4.611970000	0.730145000	5.535824000 CORE	28	O O	0.0000	28	
O	1.642349000	0.842522500	5.550709000 CORE	29	O O	0.0000	29	
O	1.644488000	4.271580000	7.688042000 CORE	30	O O	0.0000	30	
O	0.288341000	1.624328000	7.797532000 CORE	31	O O	0.0000	31	
O	-1.333926000	4.420799000	7.786684000 CORE	32	O O	0.0000	32	
O	2.996417000	1.630709000	7.787189000 CORE	33	O O	0.0000	33	
O	1.636751894	0.723575030	12.696006217 CORE	34	O O	0.0000	34	
O	-2.612897335	5.122038500	10.429025514 CORE	35	O O	0.0000	35	

O 1.682634635 2.399972501 10.597717523 CORE 36 O O 0.0000 36
O -1.328066965 2.441216386 10.538159172 CORE 37 O O 0.0000 37
O 4.653427640 0.733069276 12.640905490 CORE 38 O O 0.0000 38
O 0.024162004 3.253006631 12.830177134 CORE 39 O O 0.0000 39
O 3.342875160 3.133640554 13.342074795 CORE 40 O O 0.0000 40
C -1.739537099 3.119293522 14.407552180 CORE 41 C C 0.0000 41
H 1.618030627 0.660320222 13.668129607 CORE 42 H H 0.0000 42
H 3.801463241 2.995854680 15.415220013 CORE 43 H H 0.0000 43
O 0.578005095 3.461783300 14.998525259 CORE 44 O O 0.0000 44
C -0.385797034 3.242428594 14.158590770 CORE 45 C C 0.0000 45
end
end

CHO* + CO* + H*

!BIOSYM archive 2

PBC=ON

Energy 16 -275 -275.787732
!DATE
PBC 5.9415 5.9415 25.2282 90.0000 90.0000 120.0000
Cr 0.158058684 3.392999902 1.644235628 CORE 1 Cr Cr 0.0000 1
Cr 3.131026620 3.393598597 1.644892986 CORE 2 Cr Cr 0.0000 2
Cr 4.615554571 0.821102537 1.671078816 CORE 3 Cr Cr 0.0000 3
Cr -2.807656000 5.133964000 6.615087000 CORE 4 Cr Cr 0.0000 4
Cr 0.149101900 5.134942000 6.617609000 CORE 5 Cr Cr 0.0000 5
Cr 1.642320000 2.550568000 6.615087000 CORE 6 Cr Cr 0.0000 6
Cr 3.176598838 1.551972199 11.616869582 CORE 7 Cr Cr 0.0000 7
Cr 0.149979955 1.626587402 11.599776189 CORE 8 Cr Cr 0.0000 8
Cr -1.386753887 4.114658755 11.762924627 CORE 9 Cr Cr 0.0000 9
Zn 1.646174122 0.842947971 0.353804130 CORE 10 Zn Zn 0.0000 10
Zn 1.644164082 0.814763525 3.531987811 CORE 11 Zn Zn 0.0000 11
Zn 1.642242844 4.268522636 4.169371816 CORE 12 Zn Zn 0.0000 12
Zn -1.329284643 2.560941878 4.761483662 CORE 13 Zn Zn 0.0000 13
Zn -1.309003279 2.548058268 8.224659561 CORE 14 Zn Zn 0.0000 14
Zn 1.596040526 0.866511572 9.064290278 CORE 15 Zn Zn 0.0000 15
Zn 2.153045561 3.977288239 9.485006676 CORE 16 Zn Zn 0.0000 16
O 1.500638140 3.671044972 13.499487023 CORE 17 Zn Zn 0.0000 17
O 0.062473250 1.796250272 0.668889658 CORE 18 O O 0.0000 18
O 3.228098221 1.798104064 0.668132550 CORE 19 O O 0.0000 19
O -1.326237594 4.140469035 0.680572088 CORE 20 O O 0.0000 20
O 1.644852051 4.238808016 0.682952549 CORE 21 O O 0.0000 21
O -1.326247298 2.547288635 2.762815077 CORE 22 O O 0.0000 22
O 0.251545393 5.014582467 2.781214556 CORE 23 O O 0.0000 23
O 1.644482814 2.669081019 2.772009562 CORE 24 O O 0.0000 24
O 3.036750695 5.013234993 2.782392992 CORE 25 O O 0.0000 25
O 3.028650000 3.472434000 5.534058000 CORE 26 O O 0.0000 26
O 0.253791200 3.472434000 5.535824000 CORE 27 O O 0.0000 27
O 4.611970000 0.730145000 5.535824000 CORE 28 O O 0.0000 28
O 1.642349000 0.842522500 5.550709000 CORE 29 O O 0.0000 29
O 1.644488000 4.271580000 7.688042000 CORE 30 O O 0.0000 30
O 0.288341000 1.624328000 7.797532000 CORE 31 O O 0.0000 31
O -1.333926000 4.420799000 7.786684000 CORE 32 O O 0.0000 32
O 2.996417000 1.630709000 7.787189000 CORE 33 O O 0.0000 33
O -2.564293960 5.123467403 10.493033073 CORE 34 O O 0.0000 34
O 1.705011900 2.419305946 10.595833327 CORE 35 O O 0.0000 35
O -1.353053065 2.438812390 10.601213025 CORE 36 O O 0.0000 36
O 4.687084609 0.470915440 12.701295616 CORE 37 O O 0.0000 37
O -0.214850576 3.066344652 12.899923879 CORE 38 O O 0.0000 38
O 1.638657654 0.878071246 12.825425655 CORE 39 O O 0.0000 39
C 2.390170956 1.882166793 13.492072948 CORE 40 C C 0.0000 40
H 2.925770783 1.465728388 14.362127674 CORE 41 H H 0.0000 41
O 1.526678797 4.18921382 15.585261610 CORE 42 C C 0.0000 42
O 1.724720835 3.846242517 16.663955116 CORE 43 O O 0.0000 43
H 4.710787563 1.050981610 13.493991717 CORE 44 H H 0.0000 44
end
end

CHO* + H*

!BIOSYM archive 2

PBC=ON

Energy 17 -268 -268.589590
!DATE
PBC 5.9415 5.9415 25.2282 90.0000 90.0000 120.0000
Cr 0.152560574 3.399381898 1.656958852 CORE 1 Cr Cr 0.0000 1
Cr 3.126909382 3.399526851 1.657100676 CORE 2 Cr Cr 0.0000 2
Cr 4.610466741 0.827506413 1.683616634 CORE 3 Cr Cr 0.0000 3
Cr -2.807655825 5.133964039 6.615086322 CORE 4 Cr Cr 0.0000 4
Cr 0.149101943 5.134941682 6.617609142 CORE 5 Cr Cr 0.0000 5
Cr 1.642319723 2.550567907 6.615086322 CORE 6 Cr Cr 0.0000 6
Cr 3.235251155 1.585151541 11.577259805 CORE 7 Cr Cr 0.0000 7
Cr 0.186236571 1.631879226 11.637920555 CORE 8 Cr Cr 0.0000 8
Cr -1.251218984 4.142511233 11.663240990 CORE 9 Cr Cr 0.0000 9
Zn 1.640094475 0.849153247 0.342397078 CORE 10 Zn Zn 0.0000 10
Zn 1.639754348 0.820113012 3.551422416 CORE 11 Zn Zn 0.0000 11
Zn 1.639580562 4.269209054 4.183745469 CORE 12 Zn Zn 0.0000 12
Zn -1.329224545 2.561590986 4.786805045 CORE 13 Zn Zn 0.0000 13
Zn -1.302957614 2.545083830 8.381612136 CORE 14 Zn Zn 0.0000 14
Zn 1.598386466 0.871514842 9.080635275 CORE 15 Zn Zn 0.0000 15
Zn 2.133385754 3.988160901 9.518734104 CORE 16 Zn Zn 0.0000 16
Zn 1.674499916 4.173950505 13.419659983 CORE 17 Zn Zn 0.0000 17
O 0.057915253 1.799945958 0.684971272 CORE 18 O O 0.0000 18
O 3.221691647 1.800931193 0.684602525 CORE 19 O O 0.0000 19
O -1.331271882 4.148738844 0.694855829 CORE 20 O O 0.0000 20
O 1.639994352 4.244914015 0.696535546 CORE 21 O O 0.0000 21
O -1.330802869 2.553198145 2.773734476 CORE 22 O O 0.0000 22
O 0.249053100 5.022000648 2.788656442 CORE 23 O O 0.0000 23
O 1.639779331 2.677201897 2.782987821 CORE 24 O O 0.0000 24
O 3.029487412 5.021214558 2.790077895 CORE 25 O O 0.0000 25
O 3.028649918 3.472433884 5.534057952 CORE 26 O O 0.0000 26
O 0.253791173 3.472433884 5.535823926 CORE 27 O O 0.0000 27
O 4.611970545 0.730145022 5.535823926 CORE 28 O O 0.0000 28
O 1.642349430 0.842522522 5.550708564 CORE 29 O O 0.0000 29
O 1.644488370 4.271579926 7.688041668 CORE 30 O O 0.0000 30
O 0.288340995 1.624328263 7.797532056 CORE 31 O O 0.0000 31
O -1.333926165 4.420799134 7.786683930 CORE 32 O O 0.0000 32
O 2.996417280 1.630708671 7.787188494 CORE 33 O O 0.0000 33
O 1.720928459 0.767823479 12.68729017 CORE 34 O O 0.0000 34
O -2.547381007 5.101492184 10.488580082 CORE 35 O O 0.0000 35
O 1.742575957 2.370204018 10.511357598 CORE 36 O O 0.0000 36
O -1.264135127 2.484725092 10.520027787 CORE 37 O O 0.0000 37
O 4.666445224 0.730131889 12.574123661 CORE 38 O O 0.0000 38
O 0.101317570 3.259261900 12.692985225 CORE 39 O O 0.0000 39
O 2.440559642 1.864391885 14.981404787 CORE 40 O O 0.0000 40
C 2.556796913 3.091785858 14.874687913 CORE 41 C C 0.0000 41
H 1.879652176 1.028900922 13.651718566 CORE 42 H H 0.0000 42
H 3.110943896 3.594535681 15.711391833 CORE 43 H H 0.0000 43
end
end

CHO* + H*

!BIOSYM archive 2

PBC=ON

Energy 18 -259 -259.573173

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!DATE
PBC 5.9415 5.9415 25.2282 90.0000 90.0000 120.0000
Cr 0.158711779 3.394625863 1.641525987 CORE 1 Cr Cr 0.0000 1
Cr 3.129932914 3.392676900 1.656412855 CORE 2 Cr Cr 0.0000 2
Cr 4.611979565 0.823008332 1.681953163 CORE 3 Cr Cr 0.0000 3
Cr -2.807656000 5.133964000 6.615087000 CORE 4 Cr Cr 0.0000 4
Cr 0.149101900 5.134942000 6.617609000 CORE 5 Cr Cr 0.0000 5
Cr 1.642320000 2.550568000 6.615087000 CORE 6 Cr Cr 0.0000 6
Cr 3.167678887 1.625274194 11.611977124 CORE 7 Cr Cr 0.0000 7
Cr 0.132910658 1.565141443 11.576633462 CORE 8 Cr Cr 0.0000 8
Cr -1.209981691 4.103791593 11.642432646 CORE 9 Cr Cr 0.0000 9
Zn 1.644761508 0.847811784 0.354374093 CORE 10 Zn Zn 0.0000 10
Zn 1.639671207 0.809036534 3.544224762 CORE 11 Zn Zn 0.0000 11
Zn 1.638426033 4.267676714 4.181717345 CORE 12 Zn Zn 0.0000 12
Zn -1.327256329 2.562175817 4.781445078 CORE 13 Zn Zn 0.0000 13
Zn -1.306185136 2.550995929 8.281762463 CORE 14 Zn Zn 0.0000 14
Zn 1.605149579 0.876608930 9.066964435 CORE 15 Zn Zn 0.0000 15
Zn 2.106721621 3.991117864 9.497629753 CORE 16 Zn Zn 0.0000 16
Zn 1.323113508 4.183917277 13.302711724 CORE 17 Zn Zn 0.0000 17
O 0.070966336 1.819857134 0.668390044 CORE 18 O O 0.0000 18
O 3.229383807 1.805841955 0.682458134 CORE 19 O O 0.0000 19
O -1.305807930 4.142895760 0.687001712 CORE 20 O O 0.0000 20
O 1.639669226 4.235357629 0.686270724 CORE 21 O O 0.0000 21
O -1.319480931 2.554428470 2.768642193 CORE 22 O O 0.0000 22
O 0.245616908 4.999414466 2.786647056 CORE 23 O O 0.0000 23
O 1.632666020 2.668547206 2.770797083 CORE 24 O O 0.0000 24
O 3.036725595 5.009187905 2.777491987 CORE 25 O O 0.0000 25
O 3.028650000 3.472434000 5.534058000 CORE 26 O O 0.0000 26
O 0.253791200 3.472434000 5.535824000 CORE 27 O O 0.0000 27
O 4.611970000 0.730145000 5.535824000 CORE 28 O O 0.0000 28
O 1.642349000 0.842522500 5.550709000 CORE 29 O O 0.0000 29
O 1.644488000 4.271580000 7.688042000 CORE 30 O O 0.0000 30
O 0.288341000 1.624328000 7.797532000 CORE 31 O O 0.0000 31
O -1.333926000 4.420799000 7.786684000 CORE 32 O O 0.0000 32
O 2.996417000 1.630709000 7.787189000 CORE 33 O O 0.0000 33
O 1.672326578 0.724517343 12.702096683 CORE 34 O O 0.0000 34
O -2.527918965 5.068905261 10.471291547 CORE 35 O O 0.0000 35
O 1.656542268 2.456359543 10.593148654 CORE 36 O O 0.0000 36
O -1.284979305 2.468564658 10.556919748 CORE 37 O O 0.0000 37
O 4.615519881 0.739126262 12.644193315 CORE 38 O O 0.0000 38
O 1.597285920 1.834966794 15.087640734 CORE 39 O O 0.0000 39
C 1.390695636 3.042671681 14.958521491 CORE 40 C C 0.0000 40
H 1.687281838 0.978212099 13.673952794 CORE 41 H H 0.0000 41
H 1.151314808 3.605598589 15.901272433 CORE 42 H H 0.0000 42
end
end

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CHO* + H*

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!BIOSYM archive 2
PBC--ON
Energy 19 -268 -268.354021
!DATE
PBC 5.9415 5.9415 25.2282 90.0000 90.0000 120.0000
Cr 0.154650503 3.390962916 1.644851506 CORE 1 Cr Cr 0.0000 1
Cr 3.128530931 3.391198273 1.645115306 CORE 2 Cr Cr 0.0000 2
Cr 4.612141127 0.819340706 1.672275672 CORE 3 Cr Cr 0.0000 3
Cr -2.807655825 5.133964039 6.615086322 CORE 4 Cr Cr 0.0000 4
Cr 0.149101943 5.134941682 6.617609142 CORE 5 Cr Cr 0.0000 5
Cr 1.642319723 2.550567907 6.615086322 CORE 6 Cr Cr 0.0000 6
Cr 3.106178397 1.818926621 11.797806829 CORE 7 Cr Cr 0.0000 7
O 0.099190515 1.741089074 11.609962130 CORE 8 Cr Cr 0.0000 8
Cr -1.398448695 4.334614235 11.647596088 CORE 9 Cr Cr 0.0000 9
Zn 1.641867792 0.841971591 0.343885268 CORE 10 Zn Zn 0.0000 10
Zn 1.640992202 0.813363071 3.524640642 CORE 11 Zn Zn 0.0000 11
Zn 1.641051070 4.267535073 4.166681836 CORE 12 Zn Zn 0.0000 12
Zn -1.329621880 2.560400508 4.763727809 CORE 13 Zn Zn 0.0000 13
Zn -1.298199627 2.561676448 8.341761003 CORE 14 Zn Zn 0.0000 14
Zn 1.664401482 0.861698219 8.991341328 CORE 15 Zn Zn 0.0000 15
Zn 2.102809364 4.154704416 9.514476445 CORE 16 Zn Zn 0.0000 16
Zn 1.542176645 4.117378905 12.829064068 CORE 17 Zn Zn 0.0000 17
O 0.059775205 1.794725228 0.671095803 CORE 18 O O 0.0000 18
O 3.223270990 1.795862518 0.671009558 CORE 19 O O 0.0000 19
O -1.329333111 4.140658606 0.684361245 CORE 20 O O 0.0000 20
O 1.641815177 4.236041804 0.685002462 CORE 21 O O 0.0000 21
O -1.328965450 2.545222239 2.765416781 CORE 22 O O 0.0000 22
O 0.249059804 5.012342017 2.784047430 CORE 23 O O 0.0000 23
O 1.641433994 2.667828422 2.774171376 CORE 24 O O 0.0000 24
O 3.033352345 5.011395609 2.784801312 CORE 25 O O 0.0000 25
O 3.028649918 3.472433884 5.534057952 CORE 26 O O 0.0000 26
O 0.253791173 3.472433884 5.535823926 CORE 27 O O 0.0000 27
O 4.611970545 0.730145022 5.535823926 CORE 28 O O 0.0000 28
O 1.642349430 0.842522522 5.550708564 CORE 29 O O 0.0000 29
O 1.644488370 4.271579926 7.688041668 CORE 30 O O 0.0000 30
O 0.288340995 1.624328263 7.797532056 CORE 31 O O 0.0000 31
O -1.333926165 4.420799134 7.786683930 CORE 32 O O 0.0000 32
O 2.996417280 1.630708671 7.787188494 CORE 33 O O 0.0000 33
O 1.584699105 0.895992748 12.657786193 CORE 34 O O 0.0000 34
O 0.466664985 0.234394965 10.371650757 CORE 35 O O 0.0000 35
O 1.638563174 3.023342772 11.033891227 CORE 36 O O 0.0000 36
O -1.414712884 2.622794733 10.574117446 CORE 37 O O 0.0000 37
O 4.601608727 0.756315576 12.428237135 CORE 38 O O 0.0000 38
O -0.262023318 3.270543893 12.984356974 CORE 39 O O 0.0000 39
O 2.301541973 3.135946501 14.386084474 CORE 40 O O 0.0000 40
C 2.859807260 2.159507101 13.818346539 CORE 41 C C 0.0000 41
H 3.210233542 1.332602931 14.476337421 CORE 42 H H 0.0000 42
H -0.584185482 2.976501283 13.853016622 CORE 43 H H 0.0000 43
end
end

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CHO* + OH* + CO₂

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!BIOSYM archive 2
PBC--ON
Energy 20 -283 -283.247830
!DATE
PBC 5.9415 5.9415 25.2282 90.0000 90.0000 120.0000
Cr 0.158088941 3.395170792 1.652799022 CORE 1 Cr Cr 0.0000 1
Cr 3.131897252 3.395476951 1.653178297 CORE 2 Cr Cr 0.0000 2
Cr 4.615724461 0.823191756 1.679117619 CORE 3 Cr Cr 0.0000 3
Cr -2.807656000 5.133964000 6.615087000 CORE 4 Cr Cr 0.0000 4
Cr 0.149101900 5.134942000 6.617609000 CORE 5 Cr Cr 0.0000 5
Cr 1.642320000 2.550568000 6.615087000 CORE 6 Cr Cr 0.0000 6
Cr 3.168105699 1.626906617 11.610296695 CORE 7 Cr Cr 0.0000 7
Cr 0.132747865 1.565128886 11.575076898 CORE 8 Cr Cr 0.0000 8
Cr -1.209616452 4.102472919 11.640038944 CORE 9 Cr Cr 0.0000 9
Zn 1.646442678 0.844488088 0.352200360 CORE 10 Zn Zn 0.0000 10
Zn 1.644020433 0.815990980 3.543586637 CORE 11 Zn Zn 0.0000 11
Zn 1.642298974 4.268887222 4.179402468 CORE 12 Zn Zn 0.0000 12
Zn -1.328885504 2.561383167 4.776304020 CORE 13 Zn Zn 0.0000 13
Zn -1.306530314 2.551219139 8.281601942 CORE 14 Zn Zn 0.0000 14
Zn 1.604276402 0.876482932 9.067534298 CORE 15 Zn Zn 0.0000 15
Zn 2.101781252 3.994006725 9.499368377 CORE 16 Zn Zn 0.0000 16
Zn 1.320410489 4.186195336 13.304403608 CORE 17 Zn Zn 0.0000 17
O 0.063509486 1.796801828 0.678948324 CORE 18 O O 0.0000 18

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O	3.227857620	1.798500288	0.677803282	CORE	19	O	O	0.0000	19
O	-1.325753247	4.142209807	0.687850981	CORE	20	O	O	0.0000	20
O	1.645117320	4.240089972	0.690317073	CORE	21	O	O	0.0000	21
O	-1.325800881	2.549343012	2.769221957	CORE	22	O	O	0.0000	22
O	0.252306974	5.016638443	2.784881682	CORE	23	O	O	0.0000	23
O	1.645012543	2.671635359	2.777428051	CORE	24	O	O	0.0000	24
O	3.036321205	5.015529332	2.785788045	CORE	25	O	O	0.0000	25
O	3.028650000	3.472434000	5.534058000	CORE	26	O	O	0.0000	26
O	0.253791200	3.472434000	5.535824000	CORE	27	O	O	0.0000	27
O	4.611970000	0.730145000	5.535824000	CORE	28	O	O	0.0000	28
O	1.642349000	0.842522500	5.550709000	CORE	29	O	O	0.0000	29
O	1.644488000	4.271580000	7.688042000	CORE	30	O	O	0.0000	30
O	0.288341000	1.624328000	7.797532000	CORE	31	O	O	0.0000	31
O	-1.333926000	4.420799000	7.786684000	CORE	32	O	O	0.0000	32
O	2.996417000	1.630709000	7.787189000	CORE	33	O	O	0.0000	33
O	1.672943769	0.723615430	12.69935056	CORE	34	O	O	0.0000	34
O	-2.528464315	5.068320485	10.470567016	CORE	35	O	O	0.0000	35
O	1.655827208	2.458268864	10.593412173	CORE	36	O	O	0.0000	36
O	-1.284261994	2.467631128	10.553404176	CORE	37	O	O	0.0000	37
O	4.615122892	0.739619135	12.641539309	CORE	38	O	O	0.0000	38
O	2.179403913	3.705037816	18.848476045	CORE	39	O	O	0.0000	39
O	1.598591037	1.834771912	15.088157838	CORE	40	O	O	0.0000	40
C	1.393363855	3.043009832	14.961459200	CORE	41	C	C	0.0000	41
H	1.684984872	0.974814496	13.670967818	CORE	42	H	H	0.0000	42
H	1.161031096	3.605903910	15.906373837	CORE	43	H	H	0.0000	43
O	1.147421922	2.116366583	20.244729874	CORE	44	O	O	0.0000	44
C	1.664667008	2.911268902	19.551281576	CORE	45	C	C	0.0000	45
end									
end									

CHO* + OH* + CO*

!BIOSYM archive 2
PBC=ON

	Energy	21	-283	-283.626781					
!DATE									
PBC	5.9415	5.9415	25.2282	90.0000	90.0000	120.0000			
Cr	0.155281917	3.392217780	1.648416919	CORE	1	Cr	Cr	0.0000	1
Cr	3.128853036	3.392615040	1.648874033	CORE	2	Cr	Cr	0.0000	2
Cr	4.612748399	0.820325067	1.675671372	CORE	3	Cr	Cr	0.0000	3
Cr	-2.807656000	5.133964000	6.615087000	CORE	4	Cr	Cr	0.0000	4
Cr	0.149101900	5.134942000	6.617609000	CORE	5	Cr	Cr	0.0000	5
Cr	1.642320000	2.550568000	6.615087000	CORE	6	Cr	Cr	0.0000	6
Cr	3.132528194	1.755684887	11.813543492	CORE	7	Cr	Cr	0.0000	7
Cr	0.051476171	1.536072812	11.557217370	CORE	8	Cr	Cr	0.0000	8
Cr	-1.341330405	4.178632756	11.571546830	CORE	9	Cr	Cr	0.0000	9
Zn	1.642457713	0.842299135	0.342899038	CORE	10	Zn	Zn	0.0000	10
Zn	1.642087723	0.813910592	3.536286687	CORE	11	Zn	Zn	0.0000	11
Zn	1.641156461	4.267671986	4.174872336	CORE	12	Zn	Zn	0.0000	12
Zn	-1.328798590	2.561145912	4.769882911	CORE	13	Zn	Zn	0.0000	13
Zn	-1.309841961	2.552475650	8.266342550	CORE	14	Zn	Zn	0.0000	14
Zn	1.628861254	0.901128130	9.048226785	CORE	15	Zn	Zn	0.0000	15
Zn	2.050627559	3.973766571	9.512919158	CORE	16	Zn	Zn	0.0000	16
Zn	1.458690770	4.315659392	13.758062473	CORE	17	Zn	Zn	0.0000	17
O	0.060578258	1.795706691	0.676097828	CORE	18	O	O	0.0000	18
O	3.223364684	1.796771528	0.675584716	CORE	19	O	O	0.0000	19
O	-1.328739523	4.141112518	0.686897918	CORE	20	O	O	0.0000	20
O	1.642352599	4.237050609	0.687955503	CORE	21	O	O	0.0000	21
O	-1.328645914	2.546782430	2.766386782	CORE	22	O	O	0.0000	22
O	0.249463002	5.013310039	2.783405325	CORE	23	O	O	0.0000	23
O	1.642039412	2.669597797	2.775472350	CORE	24	O	O	0.0000	24
O	3.034067903	5.012362386	2.784267022	CORE	25	O	O	0.0000	25
O	3.028650000	3.472434000	5.534058000	CORE	26	O	O	0.0000	26
O	0.253791200	3.472434000	5.535824000	CORE	27	O	O	0.0000	27
O	4.611970000	0.730145000	5.535824000	CORE	28	O	O	0.0000	28
O	1.642349000	0.842522500	5.550709000	CORE	29	O	O	0.0000	29
O	1.644488000	4.271580000	7.688042000	CORE	30	O	O	0.0000	30
O	0.288341000	1.624328000	7.797532000	CORE	31	O	O	0.0000	31
O	-1.333926000	4.420799000	7.786684000	CORE	32	O	O	0.0000	32
O	2.996417000	1.630709000	7.787189000	CORE	33	O	O	0.0000	33
O	1.580253803	0.771938252	12.715175993	CORE	34	O	O	0.0000	34
O	0.417251683	0.005432241	10.382038237	CORE	35	O	O	0.0000	35
O	1.636954281	2.491209945	10.694192909	CORE	36	O	O	0.0000	36
O	-1.388689733	2.464182198	10.552458685	CORE	37	O	O	0.0000	37
O	4.511339695	0.468983086	12.420234364	CORE	38	O	O	0.0000	38
O	-0.312611781	3.034077989	12.946415438	CORE	39	O	O	0.0000	39
O	1.425350058	1.796585595	15.137021979	CORE	40	O	O	0.0000	40
C	1.662420998	3.002745497	15.248763772	CORE	41	C	C	0.0000	41
H	1.452293140	1.018122710	13.693271229	CORE	42	H	H	0.0000	42
H	1.973646699	3.366479739	16.256500316	CORE	43	H	H	0.0000	43
O	4.084890133	3.049196149	14.614384646	CORE	44	O	O	0.0000	44
C	-1.606239287	2.892582797	13.431642201	CORE	45	C	C	0.0000	45
end									
end									

CO*

!BIOSYM archive 2
PBC=ON

	Energy	22	-260	-260.867271					
!DATE									
PBC	5.9415	5.9415	25.2282	90.0000	90.0000	120.0000			
Cr	0.152516685	3.400435402	1.657489100	CORE	1	Cr	Cr	0.0000	1
Cr	3.127171134	3.400662148	1.657628373	CORE	2	Cr	Cr	0.0000	2
Cr	4.610676648	0.828844196	1.683762803	CORE	3	Cr	Cr	0.0000	3
Cr	-2.807655825	5.133964039	6.615086322	CORE	4	Cr	Cr	0.0000	4
Cr	0.149101943	5.134941682	6.617609142	CORE	5	Cr	Cr	0.0000	5
Cr	1.642319723	2.550567907	6.615086322	CORE	6	Cr	Cr	0.0000	6
Cr	3.237703489	1.657241516	11.648069216	CORE	7	Cr	Cr	0.0000	7
Cr	0.252005290	1.660731586	11.659718327	CORE	8	Cr	Cr	0.0000	8
Cr	-1.226288038	4.216649648	11.645441919	CORE	9	Cr	Cr	0.0000	9
Zn	1.641163235	0.850027497	0.349359269	CORE	10	Zn	Zn	0.0000	10
Zn	1.639798019	0.820751608	3.552637658	CORE	11	Zn	Zn	0.0000	11
Zn	1.639747488	4.269439694	4.183477908	CORE	12	Zn	Zn	0.0000	12
Zn	-1.329566287	2.561435001	4.788940945	CORE	13	Zn	Zn	0.0000	13
Zn	-1.303723328	2.542223737	8.420508590	CORE	14	Zn	Zn	0.0000	14
Zn	1.587207313	0.869545893	9.092251627	CORE	15	Zn	Zn	0.0000	15
Zn	2.134177130	3.988544780	9.504020684	CORE	16	Zn	Zn	0.0000	16
Zn	1.619128106	4.324187564	13.167305899	CORE	17	Zn	Zn	0.0000	17
O	0.057845800	1.800957333	0.684193685	CORE	18	O	O	0.0000	18
O	3.222788773	1.802352407	0.683042823	CORE	19	O	O	0.0000	19
O	-1.331113476	4.149061535	0.694117831	CORE	20	O	O	0.0000	20
O	1.640108202	4.246109189	0.696358738	CORE	21	O	O	0.0000	21
O	-1.330803679	2.554271954	2.774295163	CORE	22	O	O	0.0000	22
O	0.249111575	5.023148145	2.788970305	CORE	23	O	O	0.0000	23
O	1.640060724	2.677632713	2.783237131	CORE	24	O	O	0.0000	24
O	3.029651801	5.022285525	2.790585547	CORE	25	O	O	0.0000	25
O	3.028649918	3.472433884	5.534057952	CORE	26	O	O	0.0000	26
O	0.253791173	3.472433884	5.535823926	CORE	27	O	O	0.0000	27
O	4.611970545	0.730145022	5.535823926	CORE	28	O	O	0.0000	28
O	1.642349430	0.842522522	5.550708564	CORE	29	O	O	0.0000	29
O	1.644488370	4.271579926	7.688041668	CORE	30	O	O	0.0000	30
O	0.288340995	1.624328263	7.797532056	CORE	31	O	O	0.0000	31
O	-1.333926165	4.420799134	7.786683930	CORE	32	O	O	0.0000	32
O	2.996417280	1.630708671	7.787188494	CORE	33	O	O	0.0000	33

O 1.765156902 0.780823103 12.598266355 CORE 34 O O 0.0000 34
O -2.611509188 5.114689216 10.509966515 CORE 35 O O 0.0000 35
O 1.769235877 2.375946634 10.491637091 CORE 36 O O 0.0000 36
O -1.255088582 2.527120497 10.539138643 CORE 37 O O 0.0000 37
O 4.704947967 0.970945483 12.753846137 CORE 38 O O 0.0000 38
O 0.149131257 3.317145803 12.720248525 CORE 39 O O 0.0000 39
O 3.816889652 3.305576718 15.219108226 CORE 40 O O 0.0000 40
C 3.122674025 3.586427368 14.356461295 CORE 41 C C 0.0000 41
end
end

CO* + H₂*

!BIOSYM archive 2

PBC=ON

Energy 23 -268 -268.745693

!DATE

PBC 5.9415 5.9415 25.2282 90.0000 90.0000 120.0000
Cr 0.153573320 3.398098422 1.645244465 CORE 1 Cr Cr 0.0000 1
Cr 3.127766372 3.398496111 1.645534053 CORE 2 Cr Cr 0.0000 2
Cr 4.611388612 0.825460228 1.672562130 CORE 3 Cr Cr 0.0000 3
Cr -2.807655825 5.133964039 6.615086322 CORE 4 Cr Cr 0.0000 4
Cr 0.149101943 5.134941682 6.617609142 CORE 5 Cr Cr 0.0000 5
Cr 1.642319723 2.550567907 6.615086322 CORE 6 Cr Cr 0.0000 6
Cr 3.197832725 1.751978215 11.735453198 CORE 7 Cr Cr 0.0000 7
Cr 0.152943832 1.603724587 11.568389637 CORE 8 Cr Cr 0.0000 8
Cr -1.302987775 4.147669245 11.670258944 CORE 9 Cr Cr 0.0000 9
Zn 1.641225062 0.848556864 0.346570545 CORE 10 Zn Zn 0.0000 10
Zn 1.640520485 0.818543589 3.533005958 CORE 11 Zn Zn 0.0000 11
Zn 1.640831247 4.270813771 4.170910789 CORE 12 Zn Zn 0.0000 12
Zn -1.329716227 2.561384377 4.764951839 CORE 13 Zn Zn 0.0000 13
Zn -1.306346179 2.550361757 8.253965092 CORE 14 Zn Zn 0.0000 14
Zn 1.616360726 0.885018279 9.059661520 CORE 15 Zn Zn 0.0000 15
Zn 2.122688062 3.983628410 9.481056284 CORE 16 Zn Zn 0.0000 16
Zn 1.733002052 4.236059766 13.285474267 CORE 17 Zn Zn 0.0000 17
O 0.058711970 1.801111978 0.670783338 CORE 18 O O 0.0000 18
O 3.222820037 1.802303493 0.670374168 CORE 19 O O 0.0000 19
O -1.330277712 4.146598991 0.683243915 CORE 20 O O 0.0000 20
O 1.640983950 4.242601304 0.684315434 CORE 21 O O 0.0000 21
O -1.330002380 2.551834743 2.764099917 CORE 22 O O 0.0000 22
O 0.248316072 5.018567226 2.782130274 CORE 23 O O 0.0000 23
O 1.640671604 2.673411808 2.772796423 CORE 24 O O 0.0000 24
O 3.032583205 5.017816249 2.782826310 CORE 25 O O 0.0000 25
O 3.028649918 3.472433884 5.534057952 CORE 26 O O 0.0000 26
O 0.253791173 3.472433884 5.535823926 CORE 27 O O 0.0000 27
O 4.611970545 0.730145022 5.535823926 CORE 28 O O 0.0000 28
O 1.642349430 0.842522522 5.550708564 CORE 29 O O 0.0000 29
O 1.644488370 4.271579926 7.688041668 CORE 30 O O 0.0000 30
O 0.288340995 1.624328263 7.797532056 CORE 31 O O 0.0000 31
O -1.333926165 4.420799134 7.78683930 CORE 32 O O 0.0000 32
O 2.996417280 1.630708671 7.787188494 CORE 33 O O 0.0000 33
O 1.679994149 0.763084353 12.727537076 CORE 34 O O 0.0000 34
O -2.556288601 5.117975719 10.481265314 CORE 35 O O 0.0000 35
O 1.704177175 2.453080024 10.600016667 CORE 36 O O 0.0000 36
O -1.286539036 2.502091381 10.562067037 CORE 37 O O 0.0000 37
O 4.656608469 0.810267207 12.630819281 CORE 38 O O 0.0000 38
O 0.098650439 3.220673031 12.869216532 CORE 39 O O 0.0000 39
O 4.040847985 2.957903011 14.553235593 CORE 40 O O 0.0000 40
C 3.348939704 3.207292294 13.579795148 CORE 41 C C 0.0000 41
H 1.616819910 0.774427761 13.697731150 CORE 42 H H 0.0000 42
H -0.399225748 2.912450553 13.673901178 CORE 43 H H 0.0000 43
end
end

H*

!BIOSYM archive 2

PBC=ON

Energy 24 -249 -249.780498

!DATE

PBC 5.9415 5.9415 25.2282 90.0000 90.0000 120.0000
Cr 0.154664818 3.399305886 1.657267106 CORE 1 Cr Cr 0.0000 1
Cr 3.128997899 3.399425201 1.657220113 CORE 2 Cr Cr 0.0000 2
Cr 4.612561944 0.827578204 1.683407423 CORE 3 Cr Cr 0.0000 3
Cr -2.807655825 5.133964039 6.615086322 CORE 4 Cr Cr 0.0000 4
Cr 0.149101943 5.134941682 6.617609142 CORE 5 Cr Cr 0.0000 5
Cr 1.642319723 2.550567907 6.615086322 CORE 6 Cr Cr 0.0000 6
Cr 3.193377117 1.737228046 11.716588168 CORE 7 Cr Cr 0.0000 7
Cr 0.254580378 1.694675264 11.606155952 CORE 8 Cr Cr 0.0000 8
Cr -1.335099309 4.180140980 11.765254876 CORE 9 Cr Cr 0.0000 9
Zn 1.642657851 0.848761177 0.347214574 CORE 10 Zn Zn 0.0000 10
Zn 1.641504341 0.819640496 3.550334416 CORE 11 Zn Zn 0.0000 11
Zn 1.641109645 4.269582300 4.184248409 CORE 12 Zn Zn 0.0000 12
Zn -1.329431214 2.561460782 4.786232566 CORE 13 Zn Zn 0.0000 13
Zn 1.309194361 2.538711280 8.372318124 CORE 14 Zn Zn 0.0000 14
Zn 1.585806432 0.831874720 9.080152955 CORE 15 Zn Zn 0.0000 15
Zn 2.142953232 3.965695469 9.476780229 CORE 16 Zn Zn 0.0000 16
Zn 2.034275081 3.953751810 12.755124919 CORE 17 Zn Zn 0.0000 17
O 0.060136487 1.800026688 0.684646901 CORE 18 O O 0.0000 18
O 3.224129542 1.801430785 0.683768787 CORE 19 O O 0.0000 19
O -1.329238044 4.147643877 0.693917252 CORE 20 O O 0.0000 20
O 1.642071606 4.244596444 0.696165903 CORE 21 O O 0.0000 21
O -1.328964968 2.553142553 2.773373752 CORE 22 O O 0.0000 22
O 0.250634171 5.021622547 2.788229814 CORE 23 O O 0.0000 23
O 1.642034056 2.676629608 2.782783901 CORE 24 O O 0.0000 24
O 3.032056090 5.020607573 2.789289246 CORE 25 O O 0.0000 25
O 3.028649918 3.472433884 5.534057952 CORE 26 O O 0.0000 26
O 0.253791173 3.472433884 5.535823926 CORE 27 O O 0.0000 27
O 4.611970545 0.730145022 5.535823926 CORE 28 O O 0.0000 28
O 1.642349430 0.842522522 5.550708564 CORE 29 O O 0.0000 29
O 1.644488370 4.271579926 7.688041668 CORE 30 O O 0.0000 30
O 0.288340995 1.624328263 7.797532056 CORE 31 O O 0.0000 31
O -1.333926165 4.420799134 7.78683930 CORE 32 O O 0.0000 32
O 2.996417280 1.630708671 7.787188494 CORE 33 O O 0.0000 33
O 1.741722660 0.793036319 12.564279340 CORE 34 O O 0.0000 34
O -2.664919135 5.096923713 10.541508851 CORE 35 O O 0.0000 35
O 1.772345560 2.335517642 10.461146120 CORE 36 O O 0.0000 36
O -1.298443492 2.534438310 10.587248978 CORE 37 O O 0.0000 37
O 4.726701522 0.894788414 12.827108786 CORE 38 O O 0.0000 38
O 0.210484150 3.346468876 12.657401916 CORE 39 O O 0.0000 39
H 4.837249023 1.309039571 13.705016657 CORE 40 H H 0.0000 40
end
end

H₂*

!BIOSYM archive 2

PBC=ON

Energy 25 -253 -253.896237

!DATE

PBC 5.9415 5.9415 25.2282 90.0000 90.0000 120.0000
Cr 0.154267017 3.400907055 1.648181024 CORE 1 Cr Cr 0.0000 1
Cr 3.128019488 3.401297323 1.648483771 CORE 2 Cr Cr 0.0000 2
Cr 4.611970561 0.829380604 1.674547114 CORE 3 Cr Cr 0.0000 3
Cr -2.807655825 5.133964039 6.615086322 CORE 4 Cr Cr 0.0000 4

Cr	0.149101943	5.134941682	6.617609142	CORE	5	Cr	Cr	0.0000	5
Cr	1.642319723	2.550567907	6.615086322	CORE	6	Cr	Cr	0.0000	6
Cr	3.178848749	1.712241160	11.732712229	CORE	7	Cr	Cr	0.0000	7
Cr	0.102567349	1.614424477	11.610177394	CORE	8	Cr	Cr	0.0000	8
Cr	-1.330425633	4.166908113	11.684450888	CORE	9	Cr	Cr	0.0000	9
Zn	1.642245861	0.851391246	0.355528641	CORE	10	Zn	Zn	0.0000	10
Zn	1.641664243	0.821334462	3.538194741	CORE	11	Zn	Zn	0.0000	11
Zn	1.640949189	4.271356649	4.174830983	CORE	12	Zn	Zn	0.0000	12
Zn	-1.329322268	2.562004118	4.771212414	CORE	13	Zn	Zn	0.0000	13
Zn	-1.306765390	2.548834535	8.283421549	CORE	14	Zn	Zn	0.0000	14
Zn	1.610008051	0.882956836	9.066965243	CORE	15	Zn	Zn	0.0000	15
Zn	2.125783820	3.968222152	9.47892034	CORE	16	Zn	Zn	0.0000	16
Zn	2.093409272	4.021735199	12.749432848	CORE	17	Zn	Zn	0.0000	17
O	0.058183396	1.804041582	0.672109388	CORE	18	O	O	0.0000	18
O	3.224740435	1.805540646	0.671505903	CORE	19	O	O	0.0000	19
O	-1.329764093	4.148626546	0.683469453	CORE	20	O	O	0.0000	20
O	1.641394515	4.246023122	0.685924553	CORE	21	O	O	0.0000	21
O	-1.329560284	2.554942440	2.765802264	CORE	22	O	O	0.0000	22
O	0.249087158	5.021950820	2.782570093	CORE	23	O	O	0.0000	23
O	1.641217460	2.675989425	2.773396297	CORE	24	O	O	0.0000	24
O	3.033052827	5.021261597	2.783358464	CORE	25	O	O	0.0000	25
O	3.028649918	3.472433884	5.534057952	CORE	26	O	O	0.0000	26
O	0.253791173	3.472433884	5.535823926	CORE	27	O	O	0.0000	27
O	4.611970545	0.730145022	5.535823926	CORE	28	O	O	0.0000	28
O	1.642349430	0.842522522	5.550708564	CORE	29	O	O	0.0000	29
O	1.644488370	4.271579926	7.688041668	CORE	30	O	O	0.0000	30
O	0.288340995	1.624328263	7.797532056	CORE	31	O	O	0.0000	31
O	-1.333926165	4.420799134	7.78683930	CORE	32	O	O	0.0000	32
O	2.996417280	1.630708671	7.787188494	CORE	33	O	O	0.0000	33
O	1.655219137	0.776693745	12.737940970	CORE	34	O	O	0.0000	34
O	-2.587831177	5.138772163	10.478937845	CORE	35	O	O	0.0000	35
O	1.670259270	2.441633481	10.596491262	CORE	36	O	O	0.0000	36
O	-1.323347587	2.511633224	10.568280392	CORE	37	O	O	0.0000	37
O	4.641036530	0.767885735	12.690593884	CORE	38	O	O	0.0000	38
O	0.087837344	3.253454266	12.881695606	CORE	39	O	O	0.0000	39
H	1.665305902	0.760299585	13.708962871	CORE	40	H	H	0.0000	40
H	-0.295597984	2.942296111	13.724277534	CORE	41	H	H	0.0000	41
end									
end									

H2O*

!BIOSYM archive 2

PBC=ON

Energy	26	-260	-260.374154						
!DATE									
PBC	5.9415	5.9415	25.2282	90.0000	90.0000	120.0000			
Cr	0.154687012	3.392902370	1.647271917	CORE	1	Cr	Cr	0.0000	1
Cr	3.128467202	3.393212081	1.647626397	CORE	2	Cr	Cr	0.0000	2
Cr	4.612168368	0.821096134	1.674699698	CORE	3	Cr	Cr	0.0000	3
Cr	-2.807656000	5.133964000	6.615087000	CORE	4	Cr	Cr	0.0000	4
Cr	0.149101900	5.134942000	6.617609000	CORE	5	Cr	Cr	0.0000	5
Cr	1.642320000	2.550568000	6.615087000	CORE	6	Cr	Cr	0.0000	6
Cr	3.010144405	1.795759492	11.855219229	CORE	7	Cr	Cr	0.0000	7
Cr	0.000138492	1.663049564	11.528401593	CORE	8	Cr	Cr	0.0000	8
Cr	-1.537595037	4.308333959	11.712004495	CORE	9	Cr	Cr	0.0000	9
Zn	1.641886892	0.842866112	0.339060777	CORE	10	Zn	Zn	0.0000	10
Zn	1.641546833	0.814423750	3.530059405	CORE	11	Zn	Zn	0.0000	11
Zn	1.640979250	4.268412190	4.171812035	CORE	12	Zn	Zn	0.0000	12
Zn	-1.329143992	2.561141538	4.769942901	CORE	13	Zn	Zn	0.0000	13
Zn	-1.302847845	2.561130558	8.354281156	CORE	14	Zn	Zn	0.0000	14
Zn	1.664950366	0.856000074	8.995127959	CORE	15	Zn	Zn	0.0000	15
Zn	2.011195573	4.082475413	9.535237061	CORE	16	Zn	Zn	0.0000	16
Zn	1.719292993	4.050538796	12.968503081	CORE	17	Zn	Zn	0.0000	17
O	0.060360085	1.796486341	0.674817619	CORE	18	O	O	0.0000	18
O	3.222488472	1.797773188	0.674236605	CORE	19	O	O	0.0000	19
O	-1.329319034	4.142855139	0.686416959	CORE	20	O	O	0.0000	20
O	1.641799710	4.237742451	0.687165189	CORE	21	O	O	0.0000	21
O	-1.329064952	2.547285367	2.766866067	CORE	22	O	O	0.0000	22
O	0.249193796	5.013729390	2.783712170	CORE	23	O	O	0.0000	23
O	1.641499787	2.669908352	2.775015548	CORE	24	O	O	0.0000	24
O	3.033329831	5.012963600	2.784683585	CORE	25	O	O	0.0000	25
O	3.028650000	3.472434000	5.534058000	CORE	26	O	O	0.0000	26
O	0.253791200	3.472434000	5.535824000	CORE	27	O	O	0.0000	27
O	4.611970000	0.730145000	5.535824000	CORE	28	O	O	0.0000	28
O	1.642349000	0.842522500	5.550709000	CORE	29	O	O	0.0000	29
O	1.644488000	4.271580000	7.688042000	CORE	30	O	O	0.0000	30
O	0.288341000	1.624328000	7.797532000	CORE	31	O	O	0.0000	31
O	-1.333926000	4.420799000	7.78684000	CORE	32	O	O	0.0000	32
O	2.996417000	1.630709000	7.787189000	CORE	33	O	O	0.0000	33
O	1.462408950	0.899726839	12.687334923	CORE	34	O	O	0.0000	34
O	0.416146105	0.201313337	10.318105589	CORE	35	O	O	0.0000	35
O	1.505143583	2.942081245	11.012336186	CORE	36	O	O	0.0000	36
O	-1.490257893	2.602583980	10.591556880	CORE	37	O	O	0.0000	37
O	4.485420237	0.678931341	12.424095661	CORE	38	O	O	0.0000	38
O	0.261596675	2.924304382	13.926223122	CORE	39	O	O	0.0000	39
O	3.472058888	3.198592645	13.134005411	CORE	40	O	O	0.0000	40
H	-0.740982436	2.963881870	13.922372830	CORE	41	H	H	0.0000	41
H	0.588118569	1.975311082	13.858130159	CORE	42	H	H	0.0000	42
end									
end									

H* + COOH*

!BIOSYM archive 2

PBC=ON

Energy	27	-276	-276.457713						
!DATE									
PBC	5.9415	5.9415	25.2282	90.0000	90.0000	120.0000			
Cr	0.155355822	3.391047198	1.649900293	CORE	1	Cr	Cr	0.0000	1
Cr	3.128501940	3.391283077	1.650249752	CORE	2	Cr	Cr	0.0000	2
Cr	4.612323337	0.819653884	1.679328018	CORE	3	Cr	Cr	0.0000	3
Cr	-2.807656000	5.133964000	6.615087000	CORE	4	Cr	Cr	0.0000	4
Cr	0.149101900	5.134942000	6.617609000	CORE	5	Cr	Cr	0.0000	5
Cr	1.642320000	2.550568000	6.615087000	CORE	6	Cr	Cr	0.0000	6
Cr	3.143521087	1.644099880	11.652682882	CORE	7	Cr	Cr	0.0000	7
Cr	0.097148852	1.554573826	11.603934687	CORE	8	Cr	Cr	0.0000	8
Cr	-1.291836800	4.134716384	11.625286941	CORE	9	Cr	Cr	0.0000	9
Zn	1.642272705	0.842857078	0.343813423	CORE	10	Zn	Zn	0.0000	10
Zn	1.641997130	0.810510991	3.544677177	CORE	11	Zn	Zn	0.0000	11
Zn	1.640819668	4.268694908	4.182353452	CORE	12	Zn	Zn	0.0000	12
Zn	-1.329217922	2.560635802	4.780592178	CORE	13	Zn	Zn	0.0000	13
Zn	-1.310859274	2.545718303	8.273826533	CORE	14	Zn	Zn	0.0000	14
Zn	1.598381680	0.864532597	9.065626040	CORE	15	Zn	Zn	0.0000	15
Zn	2.051419056	3.965198639	9.515370436	CORE	16	Zn	Zn	0.0000	16
Zn	1.485610382	4.368605906	13.705395957	CORE	17	Zn	Zn	0.0000	17
O	0.061693519	1.799532846	0.679022990	CORE	18	O	O	0.0000	18
O	3.221776708	1.800847750	0.678665387	CORE	19	O	O	0.0000	19
O	-1.328956325	4.141765800	0.689664196	CORE	20	O	O	0.0000	20
O	1.642117795	4.234515188	0.689517754	CORE	21	O	O	0.0000	21
O	-1.328882923	2.547517899	2.767131058	CORE	22	O	O	0.0000	22
O	0.248292653	5.009196222	2.781814823	CORE	23	O	O	0.0000	23
O	1.641728495	2.668654160	2.772845872	CORE	24	O	O	0.0000	24
O	3.034876643	5.008274788	2.783027077	CORE	25	O	O	0.0000	25
O	3.028650000	3.472434000	5.534058000	CORE	26	O	O	0.0000	26

O	0.253791200	3.472434000	5.535824000	CORE	27	O	O	0.0000	27
O	4.611970000	0.730145000	5.535824000	CORE	28	O	O	0.0000	28
O	1.642349000	0.842522500	5.550709000	CORE	29	O	O	0.0000	29
O	1.644488000	4.271580000	7.688042000	CORE	30	O	O	0.0000	30
O	0.288341000	1.624328000	7.797532000	CORE	31	O	O	0.0000	31
O	-1.333926000	4.420799000	7.786684000	CORE	32	O	O	0.0000	32
O	2.996417000	1.630709000	7.787189000	CORE	33	O	O	0.0000	33
O	1.642537624	0.724563202	12.703546574	CORE	34	O	O	0.0000	34
O	-2.595026728	5.091066341	10.472414067	CORE	35	O	O	0.0000	35
O	1.640707685	2.367085158	10.554214713	CORE	36	O	O	0.0000	36
O	-1.324226599	2.448488112	10.554944135	CORE	37	O	O	0.0000	37
O	4.554321189	0.737140652	12.597486549	CORE	38	O	O	0.0000	38
O	0.015276332	3.194651896	12.955346559	CORE	39	O	O	0.0000	39
O	3.174233759	3.209459208	12.907308863	CORE	40	O	O	0.0000	40
H	-0.571408891	2.907681001	13.709733872	CORE	41	H	H	0.0000	41
H	1.622609593	0.744377729	13.676630899	CORE	42	H	H	0.0000	42
O	4.037410792	3.101115433	15.020542724	CORE	43	O	O	0.0000	43
C	3.120832876	3.411585501	14.273396340	CORE	44	C	C	0.0000	44

end
end

O*

!BIOSYM archive 2

PBC=ON

Energy	28	-253	-253.332057						
!DATE									
PBC	5.9415	5.9415	25.2282	90.0000	90.0000	120.0000			
Cr	0.152061431	3.399816318	1.658412423	CORE	1	Cr	Cr	0.0000	1
Cr	3.126619459	3.399848831	1.658166832	CORE	2	Cr	Cr	0.0000	2
Cr	4.610060894	0.828087985	1.685276848	CORE	3	Cr	Cr	0.0000	3
Cr	-2.807655825	5.133964039	6.615086322	CORE	4	Cr	Cr	0.0000	4
Cr	0.149101943	5.134941682	6.617609142	CORE	5	Cr	Cr	0.0000	5
Cr	1.642319723	2.550567907	6.615086322	CORE	6	Cr	Cr	0.0000	6
Cr	3.183019677	1.779213855	11.787987339	CORE	7	Cr	Cr	0.0000	7
Cr	0.196409013	1.654075906	11.600530546	CORE	8	Cr	Cr	0.0000	8
Cr	-1.387419786	4.152430192	11.789531991	CORE	9	Cr	Cr	0.0000	9
Zn	1.639455310	0.849729167	0.337884717	CORE	10	Zn	Zn	0.0000	10
Zn	1.639397564	0.820325421	3.551977990	CORE	11	Zn	Zn	0.0000	11
Zn	1.640009706	4.269231521	4.184494917	CORE	12	Zn	Zn	0.0000	12
Zn	-1.329347723	2.561770569	4.788612876	CORE	13	Zn	Zn	0.0000	13
Zn	-1.307790637	2.544355773	8.400294259	CORE	14	Zn	Zn	0.0000	14
Zn	1.593998708	0.863484243	9.085814105	CORE	15	Zn	Zn	0.0000	15
Zn	2.151214849	3.962385832	9.495764074	CORE	16	Zn	Zn	0.0000	16
Zn	1.606369713	4.263211496	13.020397534	CORE	17	Zn	Zn	0.0000	17
O	0.058118244	1.800348912	0.688016417	CORE	18	O	O	0.0000	18
O	3.220379712	1.801068235	0.687109191	CORE	19	O	O	0.0000	19
O	-1.331865876	4.150181821	0.697338024	CORE	20	O	O	0.0000	20
O	1.639623946	4.254243243	0.698829299	CORE	21	O	O	0.0000	21
O	-1.331184043	2.553643854	2.775063202	CORE	22	O	O	0.0000	22
O	0.249228142	5.022451683	2.790026453	CORE	23	O	O	0.0000	23
O	1.639461764	2.678247197	2.785052861	CORE	24	O	O	0.0000	24
O	3.028874164	5.021896849	2.791617480	CORE	25	O	O	0.0000	25
O	3.028649918	3.472433884	5.534057952	CORE	26	O	O	0.0000	26
O	0.253791173	3.472433884	5.535823926	CORE	27	O	O	0.0000	27
O	4.611970545	0.730145022	5.535823926	CORE	28	O	O	0.0000	28
O	1.642349430	0.842522522	5.550708564	CORE	29	O	O	0.0000	29
O	1.644488370	4.271579926	7.688041668	CORE	30	O	O	0.0000	30
O	0.288340995	1.624328263	7.797532056	CORE	31	O	O	0.0000	31
O	-1.333926165	4.420799134	7.786683930	CORE	32	O	O	0.0000	32
O	2.996417280	1.630708671	7.787188494	CORE	33	O	O	0.0000	33
O	1.742723706	0.762526934	12.516168409	CORE	34	O	O	0.0000	34
O	-2.590302571	5.101793431	10.480374045	CORE	35	O	O	0.0000	35
O	1.756906984	2.359963844	10.486171553	CORE	36	O	O	0.0000	36
O	-1.332507651	2.540822474	10.548460350	CORE	37	O	O	0.0000	37
O	4.654031885	0.921651461	12.632653210	CORE	38	O	O	0.0000	38
O	0.079244048	3.295214772	12.649483918	CORE	39	O	O	0.0000	39
O	3.240879311	3.326892010	12.852152107	CORE	40	O	O	0.0000	40

end
end

OH*

!BIOSYM archive 2

PBC=ON

Energy	29	-257	-257.834028						
!DATE									
PBC	5.9415	5.9415	25.2282	90.0000	90.0000	120.0000			
Cr	0.157686612	3.395630314	1.654187493	CORE	1	Cr	Cr	0.0000	1
Cr	3.131544242	3.396068104	1.654707196	CORE	2	Cr	Cr	0.0000	2
Cr	4.615547009	0.824270520	1.680757267	CORE	3	Cr	Cr	0.0000	3
Cr	-2.807655825	5.133964039	6.615086322	CORE	4	Cr	Cr	0.0000	4
Cr	0.149101943	5.134941682	6.617609142	CORE	5	Cr	Cr	0.0000	5
Cr	1.642319723	2.550567907	6.615086322	CORE	6	Cr	Cr	0.0000	6
Cr	3.105361308	1.680003430	11.762605523	CORE	7	Cr	Cr	0.0000	7
Cr	0.133539331	1.546475239	11.598618849	CORE	8	Cr	Cr	0.0000	8
Cr	-1.432320418	4.138613224	11.724332985	CORE	9	Cr	Cr	0.0000	9
Zn	1.645868576	0.845109394	0.348643233	CORE	10	Zn	Zn	0.0000	10
Zn	1.643853720	0.816574110	3.545418581	CORE	11	Zn	Zn	0.0000	11
Zn	1.641866929	4.268867910	4.181825138	CORE	12	Zn	Zn	0.0000	12
Zn	-1.328967618	2.561402440	4.782861203	CORE	13	Zn	Zn	0.0000	13
Zn	-1.308183215	2.544642599	8.370451231	CORE	14	Zn	Zn	0.0000	14
Zn	1.595715954	0.864689354	9.067184003	CORE	15	Zn	Zn	0.0000	15
Zn	2.092632389	3.921156857	9.479007749	CORE	16	Zn	Zn	0.0000	16
Zn	1.687174403	4.166994704	13.076747029	CORE	17	Zn	Zn	0.0000	17
O	0.063280616	1.797436323	0.681039855	CORE	18	O	O	0.0000	18
O	3.227213396	1.799220596	0.680181964	CORE	19	O	O	0.0000	19
O	-1.326178903	4.143604379	0.690816258	CORE	20	O	O	0.0000	20
O	1.644896252	4.240963204	0.692950611	CORE	21	O	O	0.0000	21
O	-1.326213854	2.550137437	2.771221731	CORE	22	O	O	0.0000	22
O	0.252445722	5.017875219	2.785849337	CORE	23	O	O	0.0000	23
O	1.644580335	2.673049854	2.779498559	CORE	24	O	O	0.0000	24
O	3.035382224	5.016431079	2.787277191	CORE	25	O	O	0.0000	25
O	3.028649918	3.472433884	5.534057952	CORE	26	O	O	0.0000	26
O	0.253791173	3.472433884	5.535823926	CORE	27	O	O	0.0000	27
O	4.611970545	0.730145022	5.535823926	CORE	28	O	O	0.0000	28
O	1.642349430	0.842522522	5.550708564	CORE	29	O	O	0.0000	29
O	1.644488370	4.271579926	7.688041668	CORE	30	O	O	0.0000	30
O	0.288340995	1.624328263	7.797532056	CORE	31	O	O	0.0000	31
O	-1.333926165	4.420799134	7.786683930	CORE	32	O	O	0.0000	32
O	2.996417280	1.630708671	7.787188494	CORE	33	O	O	0.0000	33
O	1.639870657	0.713347852	12.603855666	CORE	34	O	O	0.0000	34
O	-2.612229735	5.062420055	10.465510099	CORE	35	O	O	0.0000	35
O	1.665365262	2.378435733	10.551952179	CORE	36	O	O	0.0000	36
O	-1.349951200	2.481228288	10.569641801	CORE	37	O	O	0.0000	37
O	4.593211064	0.809681007	12.658578522	CORE	38	O	O	0.0000	38
O	0.012803761	3.185343945	12.888840155	CORE	39	O	O	0.0000	39
O	3.287608058	3.216887254	12.907157974	CORE	40	O	O	0.0000	40
H	-0.506203373	2.856236799	13.653629944	CORE	41	H	H	0.0000	41

end
end

OH* + H*

!BIOSYM archive 2

Zn	2.178250705	4.000851637	9.402734320	CORE	16	Zn	Zn	0.0000	16
Zn	1.518004297	4.369753900	13.368214532	CORE	17	Zn	Zn	0.0000	17
O	0.086398044	1.736658284	0.592350657	CORE	18	O	O	0.0000	18
O	3.265195889	1.738719015	0.585294069	CORE	19	O	O	0.0000	19
O	-1.300036926	4.107480383	0.617400992	CORE	20	O	O	0.0000	20
O	1.673557984	4.201237452	0.618694302	CORE	21	O	O	0.0000	21
O	-1.299166685	2.496815758	2.697365699	CORE	22	O	O	0.0000	22
O	0.285315153	4.982599051	2.723947507	CORE	23	O	O	0.0000	23
O	1.672874369	2.606946390	2.692759762	CORE	24	O	O	0.0000	24
O	3.047581330	4.977071167	2.750402649	CORE	25	O	O	0.0000	25
O	3.094994528	3.479299229	5.470565843	CORE	26	O	O	0.0000	26
O	0.308505255	3.488375534	5.418103270	CORE	27	O	O	0.0000	27
O	4.692997816	0.735804235	5.568173243	CORE	28	O	O	0.0000	28
O	1.710366295	0.837059262	5.522387133	CORE	29	O	O	0.0000	29
O	1.664258927	4.318590576	7.583011845	CORE	30	O	O	0.0000	30
O	0.308300984	1.660956524	7.728881290	CORE	31	O	O	0.0000	31
O	-1.328808687	4.458445006	7.620119622	CORE	32	O	O	0.0000	32
O	3.027863796	1.677843770	7.771264897	CORE	33	O	O	0.0000	33
O	1.723502180	0.828261259	12.511777732	CORE	34	O	O	0.0000	34
O	0.426377211	0.014640433	10.366455040	CORE	35	O	O	0.0000	35
O	1.757256915	2.392796729	10.387945612	CORE	36	O	O	0.0000	36
O	-1.305915148	2.590533991	10.452275927	CORE	37	O	O	0.0000	37
O	4.625291562	0.880857515	12.442673054	CORE	38	O	O	0.0000	38
O	0.125905517	3.400872752	12.503622336	CORE	39	O	O	0.0000	39
O	3.236870714	3.371556032	12.685232820	CORE	40	O	O	0.0000	40
O	1.661702312	4.796447312	16.882536721	CORE	41	O	O	0.0000	41
C	2.943083403	3.525647295	14.484058418	CORE	42	C	C	0.0000	42
C	2.327098516	4.021945461	16.347939569	CORE	43	C	C	0.0000	43
H	2.922113091	2.454520317	14.705091627	CORE	44	H	H	0.0000	44
H	-2.033720783	3.991703105	14.711039156	CORE	45	H	H	0.0000	45

end
end

TS CH₃O* + H* to CH₃O*

!BIOSYM archive 2

PBC=ON

Energy 33 -271 -271.956825

!DATE

PBC	5.9415	5.9415	25.2282	90.0000	90.0000	120.0000			
Cr	0.090589424	3.440720373	1.561643613	CORE	1	Cr	Cr	0.0000	1
Cr	3.061737441	3.439859444	1.563608944	CORE	2	Cr	Cr	0.0000	2
Cr	4.548297662	0.867910236	1.588142635	CORE	3	Cr	Cr	0.0000	3
Cr	-2.915776726	5.121686147	6.550550577	CORE	4	Cr	Cr	0.0000	4
Cr	3.031406273	0.009033739	6.573731233	CORE	5	Cr	Cr	0.0000	5
Cr	1.587943898	2.575975373	6.528494989	CORE	6	Cr	Cr	0.0000	6
Cr	3.129814056	1.689214835	11.678683339	CORE	7	Cr	Cr	0.0000	7
Cr	0.160652212	1.586606459	11.546834631	CORE	8	Cr	Cr	0.0000	8
Cr	-1.255009716	4.230318678	11.494663165	CORE	9	Cr	Cr	0.0000	9
Zn	1.579716797	0.886214672	0.260996431	CORE	10	Zn	Zn	0.0000	10
Zn	1.577375303	0.861050535	3.446397734	CORE	11	Zn	Zn	0.0000	11
Zn	1.567161786	4.328893637	4.102134725	CORE	12	Zn	Zn	0.0000	12
Zn	-1.389262262	2.614562986	4.688143106	CORE	13	Zn	Zn	0.0000	13
Zn	-1.344758180	2.537714348	8.318935274	CORE	14	Zn	Zn	0.0000	14
Zn	1.553171190	0.906717679	8.976675659	CORE	15	Zn	Zn	0.0000	15
Zn	2.079555378	3.996938506	9.423776127	CORE	16	Zn	Zn	0.0000	16
Zn	1.618128188	4.218345019	12.921822937	CORE	17	Zn	Zn	0.0000	17
O	-0.001966252	1.842255311	0.591061849	CORE	18	O	O	0.0000	18
O	3.159220132	1.844162881	0.587805299	CORE	19	O	O	0.0000	19
O	-1.394851734	4.185431169	0.597547611	CORE	20	O	O	0.0000	20
O	1.576966947	4.258085290	0.597851504	CORE	21	O	O	0.0000	21
O	-1.395939811	2.596376856	2.679244274	CORE	22	O	O	0.0000	22
O	0.184702767	5.060676896	2.686532317	CORE	23	O	O	0.0000	23
O	1.576468505	2.724209324	2.691018029	CORE	24	O	O	0.0000	24
O	2.965451294	5.058548880	2.694362847	CORE	25	O	O	0.0000	25
O	2.983453163	3.533651747	5.472515865	CORE	26	O	O	0.0000	26
O	0.190088406	3.503689874	5.454927389	CORE	27	O	O	0.0000	27
O	4.602882760	0.797461456	5.428965202	CORE	28	O	O	0.0000	28
O	1.612306210	0.878016546	5.425489869	CORE	29	O	O	0.0000	29
O	1.565605942	4.286840080	7.640387919	CORE	30	O	O	0.0000	30
O	0.224241609	1.612645744	7.686362468	CORE	31	O	O	0.0000	31
O	-1.434827587	4.402958605	7.721642974	CORE	32	O	O	0.0000	32
O	2.950387097	1.648429358	7.695010217	CORE	33	O	O	0.0000	33
O	1.680975928	0.744712961	12.531316583	CORE	34	O	O	0.0000	34
O	-2.614567642	5.139758626	10.370678481	CORE	35	O	O	0.0000	35
O	1.686456095	2.468686091	10.531396477	CORE	36	O	O	0.0000	36
O	-1.338766410	2.482950460	10.487853536	CORE	37	O	O	0.0000	37
O	4.629391504	0.860728603	12.608672255	CORE	38	O	O	0.0000	38
O	0.022326661	3.217083562	12.782097167	CORE	39	O	O	0.0000	39
O	3.261709751	3.198303955	13.064256493	CORE	40	O	O	0.0000	40
C	3.865547908	3.042629627	14.303987653	CORE	41	C	C	0.0000	41
H	3.748171476	2.059076699	14.764410625	CORE	42	H	H	0.0000	42
H	-2.123857215	3.940323851	14.931644122	CORE	43	H	H	0.0000	43
H	-0.606715688	3.053161083	13.637627649	CORE	44	H	H	0.0000	44

end
end

TS CH₃O* + CO* to CH₃CO* + O*

!BIOSYM archive 2

PBC=ON

Energy 34 -286 -286.643042

!DATE

PBC	5.9415	5.9415	25.2282	90.0000	90.0000	120.0000			
Cr	0.157295918	3.400196360	1.657981006	CORE	1	Cr	Cr	0.0000	1
Cr	3.131855905	3.400469489	1.658719557	CORE	2	Cr	Cr	0.0000	2
Cr	4.615637089	0.828708648	1.684474769	CORE	3	Cr	Cr	0.0000	3
Cr	-2.807656000	5.133964000	6.615087000	CORE	4	Cr	Cr	0.0000	4
Cr	0.149101900	5.134942000	6.617609000	CORE	5	Cr	Cr	0.0000	5
Cr	1.642320000	2.550568000	6.615087000	CORE	6	Cr	Cr	0.0000	6
Cr	3.087632815	1.827491917	11.778308468	CORE	7	Cr	Cr	0.0000	7
Cr	0.122360892	1.715995332	11.601544754	CORE	8	Cr	Cr	0.0000	8
Cr	-1.463875655	4.238164555	11.780230398	CORE	9	Cr	Cr	0.0000	9
Zn	1.646523850	0.849964005	0.353521204	CORE	10	Zn	Zn	0.0000	10
Zn	1.643881356	0.820675589	3.553538559	CORE	11	Zn	Zn	0.0000	11
Zn	1.641618067	4.269448339	4.184050800	CORE	12	Zn	Zn	0.0000	12
Zn	-1.328867460	2.561359986	4.789597357	CORE	13	Zn	Zn	0.0000	13
Zn	-1.310226618	2.546629816	8.425967257	CORE	14	Zn	Zn	0.0000	14
Zn	1.591567709	0.870441351	9.079840936	CORE	15	Zn	Zn	0.0000	15
Zn	2.124620813	3.991643873	9.512390679	CORE	16	Zn	Zn	0.0000	16
Zn	1.509536963	4.345972307	13.294144673	CORE	17	Zn	Zn	0.0000	17
O	0.062606003	1.800528823	0.684390744	CORE	18	O	O	0.0000	18
O	3.228300307	1.802393872	0.683358831	CORE	19	O	O	0.0000	19
O	-1.326394180	4.148209248	0.694281041	CORE	20	O	O	0.0000	20
O	1.645006377	4.245948899	0.696787218	CORE	21	O	O	0.0000	21
O	-1.326161472	2.554084707	2.774831505	CORE	22	O	O	0.0000	22
O	0.253164635	5.023335845	2.788929266	CORE	23	O	O	0.0000	23
O	1.644635478	2.677251385	2.783560161	CORE	24	O	O	0.0000	24
O	3.034121101	5.021706697	2.791338177	CORE	25	O	O	0.0000	25
O	3.028650000	3.472434000	5.534058000	CORE	26	O	O	0.0000	26
O	0.253791200	3.472434000	5.535824000	CORE	27	O	O	0.0000	27
O	4.611970000	0.730145000	5.535824000	CORE	28	O	O	0.0000	28
O	1.642349000	0.842522500	5.550709000	CORE	29	O	O	0.0000	29
O	1.644488000	4.271580000	7.688042000	CORE	30	O	O	0.0000	30
O	0.288341000	1.624328000	7.797532000	CORE	31	O	O	0.0000	31

O	-1.333926000	4.420799000	7.786684000 CORE	32	O	O	0.0000	32
O	2.996417000	1.630709000	7.787189000 CORE	33	O	O	0.0000	33
O	1.629747473	0.846156878	12.617458057 CORE	34	O	O	0.0000	34
O	0.337670302	0.026506770	10.470994444 CORE	35	O	O	0.0000	35
O	1.692438426	2.377531712	10.471860663 CORE	36	O	O	0.0000	36
O	-1.399211200	2.594655613	10.544177974 CORE	37	O	O	0.0000	37
O	4.557640472	0.947791199	12.583995871 CORE	38	O	O	0.0000	38
O	0.031284631	3.403225281	12.584799565 CORE	39	O	O	0.0000	39
O	3.116155718	3.417438500	12.782828555 CORE	40	O	O	0.0000	40
C	3.844464372	2.781039535	15.535111042 CORE	41	C	C	0.0000	41
H	-2.095913599	3.867631553	15.547958935 CORE	42	H	H	0.0000	42
H	-1.151334356	2.246464432	15.556164022 CORE	43	H	H	0.0000	43
H	-2.920971365	2.235906089	15.357485329 CORE	44	H	H	0.0000	44
O	0.550973294	4.658181070	16.341725825 CORE	45	O	O	0.0000	45
C	1.070122611	4.485643972	15.340225142 CORE	46	C	C	0.0000	46
end								
end								

TS CH₃O + H* + H* to CH₃OH* + H*

!BIOSYM archive 2

PBC=ON

Energy	35	0	-280.773021					
!DATE								
PBC	5.9415	5.9415	25.2282	90.0000	90.0000	120.0000		
Cr	0.156772100	3.391062000	1.648413000 CORE	1	Cr	Cr	0.0000	1
Cr	3.130434000	3.391632000	1.649024000 CORE	2	Cr	Cr	0.0000	2
Cr	4.614532000	0.819956700	1.674427000 CORE	3	Cr	Cr	0.0000	3
Cr	-2.807195000	5.134625000	6.615191000 CORE	4	Cr	Cr	0.0000	4
Cr	1.642289000	2.550383000	6.614939000 CORE	5	Cr	Cr	0.0000	5
Cr	0.149563000	5.135041000	6.617640000 CORE	6	Cr	Cr	0.0000	6
Cr	0.069216620	1.735200000	11.651350000 CORE	7	Cr	Cr	0.0000	7
Cr	3.055379000	1.688236000	11.613080000 CORE	8	Cr	Cr	0.0000	8
Cr	-1.397521000	4.307100000	11.604090000 CORE	9	Cr	Cr	0.0000	9
Zn	1.645480000	0.841170900	0.356676800 CORE	10	Zn	Zn	0.0000	10
Zn	1.643010000	0.812788500	3.532714000 CORE	11	Zn	Zn	0.0000	11
Zn	1.641801000	4.267605000	4.172160000 CORE	12	Zn	Zn	0.0000	12
Zn	-1.328680000	2.560011000	4.772124000 CORE	13	Zn	Zn	0.0000	13
Zn	-1.315592000	2.531924000	8.367731000 CORE	14	Zn	Zn	0.0000	14
Zn	1.634413000	0.840099600	9.007573000 CORE	15	Zn	Zn	0.0000	15
Zn	1.925095000	3.961162000	9.514123000 CORE	16	Zn	Zn	0.0000	16
Zn	2.001795000	4.587888000	12.938930000 CORE	17	Zn	Zn	0.0000	17
O	3.227271000	1.796288000	0.671303000 CORE	18	O	O	0.0000	18
O	0.061694100	1.794376000	0.672181700 CORE	19	O	O	0.0000	19
O	-1.327014000	4.138458000	0.684078300 CORE	20	O	O	0.0000	20
O	1.643768000	4.236227000	0.686240800 CORE	21	O	O	0.0000	21
O	-1.327200000	2.545484000	2.767580000 CORE	22	O	O	0.0000	22
O	1.643518000	2.667466000	2.775332000 CORE	23	O	O	0.0000	23
O	0.250689200	5.013025000	2.783458000 CORE	24	O	O	0.0000	24
O	3.035865000	5.011812000	2.783862000 CORE	25	O	O	0.0000	25
O	3.028768000	3.472044000	5.533926000 CORE	26	O	O	0.0000	26
O	0.253909100	3.472572000	5.535762000 CORE	27	O	O	0.0000	27
O	4.611567000	0.729454300	5.535504000 CORE	28	O	O	0.0000	28
O	1.641968000	0.842395700	5.550469000 CORE	29	O	O	0.0000	29
O	1.644812000	4.271337000	7.687988000 CORE	30	O	O	0.0000	30
O	-1.333572000	4.421117000	7.786713000 CORE	31	O	O	0.0000	31
O	2.996241000	1.630203000	7.786958000 CORE	32	O	O	0.0000	32
O	0.288164000	1.624337000	7.797369000 CORE	33	O	O	0.0000	33
O	1.546779000	2.230132000	10.397150000 CORE	34	O	O	0.0000	34
O	-1.394612000	2.586504000	10.530200000 CORE	35	O	O	0.0000	35
O	2.699317000	4.952492000	11.007600000 CORE	36	O	O	0.0000	36
O	0.294787700	3.549126000	12.655440000 CORE	37	O	O	0.0000	37
O	1.542308000	0.849868800	12.633580000 CORE	38	O	O	0.0000	38
O	4.513854000	1.375623000	13.054190000 CORE	39	O	O	0.0000	39
O	3.276354000	3.327460000	13.990670000 CORE	40	O	O	0.0000	40
C	-2.088764000	3.903403000	15.184310000 CORE	41	C	C	0.0000	41
H	-0.039467370	3.293443000	13.537780000 CORE	42	H	H	0.0000	42
H	3.863499000	2.353199000	13.659020000 CORE	43	H	H	0.0000	43
H	-1.409857000	3.171323000	15.651060000 CORE	44	H	H	0.0000	44
H	-1.541082000	4.827987000	14.937080000 CORE	45	H	H	0.0000	45
H	3.057537000	4.135762000	15.909700000 CORE	46	H	H	0.0000	46
end								
end								

TS CH₃O* + H* + H* to CH₃ + OH*

!BIOSYM archive 2

PBC=ON

Energy	36	0	-278.554055					
!DATE								
PBC	5.9415	5.9415	25.2282	90.0000	90.0000	120.0000		
Cr	0.147106930	3.419517371	1.587442765 CORE	1	Cr	Cr	0.0000	1
Cr	3.118548328	3.419474625	1.566654296 CORE	2	Cr	Cr	0.0000	2
Cr	4.605062166	0.848727867	1.566982184 CORE	3	Cr	Cr	0.0000	3
Cr	2.939362921	5.068165989	6.489755389 CORE	4	Cr	Cr	0.0000	4
Cr	1.593025163	6.550493916	6.559493910 CORE	5	Cr	Cr	0.0000	5
Cr	0.007852861	5.121886066	6.537244896 CORE	6	Cr	Cr	0.0000	6
Cr	0.193408497	1.696098529	11.548600508 CORE	7	Cr	Cr	0.0000	7
Cr	3.122421019	1.764395857	11.643357047 CORE	8	Cr	Cr	0.0000	8
Cr	-1.284620526	4.307466261	11.528436977 CORE	9	Cr	Cr	0.0000	9
Zn	1.623904499	0.841892926	0.274205892 CORE	10	Zn	Zn	0.0000	10
Zn	1.626592444	0.847621917	3.448806778 CORE	11	Zn	Zn	0.0000	11
Zn	1.569399237	4.258274657	4.077597308 CORE	12	Zn	Zn	0.0000	12
Zn	-1.389234227	2.561189045	4.657432383 CORE	13	Zn	Zn	0.0000	13
Zn	-1.322869084	2.556111734	8.335340132 CORE	14	Zn	Zn	0.0000	14
Zn	1.558694697	0.861910570	8.961608730 CORE	15	Zn	Zn	0.0000	15
Zn	2.070973738	4.069072589	9.414835405 CORE	16	Zn	Zn	0.0000	16
Zn	1.905943302	4.067390849	12.993538690 CORE	17	Zn	Zn	0.0000	17
O	3.220590938	1.765967294	0.598240833 CORE	18	O	O	0.0000	18
O	0.007990970	1.733712646	0.591733308 CORE	19	O	O	0.0000	19
O	-1.386448449	4.141775047	0.592458115 CORE	20	O	O	0.0000	20
O	1.642674589	4.282238369	0.606429661 CORE	21	O	O	0.0000	21
O	-1.351837726	2.558004317	2.684648222 CORE	22	O	O	0.0000	22
O	1.661914868	2.685699866	2.708652279 CORE	23	O	O	0.0000	23
O	0.266690312	5.099939502	2.711786815 CORE	24	O	O	0.0000	24
O	2.991224392	5.060472170	2.718941910 CORE	25	O	O	0.0000	25
O	2.995717658	3.497825474	5.479963756 CORE	26	O	O	0.0000	26
O	0.170822801	3.448364089	5.439600536 CORE	27	O	O	0.0000	27
O	4.676531202	0.777325107	5.508075210 CORE	28	O	O	0.0000	28
O	1.650360192	0.837141922	5.478007186 CORE	29	O	O	0.0000	29
O	1.537486380	4.292026568	7.649730160 CORE	30	O	O	0.0000	30
O	-1.499691725	4.389309270	7.704712879 CORE	31	O	O	0.0000	31
O	2.978874660	1.669863999	7.773317341 CORE	32	O	O	0.0000	32
O	0.222010837	1.615269015	7.742700841 CORE	33	O	O	0.0000	33
O	1.673017849	2.585116607	10.583414064 CORE	34	O	O	0.0000	34
O	-1.319405996	2.545101592	10.527520971 CORE	35	O	O	0.0000	35
O	0.299116681	0.073802507	10.423872113 CORE	36	O	O	0.0000	36
O	0.120651453	3.371202411	12.774901291 CORE	37	O	O	0.0000	37
O	1.661755052	0.846989583	12.557194114 CORE	38	O	O	0.0000	38
O	4.647448613	0.831061732	12.747002925 CORE	39	O	O	0.0000	39
O	3.471455935	3.111030377	13.209250719 CORE	40	O	O	0.0000	40
C	-1.974095587	3.860906824	15.161739882 CORE	41	C	C	0.0000	41
H	-0.528048684	3.323486658	13.514198831 CORE	42	H	H	0.0000	42
H	4.401227474	1.379041080	13.527753388 CORE	43	H	H	0.0000	43
H	-1.088007749	3.271293373	15.408212330 CORE	44	H	H	0.0000	44

H -1.820839975 4.904452915 14.887679472 CORE 45 H H 0.0000 45
H 3.066491161 3.575355044 15.702304156 CORE 46 H H 0.0000 46

end
end

TS CHOCO* + H* to CH₃CO* + O*

¹BIOSYM archive 2

PBC=ON

Energy 37 -276 -276.228167

¹DATE

PBC 5.9415 5.9415 25.2282 90.0000 90.0000 120.0000
Cr 0.177489581 3.427099607 1.682706120 CORE 1 Cr Cr 0.0000 1
Cr 3.149911092 3.426094319 1.656218083 CORE 2 Cr Cr 0.0000 2
Cr 4.633833001 0.856193063 1.656171348 CORE 3 Cr Cr 0.0000 3
Cr -2.807656000 5.133964000 6.615087000 CORE 4 Cr Cr 0.0000 4
Cr 0.149101900 5.134942000 6.617609000 CORE 5 Cr Cr 0.0000 5
Cr 1.642320000 2.550568000 6.615087000 CORE 6 Cr Cr 0.0000 6
Cr 3.161026534 1.584971229 11.456949338 CORE 7 Cr Cr 0.0000 7
Cr 0.121227304 1.663908513 11.657509193 CORE 8 Cr Cr 0.0000 8
Cr -1.360605846 4.136539498 11.747588201 CORE 9 Cr Cr 0.0000 9
Zn 1.644969332 0.843803286 0.333634223 CORE 10 Zn Zn 0.0000 10
Zn 1.667885906 0.857360793 3.548165470 CORE 11 Zn Zn 0.0000 11
Zn 1.647540174 4.277509186 4.182858207 CORE 12 Zn Zn 0.0000 12
Zn -1.331206674 2.557201531 4.783733586 CORE 13 Zn Zn 0.0000 13
Zn -1.306414122 2.549090446 8.336480860 CORE 14 Zn Zn 0.0000 14
Zn 1.574507245 0.862347774 9.078343328 CORE 15 Zn Zn 0.0000 15
Zn 2.096283174 4.034957802 9.505148872 CORE 16 Zn Zn 0.0000 16
Zn 1.799597358 3.884697632 12.920002410 CORE 17 Zn Zn 0.0000 17
O 0.030158279 1.736588640 0.685777271 CORE 18 O O 0.0000 18
O 3.242548470 1.766763595 0.695449205 CORE 19 O O 0.0000 19
O -1.361091253 4.144278129 0.685194223 CORE 20 O O 0.0000 20
O 1.674317924 4.290844135 0.696517605 CORE 21 O O 0.0000 21
O -1.317230597 2.564110485 2.772893777 CORE 22 O O 0.0000 22
O 0.305350525 5.107878274 2.787573911 CORE 23 O O 0.0000 23
O 1.697400136 2.698791921 2.788871074 CORE 24 O O 0.0000 24
O -2.910946212 5.074045671 2.782474863 CORE 25 O O 0.0000 25
O 3.028650000 3.472434000 5.534058000 CORE 26 O O 0.0000 26
O 0.253791200 3.472434000 5.535824000 CORE 27 O O 0.0000 27
O 4.611970000 0.730145000 5.535824000 CORE 28 O O 0.0000 28
O 1.642349000 0.842522500 5.550709000 CORE 29 O O 0.0000 29
O 1.644488000 4.271580000 7.688042000 CORE 30 O O 0.0000 30
O 0.288341000 1.624328000 7.797532000 CORE 31 O O 0.0000 31
O -1.333926000 4.420799000 7.786684000 CORE 32 O O 0.0000 32
O 2.996417000 1.630709000 7.787189000 CORE 33 O O 0.0000 33
O -2.613753967 5.133411950 10.528204511 CORE 34 O O 0.0000 34
O 1.636488006 2.434655339 10.518951595 CORE 35 O O 0.0000 35
O -1.306880554 2.503836070 10.532170440 CORE 36 O O 0.0000 36
O 4.568847078 0.667691777 12.658909111 CORE 37 O O 0.0000 37
O -0.011295168 3.214827235 12.792010697 CORE 38 O O 0.0000 38
O 1.741431160 0.817187229 12.738140347 CORE 39 O O 0.0000 39
C 2.385568438 1.114085615 13.977631832 CORE 40 C C 0.0000 40
H 2.085325137 0.441755075 14.794602435 CORE 41 H H 0.0000 41
C 2.544987507 2.504467975 14.315441217 CORE 42 C C 0.0000 42
O 2.933017483 3.031172433 15.342087676 CORE 43 O O 0.0000 43
H 3.762465710 0.924905791 13.540367591 CORE 44 H H 0.0000 44
end
end

TS CHOCO* + OH* to CH₃CO* + O*

¹BIOSYM archive 2

PBC=ON

Energy 38 -284 -284.753011

¹DATE

PBC 5.9415 5.9415 25.2282 90.0000 90.0000 120.0000
Cr 0.135524948 3.426364435 1.653158645 CORE 1 Cr Cr 0.0000 1
Cr 3.107968124 3.427188997 1.679816112 CORE 2 Cr Cr 0.0000 2
Cr 4.593320714 0.856184920 1.653303107 CORE 3 Cr Cr 0.0000 3
Cr -2.807656000 5.133964000 6.615087000 CORE 4 Cr Cr 0.0000 4
Cr 0.149101900 5.134942000 6.617609000 CORE 5 Cr Cr 0.0000 5
Cr 1.642320000 2.550568000 6.615087000 CORE 6 Cr Cr 0.0000 6
Cr 3.158068853 1.597841425 11.826178734 CORE 7 Cr Cr 0.0000 7
Cr 0.140157317 1.438229235 11.598008151 CORE 8 Cr Cr 0.0000 8
Cr -1.234707115 4.100203670 11.439773772 CORE 9 Cr Cr 0.0000 9
Zn 1.641002813 0.844438457 0.342627946 CORE 10 Zn Zn 0.0000 10
Zn 1.616916097 0.857109352 3.544782707 CORE 11 Zn Zn 0.0000 11
Zn 1.635305934 4.276439854 4.180906481 CORE 12 Zn Zn 0.0000 12
Zn -1.326653083 2.558089754 4.780177152 CORE 13 Zn Zn 0.0000 13
Zn -1.312686789 2.531819471 8.317576545 CORE 14 Zn Zn 0.0000 14
Zn 1.600041721 0.849106383 9.065981362 CORE 15 Zn Zn 0.0000 15
Zn 2.039482732 3.848457558 9.490862143 CORE 16 Zn Zn 0.0000 16
Zn 1.787325344 4.239599663 13.500839036 CORE 17 Zn Zn 0.0000 17
O 0.041974995 1.767053970 0.690632896 CORE 18 O O 0.0000 18
O 3.257389954 1.736744382 0.680251553 CORE 19 O O 0.0000 19
O -1.295059068 4.243631593 0.680572004 CORE 20 O O 0.0000 20
O 1.610714529 4.291575166 0.692384127 CORE 21 O O 0.0000 21
O -1.338180942 2.563933419 2.770076205 CORE 22 O O 0.0000 22
O 0.253385475 5.075045750 2.778529370 CORE 23 O O 0.0000 23
O 1.587173288 2.697693733 2.785483370 CORE 24 O O 0.0000 24
O 2.978773150 5.108731656 2.786124141 CORE 25 O O 0.0000 25
O 3.028650000 3.472434000 5.534058000 CORE 26 O O 0.0000 26
O 0.253791200 3.472434000 5.535824000 CORE 27 O O 0.0000 27
O 4.611970000 0.730145000 5.535824000 CORE 28 O O 0.0000 28
O 1.642349000 0.842522500 5.550709000 CORE 29 O O 0.0000 29
O 1.644488000 4.271580000 7.688042000 CORE 30 O O 0.0000 30
O 0.288341000 1.624328000 7.797532000 CORE 31 O O 0.0000 31
O -1.333926000 4.420799000 7.786684000 CORE 32 O O 0.0000 32
O 2.996417000 1.630709000 7.787189000 CORE 33 O O 0.0000 33
O 1.653985510 0.557442648 12.677795816 CORE 34 O O 0.0000 34
O -2.637953342 5.018905488 10.413011433 CORE 35 O O 0.0000 35
O 1.707409842 2.289529309 10.609641831 CORE 36 O O 0.0000 36
O -1.337564511 2.325781501 10.559139753 CORE 37 O O 0.0000 37
O 4.652403427 0.753806578 12.719928411 CORE 38 O O 0.0000 38
O 0.095208575 3.179918249 12.768313154 CORE 39 O O 0.0000 39
O 3.359345475 3.186024680 13.154195113 CORE 40 O O 0.0000 40
C -1.720256943 3.594642265 14.210363754 CORE 41 C C 0.0000 41
H -1.473377530 4.917531407 13.684877695 CORE 42 H H 0.0000 42
H 3.808593347 3.508918134 15.222089841 CORE 43 H H 0.0000 43
O 0.558146402 3.495414668 14.936623793 CORE 44 O O 0.0000 44
C -0.343388347 3.310723948 14.058385123 CORE 45 C C 0.0000 45
end
end

TS CHO* + CO* + H* to CHOCO* + H*

¹BIOSYM archive 2

PBC=ON

Energy 39 -274 -274.909824

¹DATE

PBC 5.9415 5.9415 25.2282 90.0000 90.0000 120.0000
Cr 0.154910888 3.390806933 1.644558378 CORE 1 Cr Cr 0.0000 1
Cr 3.128144194 3.391038374 1.644703856 CORE 2 Cr Cr 0.0000 2
Cr 4.612178204 0.818716846 1.672133809 CORE 3 Cr Cr 0.0000 3
Cr -2.807656000 5.133964000 6.615087000 CORE 4 Cr Cr 0.0000 4

Cr	0.149101900	5.134942000	6.617609000	CORE	5	Cr	Cr	0.0000	5
Cr	1.642320000	2.550568000	6.615087000	CORE	6	Cr	Cr	0.0000	6
Cr	3.204783472	1.673266602	11.680196907	CORE	7	Cr	Cr	0.0000	7
Cr	0.203017502	1.719354412	11.564755206	CORE	8	Cr	Cr	0.0000	8
Cr	-1.342436478	4.199383541	11.713699534	CORE	9	Cr	Cr	0.0000	9
Zn	1.641361834	0.840988625	0.336984633	CORE	10	Zn	Zn	0.0000	10
Zn	1.641609007	0.813073129	3.529847617	CORE	11	Zn	Zn	0.0000	11
Zn	1.641198554	4.267480576	4.169792948	CORE	12	Zn	Zn	0.0000	12
Zn	-1.329626586	2.560619373	4.761786619	CORE	13	Zn	Zn	0.0000	13
Zn	-1.308413110	2.549985216	8.226398708	CORE	14	Zn	Zn	0.0000	14
Zn	1.616369144	0.882454703	9.059108520	CORE	15	Zn	Zn	0.0000	15
Zn	2.164292023	4.034884512	9.480413891	CORE	16	Zn	Zn	0.0000	16
Zn	1.448277310	3.997420377	13.560464684	CORE	17	Zn	Zn	0.0000	17
O	0.060443767	1.794536803	0.672089900	CORE	18	O	O	0.0000	18
O	3.222040901	1.795492027	0.672270211	CORE	19	O	O	0.0000	19
O	-1.329433891	4.140435198	0.683851120	CORE	20	O	O	0.0000	20
O	1.641814389	4.235641653	0.684590928	CORE	21	O	O	0.0000	21
O	-1.329141252	2.545195810	2.763181955	CORE	22	O	O	0.0000	22
O	0.249063237	5.011653048	2.782228559	CORE	23	O	O	0.0000	23
O	1.641444594	2.668363632	2.773269648	CORE	24	O	O	0.0000	24
O	3.033731599	5.010806648	2.782833429	CORE	25	O	O	0.0000	25
O	3.028650000	3.472434000	5.534058000	CORE	26	O	O	0.0000	26
O	0.253791200	3.472434000	5.535824000	CORE	27	O	O	0.0000	27
O	4.611970000	0.730145000	5.535824000	CORE	28	O	O	0.0000	28
O	1.642349000	0.842522500	5.550709000	CORE	29	O	O	0.0000	29
O	1.644488000	4.271580000	7.688042000	CORE	30	O	O	0.0000	30
O	0.288341000	1.624328000	7.797532000	CORE	31	O	O	0.0000	31
O	-1.333926000	4.420799000	7.786684000	CORE	32	O	O	0.0000	32
O	2.996417000	1.630709000	7.787189000	CORE	33	O	O	0.0000	33
O	0.395869307	0.044850746	10.492653558	CORE	34	O	O	0.0000	34
O	1.756555892	2.467468478	10.579585214	CORE	35	O	O	0.0000	35
O	-1.325398790	2.512073483	10.594702633	CORE	36	O	O	0.0000	36
O	4.766635622	0.678767598	12.745190754	CORE	37	O	O	0.0000	37
O	-0.075091209	3.212178336	12.820085572	CORE	38	O	O	0.0000	38
O	1.632686326	0.877623788	12.792809262	CORE	39	O	O	0.0000	39
C	2.382240416	1.681551510	13.668211450	CORE	40	C	C	0.0000	40
H	2.958689604	1.036815547	14.366706491	CORE	41	H	H	0.0000	41
C	2.238037144	3.168034583	15.097280027	CORE	42	C	C	0.0000	42
O	2.851171959	2.795742867	16.027725433	CORE	43	O	O	0.0000	43
H	4.860452179	1.271491789	13.524589782	CORE	44	H	H	0.0000	44
end									
end									

TS CHO* + H* to CH₃O*

!BIOSYM archive 2

PBC=ON

	Energy		40	0	-267.514086				
!DATE									
PBC	5.9415	5.9415	25.2282	90.0000	90.0000	120.0000			
Cr	0.155161904	3.401362467	1.655615336	CORE	1	Cr	Cr	0.0000	1
Cr	3.129413344	3.401357632	1.655954514	CORE	2	Cr	Cr	0.0000	2
Cr	4.613130315	0.829480460	1.682561395	CORE	3	Cr	Cr	0.0000	3
Cr	-2.807655825	5.133964039	6.615086322	CORE	4	Cr	Cr	0.0000	4
Cr	0.149101943	5.134941682	6.617609142	CORE	5	Cr	Cr	0.0000	5
Cr	1.642319723	2.550567907	6.615086322	CORE	6	Cr	Cr	0.0000	6
Cr	3.104534219	1.732704745	11.726014880	CORE	7	Cr	Cr	0.0000	7
Cr	0.100851998	1.668776519	11.622951842	CORE	8	Cr	Cr	0.0000	8
Cr	-1.351992276	4.308410993	11.556517212	CORE	9	Cr	Cr	0.0000	9
Zn	1.642882655	0.851270382	0.344376359	CORE	10	Zn	Zn	0.0000	10
Zn	1.642260733	0.821650681	3.546411778	CORE	11	Zn	Zn	0.0000	11
Zn	1.641070351	4.269701192	4.182850180	CORE	12	Zn	Zn	0.0000	12
Zn	-1.328305511	2.561866340	4.786252548	CORE	13	Zn	Zn	0.0000	13
Zn	-1.295346963	2.558791131	8.419034339	CORE	14	Zn	Zn	0.0000	14
Zn	1.664636529	0.864017509	9.005606817	CORE	15	Zn	Zn	0.0000	15
Zn	2.048283663	4.129190963	9.545725865	CORE	16	Zn	Zn	0.0000	16
Zn	1.473303839	4.043945837	12.933948415	CORE	17	Zn	Zn	0.0000	17
O	0.060470851	1.802368704	0.682796997	CORE	18	O	O	0.0000	18
O	3.224446077	1.803468993	0.682322627	CORE	19	O	O	0.0000	19
O	-1.328661997	4.150157010	0.692999169	CORE	20	O	O	0.0000	20
O	1.642565601	4.246617575	0.694854662	CORE	21	O	O	0.0000	21
O	-1.328244597	2.555211069	2.772732195	CORE	22	O	O	0.0000	22
O	0.250974914	5.022879498	2.786813562	CORE	23	O	O	0.0000	23
O	1.642416123	2.677532681	2.779760488	CORE	24	O	O	0.0000	24
O	3.032486738	5.021896386	2.788468814	CORE	25	O	O	0.0000	25
O	3.028649918	3.472433884	5.534057952	CORE	26	O	O	0.0000	26
O	0.253791173	3.472433884	5.535823926	CORE	27	O	O	0.0000	27
O	4.611970545	0.730145022	5.535823926	CORE	28	O	O	0.0000	28
O	1.642349430	0.842522522	5.550708564	CORE	29	O	O	0.0000	29
O	1.644488370	4.271579926	7.688041668	CORE	30	O	O	0.0000	30
O	0.288340995	1.624328263	7.797532056	CORE	31	O	O	0.0000	31
O	-1.333926165	4.420799134	7.786683930	CORE	32	O	O	0.0000	32
O	2.996417280	1.630708671	7.787188494	CORE	33	O	O	0.0000	33
O	1.604337233	0.824263309	12.605194141	CORE	34	O	O	0.0000	34
O	0.445123021	0.189385598	10.334436840	CORE	35	O	O	0.0000	35
O	1.629687940	2.981188483	11.052053927	CORE	36	O	O	0.0000	36
O	-1.387486403	2.575051589	10.517304967	CORE	37	O	O	0.0000	37
O	4.579833934	0.666918550	12.413143891	CORE	38	O	O	0.0000	38
O	-0.302890821	3.203457649	12.930719484	CORE	39	O	O	0.0000	39
O	2.332685668	3.264201305	14.589003108	CORE	40	O	O	0.0000	40
C	3.378683484	2.623106002	14.383227713	CORE	41	C	C	0.0000	41
H	3.706560499	1.974516794	15.258779891	CORE	42	H	H	0.0000	42
H	-1.039019933	2.954514240	13.542466345	CORE	43	H	H	0.0000	43
end									
end									

TS CHO* + OH* + CO* to CHOCO* + OH*

!BIOSYM archive 2

PBC=ON

Energy	41	-283	-283.047353						
!DATE									
PBC	5.9415	5.9415	25.2282	90.0000	90.0000	120.0000			
Cr	0.147945293	3.399746254	1.656315728	CORE	1	Cr	Cr	0.0000	1
Cr	3.122307905	3.399449842	1.655922283	CORE	2	Cr	Cr	0.0000	2
Cr	4.605657149	0.827566737	1.683113001	CORE	3	Cr	Cr	0.0000	3
Cr	-2.807656000	5.133964000	6.615087000	CORE	4	Cr	Cr	0.0000	4
Cr	0.149101900	5.134942000	6.617609000	CORE	5	Cr	Cr	0.0000	5
Cr	1.642320000	2.550568000	6.615087000	CORE	6	Cr	Cr	0.0000	6
Cr	3.110953321	1.547518901	11.567578317	CORE	7	Cr	Cr	0.0000	7
Cr	0.063264487	1.547339710	11.603320884	CORE	8	Cr	Cr	0.0000	8
Cr	-1.397817161	4.119966191	11.644221945	CORE	9	Cr	Cr	0.0000	9
Zn	1.634182190	0.849594477	0.333466730	CORE	10	Zn	Zn	0.0000	10
Zn	1.635915956	0.819985499	3.548880954	CORE	11	Zn	Zn	0.0000	11
Zn	1.637634051	4.269016206	4.183930942	CORE	12	Zn	Zn	0.0000	12
Zn	-1.329819544	2.562095737	4.784744679	CORE	13	Zn	Zn	0.0000	13
Zn	-1.308144860	2.549953342	8.351400827	CORE	14	Zn	Zn	0.0000	14
Zn	1.602139686	0.895153779	9.072383809	CORE	15	Zn	Zn	0.0000	15
Zn	2.029707701	3.994882498	9.528284738	CORE	16	Zn	Zn	0.0000	16
Zn	1.894643318	4.254430053	13.618737992	CORE	17	Zn	Zn	0.0000	17
O	0.053331818	1.800636145	0.685528114	CORE	18	O	O	0.0000	18
O	3.215505402	1.800849287	0.685688217	CORE	19	O	O	0.0000	19
O	-1.336350820	4.150010958	0.695815141	CORE	20	O	O	0.0000	20
O	1.635409150	4.245072246	0.696574428	CORE	21	O	O	0.0000	21
O	-1.335316276	2.553464495	2.772937087	CORE	22	O	O	0.0000	22

O	0.245016620	5.021525785	2.788225523	CORE	23	O	O	0.0000	23
O	1.635329027	2.677478345	2.782057782	CORE	24	O	O	0.0000	24
O	3.025162434	5.021337842	2.789544285	CORE	25	O	O	0.0000	25
O	3.028650000	3.472434000	5.534058000	CORE	26	O	O	0.0000	26
O	0.253791200	3.472434000	5.535824000	CORE	27	O	O	0.0000	27
O	4.611970000	0.730145000	5.535824000	CORE	28	O	O	0.0000	28
O	1.642349000	0.842522500	5.550709000	CORE	29	O	O	0.0000	29
O	1.644488000	4.271580000	7.688042000	CORE	30	O	O	0.0000	30
O	0.288341000	1.624328000	7.797532000	CORE	31	O	O	0.0000	31
O	-1.333926000	4.420799000	7.786684000	CORE	32	O	O	0.0000	32
O	2.996417000	1.630709000	7.787189000	CORE	33	O	O	0.0000	33
O	1.595259138	0.734911547	12.684170097	CORE	34	O	O	0.0000	34
O	-2.588180948	5.128746367	10.427360079	CORE	35	O	O	0.0000	35
O	1.599505798	2.448291071	10.589064665	CORE	36	O	O	0.0000	36
O	-1.354343688	2.453945276	10.534387098	CORE	37	O	O	0.0000	37
O	4.569342390	0.586697174	12.514654622	CORE	38	O	O	0.0000	38
O	-0.120354417	3.164870630	12.984370335	CORE	39	O	O	0.0000	39
O	2.613250798	1.729584311	14.827637685	CORE	40	O	O	0.0000	40
C	2.903088362	2.943786708	14.806687911	CORE	41	C	C	0.0000	41
H	1.892344372	1.023294307	13.626722972	CORE	42	H	H	0.0000	42
H	3.296891335	3.410920506	15.735161403	CORE	43	H	H	0.0000	43
O	-0.263361141	3.758968987	15.129690928	CORE	44	O	O	0.0000	44
C	-0.814680975	3.325537058	14.137246202	CORE	45	C	C	0.0000	45
end									
end									

TS CO* + H* + H* to CHO* + H*

!BIOSYM archive 2

PBC=ON

	Energy		42	-268	-268.081917				
!DATE									
PBC	5.9415	5.9415	25.2282	90.0000	90.0000	120.0000			
Cr	0.108150341	3.395620853	1.708739691	CORE	1	Cr	Cr	0.0000	1
Cr	3.081568217	3.395577545	1.709860229	CORE	2	Cr	Cr	0.0000	2
Cr	4.566431239	0.823575777	1.735668474	CORE	3	Cr	Cr	0.0000	3
Cr	2.868441123	5.111401027	6.667129378	CORE	4	Cr	Cr	0.0000	4
Cr	0.092587203	5.123605011	6.675514064	CORE	5	Cr	Cr	0.0000	5
Cr	1.595960552	2.544330892	6.675499610	CORE	6	Cr	Cr	0.0000	6
Cr	3.081543156	1.644032988	11.711560652	CORE	7	Cr	Cr	0.0000	7
Cr	0.012564743	1.595752562	11.696729455	CORE	8	Cr	Cr	0.0000	8
Cr	-1.332998489	4.154443977	11.654297229	CORE	9	Cr	Cr	0.0000	9
Zn	1.596738448	0.847122116	0.398957680	CORE	10	Zn	Zn	0.0000	10
Zn	1.595365593	0.816507250	3.600291812	CORE	11	Zn	Zn	0.0000	11
Zn	1.589307398	4.271214732	4.236439246	CORE	12	Zn	Zn	0.0000	12
Zn	-1.378158719	2.558889553	4.831337471	CORE	13	Zn	Zn	0.0000	13
Zn	-1.343713905	2.539486871	8.397097280	CORE	14	Zn	Zn	0.0000	14
Zn	1.580596095	0.868560654	9.094248602	CORE	15	Zn	Zn	0.0000	15
Zn	2.060258500	4.046252845	9.562446311	CORE	16	Zn	Zn	0.0000	16
Zn	1.722236537	3.850001530	12.829153557	CORE	17	Zn	Zn	0.0000	17
O	0.014340556	1.798534228	0.736441128	CORE	18	O	O	0.0000	18
O	3.177996949	1.800118734	0.734754373	CORE	19	O	O	0.0000	19
O	-1.375905612	4.145840755	0.748675703	CORE	20	O	O	0.0000	20
O	1.595514484	4.240527740	0.748073534	CORE	21	O	O	0.0000	21
O	-1.376403266	2.549563667	2.826755977	CORE	22	O	O	0.0000	22
O	0.202987344	5.017058933	2.842453626	CORE	23	O	O	0.0000	23
O	1.595110084	2.672319325	2.835213034	CORE	24	O	O	0.0000	24
O	2.985974302	5.015310592	2.845438791	CORE	25	O	O	0.0000	25
O	2.983831486	3.472661088	5.595847432	CORE	26	O	O	0.0000	26
O	0.204594670	3.462121787	5.592118168	CORE	27	O	O	0.0000	27
O	4.577468625	0.735775077	5.600279073	CORE	28	O	O	0.0000	28
O	1.603176700	0.836886506	5.609320578	CORE	29	O	O	0.0000	29
O	1.590890493	4.264745240	7.750274963	CORE	30	O	O	0.0000	30
O	0.240769869	1.611655561	7.856776010	CORE	31	O	O	0.0000	31
O	-1.392471420	4.402596058	7.843181562	CORE	32	O	O	0.0000	32
O	2.952763225	1.628330971	7.851784336	CORE	33	O	O	0.0000	33
O	1.564880449	0.732595744	12.765770125	CORE	34	O	O	0.0000	34
O	0.413046520	0.051064064	10.473658366	CORE	35	O	O	0.0000	35
O	1.577024675	2.668338379	10.842363306	CORE	36	O	O	0.0000	36
O	-1.403826005	2.463804738	10.590052246	CORE	37	O	O	0.0000	37
O	4.524051674	0.592932387	12.560007531	CORE	38	O	O	0.0000	38
O	-0.173646379	3.142747212	12.973574517	CORE	39	O	O	0.0000	39
O	2.984011467	2.349417845	15.135016791	CORE	40	O	O	0.0000	40
C	3.478905640	2.866991372	14.182269360	CORE	41	C	C	0.0000	41
H	1.625137304	0.744086312	13.737477533	CORE	42	H	H	0.0000	42
H	-1.222760197	2.997582622	13.819391584	CORE	43	H	H	0.0000	43
end									
end									

TS OH* + H* + CO* to H* + COOH*

!BIOSYM archive 2

PBC=ON

	Energy		43	-276	-276.220334				
!DATE									
PBC	5.9415	5.9415	25.2282	90.0000	90.0000	120.0000			
Cr	0.155889307	3.395325083	1.647917157	CORE	1	Cr	Cr	0.0000	1
Cr	3.129394798	3.395688633	1.648410418	CORE	2	Cr	Cr	0.0000	2
Cr	4.613463001	0.823317997	1.674998247	CORE	3	Cr	Cr	0.0000	3
Cr	-2.807656000	5.133964000	6.615087000	CORE	4	Cr	Cr	0.0000	4
Cr	0.149101900	5.134942000	6.617609000	CORE	5	Cr	Cr	0.0000	5
Cr	1.642320000	2.550568000	6.615087000	CORE	6	Cr	Cr	0.0000	6
Cr	3.127028338	1.754317971	11.748621546	CORE	7	Cr	Cr	0.0000	7
Cr	0.081010653	1.615720382	11.584669326	CORE	8	Cr	Cr	0.0000	8
Cr	-1.345107582	4.202231700	11.647274151	CORE	9	Cr	Cr	0.0000	9
Zn	1.643133348	0.845514493	0.346324821	CORE	10	Zn	Zn	0.0000	10
Zn	1.642961348	0.816463878	3.536931751	CORE	11	Zn	Zn	0.0000	11
Zn	1.641783986	4.268903568	4.174579494	CORE	12	Zn	Zn	0.0000	12
Zn	-1.328854738	2.561452014	4.768168001	CORE	13	Zn	Zn	0.0000	13
Zn	-1.312258899	2.548970498	8.239461537	CORE	14	Zn	Zn	0.0000	14
Zn	1.604021336	0.872651299	9.068145841	CORE	15	Zn	Zn	0.0000	15
Zn	2.056284251	3.984378693	9.506759291	CORE	16	Zn	Zn	0.0000	16
Zn	1.573105246	4.337532564	13.517384167	CORE	17	Zn	Zn	0.0000	17
O	0.060823256	1.798451819	0.674409250	CORE	18	O	O	0.0000	18
O	3.224547074	1.799746616	0.674426017	CORE	19	O	O	0.0000	19
O	-1.328237991	4.143852360	0.685541211	CORE	20	O	O	0.0000	20
O	1.642935588	4.240112758	0.687054478	CORE	21	O	O	0.0000	21
O	-1.328050680	2.549540081	2.765507435	CORE	22	O	O	0.0000	22
O	0.250399248	5.016199637	2.783024245	CORE	23	O	O	0.0000	23
O	1.642606872	2.671847572	2.774639856	CORE	24	O	O	0.0000	24
O	3.034669806	5.015403748	2.783862744	CORE	25	O	O	0.0000	25
O	3.028650000	3.472434000	5.534058000	CORE	26	O	O	0.0000	26
O	0.253791200	3.472434000	5.535824000	CORE	27	O	O	0.0000	27
O	4.611970000	0.730145000	5.535824000	CORE	28	O	O	0.0000	28
O	1.642349000	0.842522500	5.550709000	CORE	29	O	O	0.0000	29
O	1.644488000	4.271580000	7.688042000	CORE	30	O	O	0.0000	30
O	0.288341000	1.624328000	7.797532000	CORE	31	O	O	0.0000	31
O	-1.333926000	4.420799000	7.786684000	CORE	32	O	O	0.0000	32
O	2.996417000	1.630709000	7.787189000	CORE	33	O	O	0.0000	33
O	1.618076466	0.793464184	12.724646036	CORE	34	O	O	0.0000	34
O	0.337734539	0.003184126	10.472587806	CORE	35	O	O	0.0000	35
O	1.650656614	2.409459324	10.580756612	CORE	36	O	O	0.0000	36
O	-1.366887418	2.507129653	10.588812546	CORE	37	O	O	0.0000	37
O	4.574475107	0.838180785	12.662079802	CORE	38	O	O	0.0000	38
O	0.006375146	3.249692746	12.919284607	CORE	39	O	O	0.0000	39

O	3.219051190	3.236195357	13.024763990 CORE	40	O	O	0.0000	40
H	-0.614528491	2.909714041	13.601131868 CORE	41	H	H	0.0000	41
H	1.568565141	0.787047883	13.695513920 CORE	42	H	H	0.0000	42
O	3.438864494	2.713641034	15.492970653 CORE	43	O	O	0.0000	43
C	2.784174527	3.331767911	14.737310304 CORE	44	C	C	0.0000	44

end
end

Completed surface

'BIOSYM archive 2

PBC=ON

	Energy	44	-245	-245.621366				
'DATE								
PBC	5.9415	5.9415	25.2282	90.0000	90.0000	120.0000		
Cr	0.152879929	3.400433239	1.656551828 CORE	1	Cr	Cr	0.0000	1
Cr	3.126937152	3.400521257	1.656625400 CORE	2	Cr	Cr	0.0000	2
Cr	4.610700304	0.828419670	1.683488768 CORE	3	Cr	Cr	0.0000	3
Cr	-2.807656000	5.133964000	6.615087000 CORE	4	Cr	Cr	0.0000	4
Cr	0.149101900	5.134942000	6.617609000 CORE	5	Cr	Cr	0.0000	5
Cr	1.642320000	2.550568000	6.615087000 CORE	6	Cr	Cr	0.0000	6
Cr	3.271760501	1.653102128	11.649800610 CORE	7	Cr	Cr	0.0000	7
Cr	0.292630819	1.577049444	11.668721311 CORE	8	Cr	Cr	0.0000	8
Cr	-1.266861430	4.104249372	11.659787931 CORE	9	Cr	Cr	0.0000	9
Zn	1.640399292	0.850161232	0.342330020 CORE	10	Zn	Zn	0.0000	10
Zn	1.639997162	0.820725536	3.551513600 CORE	11	Zn	Zn	0.0000	11
Zn	1.640006508	4.269174732	4.183660377 CORE	12	Zn	Zn	0.0000	12
Zn	-1.329366822	2.561827755	4.788303690 CORE	13	Zn	Zn	0.0000	13
Zn	-1.302168325	2.541713779	8.400729171 CORE	14	Zn	Zn	0.0000	14
Zn	1.594906812	0.870336103	9.087503713 CORE	15	Zn	Zn	0.0000	15
Zn	2.134880305	3.972667818	9.498290054 CORE	16	Zn	Zn	0.0000	16
Zn	1.157163542	4.464337137	13.160753892 CORE	17	Zn	Zn	0.0000	17
O	0.058364930	1.800888326	0.685621430 CORE	18	O	O	0.0000	18
O	3.222182884	1.802214537	0.684571665 CORE	19	O	O	0.0000	19
O	-1.331166819	4.149378871	0.694885975 CORE	20	O	O	0.0000	20
O	1.640201001	4.246017184	0.697053039 CORE	21	O	O	0.0000	21
O	-1.330777831	2.554314667	2.774210930 CORE	22	O	O	0.0000	22
O	0.249281119	5.022936540	2.788719388 CORE	23	O	O	0.0000	23
O	1.640154203	2.677930390	2.783137413 CORE	24	O	O	0.0000	24
O	3.029707440	5.022075252	2.790381862 CORE	25	O	O	0.0000	25
O	3.028650000	3.472434000	5.534058000 CORE	26	O	O	0.0000	26
O	0.253791200	3.472434000	5.535824000 CORE	27	O	O	0.0000	27
O	4.611970000	0.730145000	5.535824000 CORE	28	O	O	0.0000	28
O	1.642349000	0.842522500	5.550709000 CORE	29	O	O	0.0000	29
O	1.644488000	4.271580000	7.688042000 CORE	30	O	O	0.0000	30
O	0.288341000	1.624328000	7.797532000 CORE	31	O	O	0.0000	31
O	-1.333926000	4.420799000	7.786684000 CORE	32	O	O	0.0000	32
O	2.996417000	1.630709000	7.787189000 CORE	33	O	O	0.0000	33
O	1.859614608	0.675491587	12.579322655 CORE	34	O	O	0.0000	34
O	-2.565070371	5.071676585	10.487247969 CORE	35	O	O	0.0000	35
O	1.780922993	2.372606032	10.521569834 CORE	36	O	O	0.0000	36
O	-1.220778578	2.456592742	10.524613946 CORE	37	O	O	0.0000	37
O	4.752803118	0.931172697	12.789259093 CORE	38	O	O	0.0000	38
O	0.026352871	3.136410318	12.854529331 CORE	39	O	O	0.0000	39

end
end

➤ ZnCr₂O₄ (11) surfaceCH₃CO* + O*

'BIOSYM archive 2

PBC=ON

Energy	0	-310	-310.212153			
'DATE						
PBC	5.9865	5.9865	25.4420	90.0000	90.0000	120.0000
Cr	3.489767467	1.446281255	1.802675553	CORE	1 Cr Cr	0.0000 1
Cr	-1.007014831	4.027236884	1.803335009	CORE	2 Cr Cr	0.0000 2
Cr	0.473947195	1.451444190	1.777033307	CORE	3 Cr Cr	0.0000 3
Cr	1.987462822	0.577701438	4.260817821	CORE	4 Cr Cr	0.0000 4
Cr	-2.499936800	4.896568000	6.721013000	CORE	5 Cr Cr	0.0000 5
Cr	0.493317500	4.896568000	6.721013000	CORE	6 Cr Cr	0.0000 6
Cr	1.989943000	2.304338000	6.721013000	CORE	7 Cr Cr	0.0000 7
Cr	1.991742191	4.027582673	9.165687567	CORE	8 Cr Cr	0.0000 8
Cr	3.473771135	3.176476979	11.676238215	CORE	9 Cr Cr	0.0000 9
Cr	4.938944775	0.565746182	11.614768234	CORE	10 Cr Cr	0.0000 10
Cr	0.476515254	3.203227852	11.624759558	CORE	11 Cr Cr	0.0000 11
Zn	2.005629443	4.023022104	0.495725267	CORE	12 Zn Zn	0.0000 12
Zn	1.982441126	4.036261166	3.673078615	CORE	13 Zn Zn	0.0000 13
Zn	-1.001654142	2.303489553	4.883787870	CORE	14 Zn Zn	0.0000 14
Zn	-1.003558698	2.304571864	8.575210087	CORE	15 Zn Zn	0.0000 15
Zn	1.973566103	0.583299580	9.778672694	CORE	16 Zn Zn	0.0000 16
Zn	2.172498352	0.474759158	13.331846750	CORE	17 Zn Zn	0.0000 17
O	5.009531604	0.684938202	0.841570688	CORE	18 O O	0.0000 18
O	0.411803389	3.091150284	0.841222657	CORE	19 O O	0.0000 19
O	3.599317374	3.103513217	0.814512926	CORE	20 O O	0.0000 20
O	1.980630154	0.581576599	0.879143509	CORE	21 O O	0.0000 21
O	-1.004406146	2.305157993	2.891631053	CORE	22 O O	0.0000 22
O	-2.374123936	4.994219159	2.991601909	CORE	23 O O	0.0000 23
O	1.968563211	2.146403190	2.990963349	CORE	24 O O	0.0000 24
O	0.354891681	4.978666550	3.000199931	CORE	25 O O	0.0000 25
O	3.351662000	1.362373000	5.553988000	CORE	26 O O	0.0000 26
O	-1.003367000	4.188267000	5.553988000	CORE	27 O O	0.0000 27
O	0.628163500	1.362373000	5.553988000	CORE	28 O O	0.0000 28
O	1.989883000	4.032526000	5.664153000	CORE	29 O O	0.0000 29
O	1.989913000	0.576201000	7.777874000	CORE	30 O O	0.0000 30
O	4.983162000	0.420459800	7.888038000	CORE	31 O O	0.0000 31
O	0.628163500	3.246302000	7.888038000	CORE	32 O O	0.0000 32
O	3.351662000	3.246302000	7.888038000	CORE	33 O O	0.0000 33
O	-2.650821947	4.814667683	10.457491476	CORE	34 O O	0.0000 34
O	0.625255791	4.811592950	10.422224129	CORE	35 O O	0.0000 35
O	1.981437256	2.471030892	10.460202760	CORE	36 O O	0.0000 36
O	-1.006303927	2.305208553	10.571431788	CORE	37 O O	0.0000 37
O	1.954432314	4.050644241	12.614194716	CORE	38 O O	0.0000 38
O	3.553385622	1.515816153	12.614244833	CORE	39 O O	0.0000 39
O	-1.035519566	3.935775312	12.632457192	CORE	40 O O	0.0000 40
O	0.336158539	1.509187485	12.839346593	CORE	41 O O	0.0000 41
C	-0.011707979	1.665266696	14.212761063	CORE	42 C C	0.0000 42
H	5.110995923	1.031927185	14.483763975	CORE	43 H H	0.0000 43
H	-0.237638545	2.715732172	14.463979593	CORE	44 H H	0.0000 44
C	1.172029647	1.165320315	15.041489800	CORE	45 C C	0.0000 45
O	1.353735989	1.217575772	16.223630435	CORE	46 O O	0.0000 46
end						
end						

CH₃CO* + OH*

'BIOSYM archive 2

PBC=ON

Energy	1	-315	-315.124202			
'DATE						
PBC	5.9865	5.9865	25.4420	90.0000	90.0000	120.0000
Cr	0.479965894	1.448434501	1.776721568	CORE	1 Cr Cr	0.0000 1
Cr	-1.004254797	4.020030283	1.777922092	CORE	2 Cr Cr	0.0000 2
Cr	3.496514565	1.447499009	1.778341073	CORE	3 Cr Cr	0.0000 3
Cr	1.989100798	0.576947975	4.264245318	CORE	4 Cr Cr	0.0000 4
Cr	-2.499932467	4.896567956	6.721013140	CORE	5 Cr Cr	0.0000 5
Cr	0.493317533	4.896567956	6.721013140	CORE	6 Cr Cr	0.0000 6
Cr	1.989942533	2.304337416	6.721013140	CORE	7 Cr Cr	0.0000 7
Cr	1.989273633	4.030227813	9.168114860	CORE	8 Cr Cr	0.0000 8
Cr	5.048975912	0.568838843	11.611786420	CORE	9 Cr Cr	0.0000 9
Cr	3.519103144	3.221420725	11.613188002	CORE	10 Cr Cr	0.0000 10
Cr	0.512923067	3.175152092	11.681717128	CORE	11 Cr Cr	0.0000 11
Zn	1.990859408	4.032927428	0.509209150	CORE	12 Zn Zn	0.0000 12
Zn	1.988000175	4.034023885	3.666308556	CORE	13 Zn Zn	0.0000 13
Zn	-1.003848003	2.304668236	4.873618167	CORE	14 Zn Zn	0.0000 14
Zn	-0.999824086	2.306126691	8.575098412	CORE	15 Zn Zn	0.0000 15
Zn	2.023424448	0.593295983	9.771670930	CORE	16 Zn Zn	0.0000 16
Zn	1.941367327	0.545152542	13.207698420	CORE	17 Zn Zn	0.0000 17
O	3.587995844	3.110578963	0.812120710	CORE	18 O O	0.0000 18
O	4.983543361	0.693694938	0.813532897	CORE	19 O O	0.0000 19
O	0.392454313	3.110510721	0.813988971	CORE	20 O O	0.0000 20
O	1.988234363	0.577170842	0.867828468	CORE	21 O O	0.0000 21
O	-1.004859164	2.305253499	2.880626590	CORE	22 O O	0.0000 22
O	-2.357937975	4.981824787	2.990432289	CORE	23 O O	0.0000 23
O	1.987063438	2.139322649	2.990391217	CORE	24 O O	0.0000 24
O	0.348468049	4.979995478	2.990323299	CORE	25 O O	0.0000 25
O	3.351661755	1.362372683	5.553988600	CORE	26 O O	0.0000 26
O	-1.003367332	4.188266883	5.553988600	CORE	27 O O	0.0000 27
O	0.628163445	1.362372683	5.553988600	CORE	28 O O	0.0000 28
O	1.989882668	4.032525672	5.664152460	CORE	29 O O	0.0000 29
O	1.989912600	0.576201004	7.777873820	CORE	30 O O	0.0000 30
O	4.983162600	0.420459794	7.888037680	CORE	31 O O	0.0000 31
O	0.628163445	3.246302150	7.888037680	CORE	32 O O	0.0000 32
O	3.351661755	3.246302150	7.888037680	CORE	33 O O	0.0000 33
O	-2.618072673	4.822838285	10.417446053	CORE	34 O O	0.0000 34
O	2.009938620	2.472219984	10.465433538	CORE	35 O O	0.0000 35
O	0.649379585	4.823874906	10.466063110	CORE	36 O O	0.0000 36
O	-0.984724645	2.310015436	10.571165335	CORE	37 O O	0.0000 37
O	2.036906718	4.054678540	12.610659156	CORE	38 O O	0.0000 38
O	0.415326938	1.519714318	12.683493851	CORE	39 O O	0.0000 39
O	-0.967895813	3.916698605	12.687728241	CORE	40 O O	0.0000 40
O	3.640636736	1.522250262	12.828930209	CORE	41 O O	0.0000 41
O	0.697262373	4.468964476	16.298568743	CORE	42 O O	0.0000 42
C	1.632744618	0.469274901	15.521745033	CORE	43 C C	0.0000 43
C	-0.281325847	5.017557298	15.972905427	CORE	44 C C	0.0000 44
H	4.219570678	1.854001240	13.544884182	CORE	45 H H	0.0000 45
H	1.532655337	1.526922048	15.775881490	CORE	46 H H	0.0000 46
H	-2.273779620	5.062950352	15.399622523	CORE	47 H H	0.0000 47
end						
end						

CH₃O*

'BIOSYM archive 2

PBC=ON

Energy	2	-294	-294.529977			
'DATE						
PBC	5.9865	5.9865	25.4420	90.0000	90.0000	120.0000
Cr	3.497929670	1.447238556	1.778985599	CORE	1 Cr Cr	0.0000 1
Cr	-1.003259122	4.019605975	1.778851012	CORE	2 Cr Cr	0.0000 2
Cr	0.480992928	1.447839389	1.777631597	CORE	3 Cr Cr	0.0000 3

Cr	1.989529344	0.576541202	4.264182957	CORE	4	Cr	Cr	0.0000	4
Cr	-2.499932467	4.896567956	6.721013140	CORE	5	Cr	Cr	0.0000	5
Cr	0.493317533	4.896567956	6.721013140	CORE	6	Cr	Cr	0.0000	6
Cr	1.989942533	2.304337416	6.721013140	CORE	7	Cr	Cr	0.0000	7
Cr	1.994451229	4.028659325	9.166929401	CORE	8	Cr	Cr	0.0000	8
Cr	3.475094135	3.170180136	11.68888417	CORE	9	Cr	Cr	0.0000	9
Cr	4.936034860	0.560846062	11.620371921	CORE	10	Cr	Cr	0.0000	10
Cr	0.478327667	3.210711254	11.617471401	CORE	11	Cr	Cr	0.0000	11
Zn	1.991558648	4.032489854	0.498733830	CORE	12	Zn	Zn	0.0000	12
Zn	1.989052948	4.033200199	3.665619327	CORE	13	Zn	Zn	0.0000	13
Zn	-1.003556498	2.304527625	4.874604775	CORE	14	Zn	Zn	0.0000	14
Zn	-1.003962676	2.304834640	8.578033142	CORE	15	Zn	Zn	0.0000	15
Zn	1.965181026	0.586554252	9.783447892	CORE	16	Zn	Zn	0.0000	16
Zn	2.253062602	0.419356063	13.402687240	CORE	17	Zn	Zn	0.0000	17
O	4.984325941	0.691742962	0.816202529	CORE	18	O	O	0.0000	18
O	0.394624604	3.110799111	0.816637975	CORE	19	O	O	0.0000	19
O	3.587684713	3.110693924	0.814981446	CORE	20	O	O	0.0000	20
O	1.989704958	0.576674060	0.869912144	CORE	21	O	O	0.0000	21
O	-1.003767437	2.304908363	2.881268903	CORE	22	O	O	0.0000	22
O	-2.356581585	4.981378574	2.990637562	CORE	23	O	O	0.0000	23
O	1.988382163	2.138128118	2.990868501	CORE	24	O	O	0.0000	24
O	0.349077570	4.980088702	2.991303551	CORE	25	O	O	0.0000	25
O	3.351661755	1.362372683	5.553988600	CORE	26	O	O	0.0000	26
O	-1.003367332	4.188266883	5.553988600	CORE	27	O	O	0.0000	27
O	0.628163445	1.362372683	5.553988600	CORE	28	O	O	0.0000	28
O	1.989882668	4.032525672	5.664152460	CORE	29	O	O	0.0000	29
O	1.989912600	0.576201004	7.777873820	CORE	30	O	O	0.0000	30
O	4.983162600	0.420459794	7.888037680	CORE	31	O	O	0.0000	31
O	0.628163445	3.246302150	7.888037680	CORE	32	O	O	0.0000	32
O	3.351661755	3.246302150	7.888037680	CORE	33	O	O	0.0000	33
O	-2.651631104	4.808170008	10.468329604	CORE	34	O	O	0.0000	34
O	0.623263084	4.818311555	10.426369812	CORE	35	O	O	0.0000	35
O	1.986486883	2.475397634	10.465168778	CORE	36	O	O	0.0000	36
O	-1.007616718	2.301986760	10.577261385	CORE	37	O	O	0.0000	37
O	1.950307178	4.049520882	12.625175643	CORE	38	O	O	0.0000	38
O	3.554571907	1.503943461	12.641402512	CORE	39	O	O	0.0000	39
O	1.028984299	3.932798051	12.645848843	CORE	40	O	O	0.0000	40
O	0.285260372	1.558925146	12.780634516	CORE	41	O	O	0.0000	41
C	0.558685477	1.423118292	14.100652178	CORE	42	C	C	0.0000	42
H	0.875341058	2.344291178	14.604646362	CORE	43	H	H	0.0000	43
H	-0.088034016	0.721396867	14.641183793	CORE	44	H	H	0.0000	44

end
end

CH₂O* + H*

!BIOSYM archive 2
PBC=ON

Energy	3	-299	-299.123381						
!DATE									
PBC	5.9865	5.9865	25.4420	90.0000	90.0000	120.0000			
Cr	3.497855575	1.447331521	1.777632780	CORE	1	Cr	Cr	0.0000	1
Cr	-1.00379082	4.019778198	1.777606742	CORE	2	Cr	Cr	0.0000	2
Cr	0.481224135	1.447633707	1.776743273	CORE	3	Cr	Cr	0.0000	3
Cr	1.989713483	0.576503991	4.261120499	CORE	4	Cr	Cr	0.0000	4
Cr	-2.499932467	4.896567956	6.721013140	CORE	5	Cr	Cr	0.0000	5
Cr	0.493317533	4.896567956	6.721013140	CORE	6	Cr	Cr	0.0000	6
Cr	1.989942533	2.304337416	6.721013140	CORE	7	Cr	Cr	0.0000	7
Cr	1.984001086	4.033518204	9.158444450	CORE	8	Cr	Cr	0.0000	8
Cr	3.474729539	3.219176269	11.625608852	CORE	9	Cr	Cr	0.0000	9
Cr	4.978507400	0.589531189	11.612290078	CORE	10	Cr	Cr	0.0000	10
Cr	0.490760716	3.205139843	11.635843232	CORE	11	Cr	Cr	0.0000	11
Zn	1.990828372	4.032519574	0.494356995	CORE	12	Zn	Zn	0.0000	12
Zn	1.989470791	4.033215279	3.658840515	CORE	13	Zn	Zn	0.0000	13
Zn	-1.003017956	2.304654046	4.867210751	CORE	14	Zn	Zn	0.0000	14
Zn	-1.003911553	2.303848729	8.573765768	CORE	15	Zn	Zn	0.0000	15
Zn	1.983637923	0.604946875	9.765941271	CORE	16	Zn	Zn	0.0000	16
Zn	2.148644137	0.308618979	13.588889768	CORE	17	Zn	Zn	0.0000	17
O	4.984009470	0.691529011	0.814816344	CORE	18	O	O	0.0000	18
O	0.394581743	3.111070368	0.815161557	CORE	19	O	O	0.0000	19
O	3.587118213	3.111036531	0.813881526	CORE	20	O	O	0.0000	20
O	1.989739697	0.576753986	0.867852353	CORE	21	O	O	0.0000	21
O	-1.003692594	2.304972322	2.881104124	CORE	22	O	O	0.0000	22
O	-2.356285568	4.981285796	2.993069592	CORE	23	O	O	0.0000	23
O	1.988594630	2.138088313	2.993198612	CORE	24	O	O	0.0000	24
O	0.349135809	4.980202911	2.993298619	CORE	25	O	O	0.0000	25
O	3.351661755	1.362372683	5.553988600	CORE	26	O	O	0.0000	26
O	-1.003367332	4.188266883	5.553988600	CORE	27	O	O	0.0000	27
O	0.628163445	1.362372683	5.553988600	CORE	28	O	O	0.0000	28
O	1.989882668	4.032525672	5.664152460	CORE	29	O	O	0.0000	29
O	1.989912600	0.576201004	7.777873820	CORE	30	O	O	0.0000	30
O	4.983162600	0.420459794	7.888037680	CORE	31	O	O	0.0000	31
O	0.628163445	3.246302150	7.888037680	CORE	32	O	O	0.0000	32
O	3.351661755	3.246302150	7.888037680	CORE	33	O	O	0.0000	33
O	-2.649205706	4.836088084	10.442525890	CORE	34	O	O	0.0000	34
O	0.621532094	4.839235046	10.452800470	CORE	35	O	O	0.0000	35
O	1.988071030	2.477113538	10.454137706	CORE	36	O	O	0.0000	36
O	-1.012186365	2.303743426	10.583090735	CORE	37	O	O	0.0000	37
O	1.978630219	4.063136289	12.615361046	CORE	38	O	O	0.0000	38
O	3.593794848	1.498653133	12.851796427	CORE	39	O	O	0.0000	39
O	-0.999316388	3.859357528	12.735014524	CORE	40	O	O	0.0000	40
O	0.342057461	1.533618609	12.747139844	CORE	41	O	O	0.0000	41
C	0.577405471	1.431762841	14.122551264	CORE	42	C	C	0.0000	42
H	4.107083111	1.954783149	13.554546110	CORE	43	H	H	0.0000	43
H	0.809412997	2.398789252	14.586160472	CORE	44	H	H	0.0000	44
H	-0.178043995	0.830546395	14.649476166	CORE	45	H	H	0.0000	45

end
end

CH₂O + H* + CO*

!BIOSYM archive 2
PBC=ON

Energy	4	-314	-314.220539						
!DATE									
PBC	5.9865	5.9865	25.4420	90.0000	90.0000	120.0000			
Cr	0.482312105	1.447739802	1.775247772	CORE	1	Cr	Cr	0.0000	1
Cr	3.499057996	1.447326499	1.776305336	CORE	2	Cr	Cr	0.0000	2
Cr	-1.002167719	4.019894677	1.776185161	CORE	3	Cr	Cr	0.0000	3
Cr	1.990209647	0.576559400	4.261086931	CORE	4	Cr	Cr	0.0000	4
Cr	-2.499932467	4.896567956	6.721013140	CORE	5	Cr	Cr	0.0000	5
Cr	0.493317533	4.896567956	6.721013140	CORE	6	Cr	Cr	0.0000	6
Cr	1.989942533	2.304337416	6.721013140	CORE	7	Cr	Cr	0.0000	7
Cr	1.989125478	4.027527240	9.157869131	CORE	8	Cr	Cr	0.0000	8
Cr	4.996500680	0.544380143	11.606467717	CORE	9	Cr	Cr	0.0000	9
Cr	3.489862170	3.210129987	11.626319994	CORE	10	Cr	Cr	0.0000	10
Cr	0.506342671	3.190519941	11.635268196	CORE	11	Cr	Cr	0.0000	11
Zn	1.992088164	4.032753787	0.500326201	CORE	12	Zn	Zn	0.0000	12
Zn	1.990244529	4.033285219	3.660482301	CORE	13	Zn	Zn	0.0000	13
Zn	-1.003102201	2.304769986	4.867757428	CORE	14	Zn	Zn	0.0000	14
Zn	-1.002695498	2.302767711	8.575310525	CORE	15	Zn	Zn	0.0000	15
Zn	1.995570166	0.595655122	9.772241187	CORE	16	Zn	Zn	0.0000	16
Zn	2.335726163	0.199566991	13.755709737	CORE	17	Zn	Zn	0.0000	17
O	3.588679469	3.110908162	0.812513738	CORE	18	O	O	0.0000	18
O	4.985114589	0.692265491	0.813340037	CORE	19	O	O	0.0000	19

O 0.395220230 3.111045951 0.813706696 CORE 20 O O 0.0000 20
O 1.990985899 0.576851087 0.867353663 CORE 21 O O 0.0000 21
O -1.002612186 2.305031591 2.879761805 CORE 22 O O 0.0000 22
O -2.355509767 4.981244620 2.991025840 CORE 23 O O 0.0000 23
O 1.989649060 2.138247101 2.991439279 CORE 24 O O 0.0000 24
O 0.350117318 4.980292798 2.991432527 CORE 25 O O 0.0000 25
O 3.351661755 1.362372683 5.553988600 CORE 26 O O 0.0000 26
O -1.003367332 4.188266883 5.553988600 CORE 27 O O 0.0000 27
O 0.628163445 1.362372683 5.553988600 CORE 28 O O 0.0000 28
O 1.989882668 4.032525672 5.664152460 CORE 29 O O 0.0000 29
O 1.989912600 0.576201004 7.777873820 CORE 30 O O 0.0000 30
O 4.983162600 0.420459794 7.888037680 CORE 31 O O 0.0000 31
O 0.628163445 3.246302150 7.888037680 CORE 32 O O 0.0000 32
O 3.351661755 3.246302150 7.888037680 CORE 33 O O 0.0000 33
O -2.637070519 4.820719867 10.436886362 CORE 34 O O 0.0000 34
O 0.631734137 4.827294669 10.456237984 CORE 35 O O 0.0000 35
O 2.003350143 2.470124608 10.451353951 CORE 36 O O 0.0000 36
O -0.996304049 2.292177647 10.584196405 CORE 37 O O 0.0000 37
O 1.991854612 4.050912873 12.619678564 CORE 38 O O 0.0000 38
O -0.986320559 3.846449707 12.743087220 CORE 39 O O 0.0000 39
O 0.381853616 1.498246610 12.736673104 CORE 40 O O 0.0000 40
O 3.620980842 1.488948175 12.855316477 CORE 41 O O 0.0000 41
O 2.791847169 0.016290793 16.841427602 CORE 42 O O 0.0000 42
C 0.642108467 1.341631087 14.071067975 CORE 43 C C 0.0000 43
C 0.050119381 5.135907510 15.718672203 CORE 44 C C 0.0000 44
H 4.170916230 1.977596992 13.508737474 CORE 45 H H 0.0000 45
H 0.900500568 2.280704760 14.582641808 CORE 46 H H 0.0000 46
H -0.079869031 0.694097812 14.596655418 CORE 47 H H 0.0000 47
end
end

CH₃CO* + O*

!BIOSYM archive 2
PBC=ON

Energy 5 -313 -313.686783
!DATE
PBC 5.9865 5.9865 25.4420 90.0000 90.0000 120.0000
Cr 3.497988340 1.447033219 1.778728512 CORE 1 Cr Cr 0.0000 1
Cr -1.003185714 4.019374126 1.778426787 CORE 2 Cr Cr 0.0000 2
Cr 0.481057848 1.447571424 1.777193554 CORE 3 Cr Cr 0.0000 3
Cr 1.989621427 0.576384352 4.265198380 CORE 4 Cr Cr 0.0000 4
Cr -2.499932468 4.896567956 6.721013140 CORE 5 Cr Cr 0.0000 5
Cr 0.493317532 4.896567956 6.721013140 CORE 6 Cr Cr 0.0000 6
Cr 1.989942532 2.304337416 6.721013140 CORE 7 Cr Cr 0.0000 7
Cr 1.994373769 4.030673914 9.168887374 CORE 8 Cr Cr 0.0000 8
Cr 3.511796488 3.154202584 11.680787848 CORE 9 Cr Cr 0.0000 9
Cr 4.991542666 0.574458387 11.650497749 CORE 10 Cr Cr 0.0000 10
Cr 0.501026087 3.164218480 11.646748861 CORE 11 Cr Cr 0.0000 11
Zn 1.991702327 4.032194607 0.498737392 CORE 12 Zn Zn 0.0000 12
Zn 1.989088087 4.032874635 3.667577343 CORE 13 Zn Zn 0.0000 13
Zn -1.003576331 2.304527625 4.876270721 CORE 14 Zn Zn 0.0000 14
Zn -1.004581913 2.304765196 8.569232543 CORE 15 Zn Zn 0.0000 15
Zn 1.998194081 0.573439746 9.794446341 CORE 16 Zn Zn 0.0000 16
Zn 1.980189655 0.577975664 13.300745255 CORE 17 Zn Zn 0.0000 17
O 4.984604033 0.691596560 0.815627602 CORE 18 O O 0.0000 18
O 0.394605926 3.110267058 0.815899535 CORE 19 O O 0.0000 19
O 3.587993702 3.110391319 0.814110498 CORE 20 O O 0.0000 20
O 1.989796818 0.576473527 0.869409066 CORE 21 O O 0.0000 21
O -1.003604342 2.304725896 2.880513909 CORE 22 O O 0.0000 22
O -2.356437226 4.981212241 2.989492384 CORE 23 O O 0.0000 23
O 1.988315916 2.137885052 2.989686091 CORE 24 O O 0.0000 24
O 0.349098931 4.979829717 2.990014752 CORE 25 O O 0.0000 25
O 3.351661755 1.362372683 5.553988600 CORE 26 O O 0.0000 26
O -1.003367333 4.188266883 5.553988600 CORE 27 O O 0.0000 27
O 0.628163445 1.362372683 5.553988600 CORE 28 O O 0.0000 28
O 1.989882667 4.032525672 5.664152460 CORE 29 O O 0.0000 29
O 1.989912600 0.576201004 7.777873820 CORE 30 O O 0.0000 30
O 4.983162600 0.420459794 7.888037680 CORE 31 O O 0.0000 31
O 0.628163445 3.246302150 7.888037680 CORE 32 O O 0.0000 32
O 3.351661755 3.246302150 7.888037680 CORE 33 O O 0.0000 33
O -2.641334428 4.787683956 10.447460206 CORE 34 O O 0.0000 34
O 0.650969567 4.808787995 10.441517045 CORE 35 O O 0.0000 35
O 2.015822564 2.482535484 10.446099085 CORE 36 O O 0.0000 36
O -0.996361184 2.301292599 10.562346803 CORE 37 O O 0.0000 37
O 2.005919147 4.024213545 12.603971974 CORE 38 O O 0.0000 38
O 3.529887939 1.497083467 12.562745961 CORE 39 O O 0.0000 39
O -1.034407955 3.961658790 12.569384215 CORE 40 O O 0.0000 40
O 0.417539438 1.480235095 12.582867814 CORE 41 O O 0.0000 41
O 2.805621976 0.092420627 16.031550820 CORE 42 O O 0.0000 42
C 0.819324973 1.465792228 16.029770007 CORE 43 C C 0.0000 43
C 1.943445651 0.665148982 15.413025098 CORE 44 C C 0.0000 44
H 0.176144707 1.912438056 15.265696706 CORE 45 H H 0.0000 45
H 1.264860240 2.247082858 16.665953875 CORE 46 H H 0.0000 46
H 0.236775160 0.785137259 16.671767245 CORE 47 H H 0.0000 47
end
end

CH₃O*

!BIOSYM archive 2
PBC=ON

Energy 6 -299 -299.599349
!DATE
PBC 5.9865 5.9865 25.4420 90.0000 90.0000 120.0000
Cr 3.498099332 1.446790324 1.784263082 CORE 1 Cr Cr 0.0000 1
Cr -1.003242765 4.018811236 1.783989182 CORE 2 Cr Cr 0.0000 2
Cr 0.480895185 1.447243639 1.782852227 CORE 3 Cr Cr 0.0000 3
Cr 1.989574910 0.576213852 4.265767124 CORE 4 Cr Cr 0.0000 4
Cr -2.499932467 4.896567956 6.721013140 CORE 5 Cr Cr 0.0000 5
Cr 0.493317533 4.896567956 6.721013140 CORE 6 Cr Cr 0.0000 6
Cr 1.989942533 2.304337416 6.721013140 CORE 7 Cr Cr 0.0000 7
Cr 1.991935744 4.026568084 9.173402611 CORE 8 Cr Cr 0.0000 8
Cr 3.479837064 3.159614041 11.668650643 CORE 9 Cr Cr 0.0000 9
Cr 4.946011898 0.559646491 11.641939163 CORE 10 Cr Cr 0.0000 10
Cr 0.477846400 3.188390042 11.644174268 CORE 11 Cr Cr 0.0000 11
Zn 1.991405628 4.032227322 0.501512164 CORE 12 Zn Zn 0.0000 12
Zn 1.989181126 4.032480250 3.666130261 CORE 13 Zn Zn 0.0000 13
Zn -1.003672507 2.304526582 4.877509651 CORE 14 Zn Zn 0.0000 14
Zn -1.001917372 2.303073090 8.582022246 CORE 15 Zn Zn 0.0000 15
Zn 1.973897456 0.576917864 9.753757250 CORE 16 Zn Zn 0.0000 16
Zn 2.064074179 0.516409361 12.866530927 CORE 17 Zn Zn 0.0000 17
O 4.984286015 0.691008153 0.822166341 CORE 18 O O 0.0000 18
O 0.394662419 3.110338869 0.822714480 CORE 19 O O 0.0000 19
O 3.587297456 3.110479370 0.821216292 CORE 20 O O 0.0000 20
O 1.989766118 0.576024676 0.876090780 CORE 21 O O 0.0000 21
O -1.003590758 2.304335175 2.886423213 CORE 22 O O 0.0000 22
O -2.35684732 4.980566907 2.995546364 CORE 23 O O 0.0000 23
O 1.988391088 2.137847750 2.995630546 CORE 24 O O 0.0000 24
O 0.349297626 4.979374640 2.996153643 CORE 25 O O 0.0000 25
O 3.351661755 1.362372683 5.553988600 CORE 26 O O 0.0000 26
O -1.003367332 4.188266883 5.553988600 CORE 27 O O 0.0000 27
O 0.628163445 1.362372683 5.553988600 CORE 28 O O 0.0000 28
O 1.989882668 4.032525672 5.664152460 CORE 29 O O 0.0000 29
O 1.989912600 0.576201004 7.777873820 CORE 30 O O 0.0000 30

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O      4.983162600    0.420459794    7.888037680 CORE   31  O  O  0.0000  31
O      0.628163445    3.246302150    7.888037680 CORE   32  O  O  0.0000  32
O      3.351661755    3.246302150    7.888037680 CORE   33  O  O  0.0000  33
O      -2.638367943    4.815518630    10.468688073 CORE   34  O  O  0.0000  34
O      0.621876754    4.809167213    10.444457694 CORE   35  O  O  0.0000  35
O      1.980934516    2.452116448    10.465155325 CORE   36  O  O  0.0000  36
O      -0.994469912    2.287340530    10.579729013 CORE   37  O  O  0.0000  37
O      1.969176029    4.031611415    12.609780616 CORE   38  O  O  0.0000  38
O      3.586830075    1.520748443    12.676638637 CORE   39  O  O  0.0000  39
O      -1.033528484    3.879521332    12.682811039 CORE   40  O  O  0.0000  40
O      0.362609169    1.496371104    12.881675536 CORE   41  O  O  0.0000  41
C      0.011033190    1.283505719    14.283505799 CORE   42  C  C  0.0000  42
H      -0.933316864    2.228175098    14.346054765 CORE   43  H  H  0.0000  43
H      0.811596642    2.249333570    14.777104684 CORE   44  H  H  0.0000  44
H      -0.104827103    0.684110769    14.746345829 CORE   45  H  H  0.0000  45
end
end

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CH₃OH*

!BIOSYM archive 2

PBC=ON

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Energy      7      -302      -302.342687

!DATE
PBC      5.9865      5.9865      25.4420      90.0000      90.0000      120.0000
Cr      3.498822066    1.445726967    1.764679838 CORE   1  Cr Cr  0.0000  1
Cr      -1.001737792    4.018978001    1.764180128 CORE   2  Cr Cr  0.0000  2
Cr      0.483007132    1.446262667    1.763317442 CORE   3  Cr Cr  0.0000  3
Cr      1.990265708    0.575589824    4.247585997 CORE   4  Cr Cr  0.0000  4
Cr      -2.499932467    4.896567956    6.721013140 CORE   5  Cr Cr  0.0000  5
Cr      0.493317533    4.896567956    6.721013140 CORE   6  Cr Cr  0.0000  6
Cr      1.989942533    2.304337416    6.721013140 CORE   7  Cr Cr  0.0000  7
Cr      2.003440701    4.025489331    9.152490761 CORE   8  Cr Cr  0.0000  8
Cr      3.459050307    3.164611848    11.696076616 CORE   9  Cr Cr  0.0000  9
Cr      4.890669718    0.549581802    11.590429940 CORE   10 Cr Cr  0.0000  10
Cr      4.890669718    3.239500450    11.567763789 CORE   11 Cr Cr  0.0000  11
Zn      1.992411860    4.032361757    0.496734226 CORE   12 Zn Zn  0.0000  12
Zn      1.991362195    4.031430655    3.639318087 CORE   13 Zn Zn  0.0000  13
Zn      -1.002758840    2.304265195    4.843062999 CORE   14 Zn Zn  0.0000  14
Zn      -1.003775306    2.302847880    8.552873154 CORE   15 Zn Zn  0.0000  15
Zn      1.920602104    0.610156892    9.738958246 CORE   16 Zn Zn  0.0000  16
Zn      2.291597354    0.381445004    13.220430616 CORE   17 Zn Zn  0.0000  17
O      4.984704362    0.691339735    0.800378919 CORE   18  O  O  0.0000  18
O      0.395076500    3.110166732    0.801209856 CORE   19  O  O  0.0000  19
O      3.588374301    3.110089318    0.800956829 CORE   20  O  O  0.0000  20
O      1.991273742    0.575447772    0.852412838 CORE   21  O  O  0.0000  21
O      -1.002263988    2.303805120    2.872485178 CORE   22  O  O  0.0000  22
O      -2.354604941    4.979875811    2.991200995 CORE   23  O  O  0.0000  23
O      1.990055203    2.136563494    2.991737995 CORE   24  O  O  0.0000  24
O      0.350092835    4.978983513    2.992530609 CORE   25  O  O  0.0000  25
O      3.351661755    1.362372683    5.553988600 CORE   26  O  O  0.0000  26
O      -1.003367332    4.188266883    5.553988600 CORE   27  O  O  0.0000  27
O      0.628163445    1.362372683    5.553988600 CORE   28  O  O  0.0000  28
O      1.989882668    4.032525672    5.664152460 CORE   29  O  O  0.0000  29
O      1.989912600    0.576201004    7.777873820 CORE   30  O  O  0.0000  30
O      4.983162600    0.420459794    7.888037680 CORE   31  O  O  0.0000  31
O      0.628163445    3.246302150    7.888037680 CORE   32  O  O  0.0000  32
O      3.351661755    3.246302150    7.888037680 CORE   33  O  O  0.0000  33
O      -2.646441198    4.823973872    10.490811384 CORE   34  O  O  0.0000  34
O      0.603858975    4.827865821    10.400332313 CORE   35  O  O  0.0000  35
O      1.964496720    2.462469677    10.472200844 CORE   36  O  O  0.0000  36
O      -1.009092631    2.288617632    10.590735195 CORE   37  O  O  0.0000  37
O      1.920059233    4.027379709    12.648601225 CORE   38  O  O  0.0000  38
O      3.663225401    1.509728372    12.759286817 CORE   39  O  O  0.0000  39
O      -0.984911154    3.807899712    12.794137693 CORE   40  O  O  0.0000  40
O      1.110775988    1.451599771    14.517462045 CORE   41  O  O  0.0000  41
C      0.088700637    0.912794123    15.397457544 CORE   42  C  C  0.0000  42
H      5.131865771    1.455327552    15.256210826 CORE   43  H  H  0.0000  43
H      0.434970172    0.977920191    16.439696957 CORE   44  H  H  0.0000  44
H      2.936032788    5.047968777    15.107005825 CORE   45  H  H  0.0000  45
H      0.997457129    2.408427281    14.321269569 CORE   46  H  H  0.0000  46
end
end

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CH₃O* + CO*

!BIOSYM archive 2

PBC=ON

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Energy      8      -314      -314.574378

!DATE
PBC      5.9865      5.9865      25.4420      90.0000      90.0000      120.0000
Cr      3.498041666    1.447534245    1.777614563 CORE   1  Cr Cr  0.0000  1
Cr      -1.003141856    4.019799040    1.777304426 CORE   2  Cr Cr  0.0000  2
Cr      0.481343891    1.447966970    1.776636515 CORE   3  Cr Cr  0.0000  3
Cr      1.989648007    0.576526597    4.262740555 CORE   4  Cr Cr  0.0000  4
Cr      -2.499932467    4.896567956    6.721013140 CORE   5  Cr Cr  0.0000  5
Cr      0.493317533    4.896567956    6.721013140 CORE   6  Cr Cr  0.0000  6
Cr      1.989942533    2.304337416    6.721013140 CORE   7  Cr Cr  0.0000  7
Cr      1.991373165    4.029932570    9.167874748 CORE   8  Cr Cr  0.0000  8
Cr      3.471653966    3.171974979    11.657740542 CORE   9  Cr Cr  0.0000  9
Cr      4.938427956    0.564445575    11.636445315 CORE   10 Cr Cr  0.0000  10
Cr      0.476748089    3.205065543    11.636813212 CORE   11 Cr Cr  0.0000  11
Zn      1.991344281    4.033252987    0.504267487 CORE   12 Zn Zn  0.0000  12
Zn      1.989322687    4.033200298    3.664039560 CORE   13 Zn Zn  0.0000  13
Zn      -1.003574486    2.304672355    4.871611292 CORE   14 Zn Zn  0.0000  14
Zn      -1.001848899    2.303751582    8.579970276 CORE   15 Zn Zn  0.0000  15
Zn      1.975589813    0.580789822    9.769142910 CORE   16 Zn Zn  0.0000  16
Zn      2.049559237    0.535414947    13.131829201 CORE   17 Zn Zn  0.0000  17
O      4.984108155    0.693085064    0.813424829 CORE   18  O  O  0.0000  18
O      0.393949024    3.110926662    0.813948665 CORE   19  O  O  0.0000  19
O      3.588143482    3.110723289    0.812794362 CORE   20  O  O  0.0000  20
O      1.989896316    0.576942152    0.867772662 CORE   21  O  O  0.0000  21
O      -1.003587125    2.305168333    2.880224361 CORE   22  O  O  0.0000  22
O      -2.356476517    4.981230062    2.990240142 CORE   23  O  O  0.0000  23
O      1.988755793    2.138365253    2.990699759 CORE   24  O  O  0.0000  24
O      0.349439028    4.980124222    2.990575311 CORE   25  O  O  0.0000  25
O      3.351661755    1.362372683    5.553988600 CORE   26  O  O  0.0000  26
O      -1.003367332    4.188266883    5.553988600 CORE   27  O  O  0.0000  27
O      0.628163445    1.362372683    5.553988600 CORE   28  O  O  0.0000  28
O      1.989882668    4.032525672    5.664152460 CORE   29  O  O  0.0000  29
O      1.989912600    0.576201004    7.777873820 CORE   30  O  O  0.0000  30
O      4.983162600    0.420459794    7.888037680 CORE   31  O  O  0.0000  31
O      0.628163445    3.246302150    7.888037680 CORE   32  O  O  0.0000  32
O      3.351661755    3.246302150    7.888037680 CORE   33  O  O  0.0000  33
O      -2.646270663    4.820188284    10.467117083 CORE   34  O  O  0.0000  34
O      0.628845114    4.813361773    10.435500553 CORE   35  O  O  0.0000  35
O      1.978957139    2.464192398    10.465410979 CORE   36  O  O  0.0000  36
O      -0.995619693    2.295105352    10.580595691 CORE   37  O  O  0.0000  37
O      1.963922499    4.042285559    12.630986396 CORE   38  O  O  0.0000  38
O      3.550613819    1.522036486    12.630124260 CORE   39  O  O  0.0000  39
O      -1.046499163    3.925860369    12.632350421 CORE   40  O  O  0.0000  40
O      0.336782320    1.523918165    12.943110871 CORE   41  O  O  0.0000  41
O      0.036898590    5.155078296    16.249664009 CORE   42  O  O  0.0000  42
C      -0.129943257    1.787789437    14.287102704 CORE   43  C  C  0.0000  43
C      2.471932615    0.292222334    15.306628017 CORE   44  C  C  0.0000  44

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H -1.077860390 2.337078007 14.244625085 CORE 45 H H 0.0000 45
H 0.625148601 2.392550343 14.817528280 CORE 46 H H 0.0000 46
H -0.280953514 0.828069917 14.809547348 CORE 47 H H 0.0000 47

end
end

CH₃O* + H* + H*

!BIOSYM archive 2

PBC=ON

Energy	9	-303	-303.813547			
!DATE						
PBC	5.9865	5.9865	25.4420	90.0000	90.0000	120.0000
Cr	3.496421294	1.445746112	1.746125328	CORE	1 Cr Cr	0.0000 1
Cr	-1.002845661	4.021744096	1.746219677	CORE	2 Cr Cr	0.0000 2
Cr	0.483992788	1.445983035	1.745874370	CORE	3 Cr Cr	0.0000 3
Cr	1.989908750	0.576157137	4.227348533	CORE	4 Cr Cr	0.0000 4
Cr	-2.499932467	4.896567956	6.721013140	CORE	5 Cr Cr	0.0000 5
Cr	0.493317533	4.896567956	6.721013140	CORE	6 Cr Cr	0.0000 6
Cr	1.989942533	2.304337416	6.721013140	CORE	7 Cr Cr	0.0000 7
Cr	1.988314282	4.033183299	9.150122294	CORE	8 Cr Cr	0.0000 8
Cr	3.505380092	3.156211790	11.615970774	CORE	9 Cr Cr	0.0000 9
Cr	4.935084917	0.623946502	11.608059615	CORE	10 Cr Cr	0.0000 10
Cr	0.426552037	3.182371610	11.606764378	CORE	11 Cr Cr	0.0000 11
Zn	1.991014155	4.032601029	0.471097622	CORE	12 Zn Zn	0.0000 12
Zn	1.989675495	4.032633363	3.599489909	CORE	13 Zn Zn	0.0000 13
Zn	-1.003519506	2.304234940	4.802075514	CORE	14 Zn Zn	0.0000 14
Zn	-1.002795360	2.303944939	8.462843793	CORE	15 Zn Zn	0.0000 15
Zn	1.957030572	0.594582221	9.702651885	CORE	16 Zn Zn	0.0000 16
Zn	2.077569433	0.523596431	12.708093523	CORE	17 Zn Zn	0.0000 17
O	4.983757656	0.689590328	0.786310526	CORE	18 O O	0.0000 18
O	0.396102229	3.112169288	0.786898229	CORE	19 O O	0.0000 19
O	3.585411127	3.111780059	0.785954591	CORE	20 O O	0.0000 20
O	1.990267023	0.576319961	0.829117491	CORE	21 O O	0.0000 21
O	-1.003323029	2.304515339	2.860755804	CORE	22 O O	0.0000 22
O	-2.354109829	4.981415032	2.994001937	CORE	23 O O	0.0000 23
O	1.989562113	2.135728507	2.994198895	CORE	24 O O	0.0000 24
O	0.347688728	4.980953243	2.994306947	CORE	25 O O	0.0000 25
O	3.351661755	1.362372683	5.553988600	CORE	26 O O	0.0000 26
O	-1.003367332	4.188266883	5.553988600	CORE	27 O O	0.0000 27
O	0.628163445	1.362372683	5.553988600	CORE	28 O O	0.0000 28
O	1.989882668	4.032525672	5.664152460	CORE	29 O O	0.0000 29
O	1.989912600	0.576201004	7.777873820	CORE	30 O O	0.0000 30
O	4.983162600	0.420459794	7.888037680	CORE	31 O O	0.0000 31
O	0.628163445	3.246302150	7.888037680	CORE	32 O O	0.0000 32
O	3.351661755	3.246302150	7.888037680	CORE	33 O O	0.0000 33
O	-2.650624169	4.846236956	10.491842913	CORE	34 O O	0.0000 34
O	0.613728733	4.825124897	10.468570551	CORE	35 O O	0.0000 35
O	1.958071331	2.458888467	10.490012445	CORE	36 O O	0.0000 36
O	-1.006690404	2.304193644	10.552987712	CORE	37 O O	0.0000 37
O	1.961018339	4.044057985	12.687261752	CORE	38 O O	0.0000 38
O	3.608845961	1.539133209	12.717422050	CORE	39 O O	0.0000 39
O	-1.027217838	3.873277823	12.718404508	CORE	40 O O	0.0000 40
O	0.371201108	1.506638709	12.883049871	CORE	41 O O	0.0000 41
C	0.043423226	1.681884962	14.283191040	CORE	42 C C	0.0000 42
H	-0.903117362	2.223811012	14.368998133	CORE	43 H H	0.0000 43
H	0.849882740	2.241890357	14.785700817	CORE	44 H H	0.0000 44
H	-0.039878199	0.694353429	14.768474288	CORE	45 H H	0.0000 45
H	1.953272794	4.035048126	13.658433656	CORE	46 H H	0.0000 46

end
end

CHOCO* + H*

!BIOSYM archive 2

PBC=ON

Energy	10	-309	-309.468662			
!DATE						
PBC	5.9865	5.9865	25.4420	90.0000	90.0000	120.0000
Cr	3.498972896	1.451037389	1.763221577	CORE	1 Cr Cr	0.0000 1
Cr	-1.001550524	4.025077787	1.763897845	CORE	2 Cr Cr	0.0000 2
Cr	0.483692325	1.451521318	1.762393208	CORE	3 Cr Cr	0.0000 3
Cr	1.990622696	0.583477174	4.246429321	CORE	4 Cr Cr	0.0000 4
Cr	-2.499933000	4.896568000	6.721013000	CORE	5 Cr Cr	0.0000 5
Cr	0.493317500	4.896568000	6.721013000	CORE	6 Cr Cr	0.0000 6
Cr	1.989943000	2.304338000	6.721013000	CORE	7 Cr Cr	0.0000 7
Cr	1.993636790	4.026508335	9.136964771	CORE	8 Cr Cr	0.0000 8
Cr	3.463177222	3.138433307	11.602660745	CORE	9 Cr Cr	0.0000 9
Cr	4.979445401	0.544395791	11.624472209	CORE	10 Cr Cr	0.0000 10
Cr	0.537616272	3.160270010	11.593384171	CORE	11 Cr Cr	0.0000 11
Zn	1.992510876	4.036170196	0.484348772	CORE	12 Zn Zn	0.0000 12
Zn	1.991629212	4.038078300	3.629192426	CORE	13 Zn Zn	0.0000 13
Zn	-1.003218102	2.305477828	4.834080976	CORE	14 Zn Zn	0.0000 14
Zn	-1.001137579	2.302584896	8.537871745	CORE	15 Zn Zn	0.0000 15
Zn	1.973475744	0.549254659	9.729716860	CORE	16 Zn Zn	0.0000 16
Zn	2.318485733	0.521709883	13.347722550	CORE	17 Zn Zn	0.0000 17
O	4.985088541	0.693935182	0.803229990	CORE	18 O O	0.0000 18
O	0.396841935	3.116079436	0.803052560	CORE	19 O O	0.0000 19
O	3.587588332	3.115599786	0.802425070	CORE	20 O O	0.0000 20
O	1.991442209	0.581116395	0.851883183	CORE	21 O O	0.0000 21
O	-1.002129655	2.308912777	2.873180531	CORE	22 O O	0.0000 22
O	-2.353039426	4.986394280	2.996919745	CORE	23 O O	0.0000 23
O	1.990610348	2.141979954	2.997132526	CORE	24 O O	0.0000 24
O	0.349006700	4.985524448	2.997612341	CORE	25 O O	0.0000 25
O	3.351662000	1.362373000	5.553988000	CORE	26 O O	0.0000 26
O	-1.003367000	4.188267000	5.553988000	CORE	27 O O	0.0000 27
O	0.628163500	1.362373000	5.553988000	CORE	28 O O	0.0000 28
O	1.989883000	4.032526000	5.664153000	CORE	29 O O	0.0000 29
O	1.989913000	0.576201000	7.777874000	CORE	30 O O	0.0000 30
O	4.983162000	0.420459800	7.888038000	CORE	31 O O	0.0000 31
O	0.628163500	3.246302000	7.888038000	CORE	32 O O	0.0000 32
O	3.351662000	3.246302000	7.888038000	CORE	33 O O	0.0000 33
O	-2.631796292	4.795645781	10.452238391	CORE	34 O O	0.0000 34
O	0.616984916	4.808317247	10.469262677	CORE	35 O O	0.0000 35
O	1.993226354	2.444061287	10.440317468	CORE	36 O O	0.0000 36
O	-0.977430857	2.293107420	10.582659262	CORE	37 O O	0.0000 37
O	1.984791228	4.004383704	12.619120764	CORE	38 O O	0.0000 38
O	3.729233380	1.554827542	12.795977656	CORE	39 O O	0.0000 39
O	-0.985081020	3.864696785	12.864392651	CORE	40 O O	0.0000 40
O	0.498460631	1.445145497	12.747098851	CORE	41 O O	0.0000 41
C	0.520413941	1.378294565	14.171229217	CORE	42 C C	0.0000 42
H	-0.149852361	0.636304201	14.621769408	CORE	43 H H	0.0000 43
H	-1.173532489	3.193688704	13.558931228	CORE	44 H H	0.0000 44
C	0.949455722	2.400572187	14.946961814	CORE	45 C C	0.0000 45
O	1.352062446	3.193379799	15.723503646	CORE	46 O O	0.0000 46

end
end

CHOCO* + H*

!BIOSYM archive 2

PBC=ON

Energy	11	-310	-310.531233			
!DATE						
PBC	5.9865	5.9865	25.4420	90.0000	90.0000	120.0000

Cr	3.498151859	1.446620434	1.761096200	CORE	1 Cr Cr	0.0000	1
Cr	-1.002408749	4.020187137	1.760715585	CORE	2 Cr Cr	0.0000	2
Cr	0.483349081	1.446854063	1.760395674	CORE	3 Cr Cr	0.0000	3
Cr	1.989996701	0.576251724	4.242148917	CORE	4 Cr Cr	0.0000	4
Cr	-2.499933000	4.896568000	6.721013000	CORE	5 Cr Cr	0.0000	5
Cr	0.493317500	4.896568000	6.721013000	CORE	6 Cr Cr	0.0000	6
Cr	1.989943000	2.304338000	6.721013000	CORE	7 Cr Cr	0.0000	7
Cr	1.991422047	4.031461567	9.141849005	CORE	8 Cr Cr	0.0000	8
Cr	3.455098341	3.136902045	11.604080429	CORE	9 Cr Cr	0.0000	9
Cr	4.970871891	0.543688284	11.625921073	CORE	10 Cr Cr	0.0000	10
Cr	0.527907156	3.160261894	11.592892871	CORE	11 Cr Cr	0.0000	11
Zn	1.992809152	4.032689113	0.479772501	CORE	12 Zn Zn	0.0000	12
Zn	1.990462871	4.032339451	3.629146636	CORE	13 Zn Zn	0.0000	13
Zn	-1.003268387	2.304335032	4.832847774	CORE	14 Zn Zn	0.0000	14
Zn	-1.002622463	2.302938466	8.534537965	CORE	15 Zn Zn	0.0000	15
Zn	1.967377233	0.550059591	9.729733584	CORE	16 Zn Zn	0.0000	16
Zn	2.304598332	0.526955612	13.347077039	CORE	17 Zn Zn	0.0000	17
O	4.985056931	0.689737141	0.800669269	CORE	18 O O	0.0000	18
O	0.397374057	3.111833943	0.801203637	CORE	19 O O	0.0000	19
O	3.587258551	3.111150981	0.799220584	CORE	20 O O	0.0000	20
O	1.990882616	0.576264081	0.849389651	CORE	21 O O	0.0000	21
O	-1.002670049	2.304646347	2.871119673	CORE	22 O O	0.0000	22
O	-2.354704622	4.981137323	2.994148027	CORE	23 O O	0.0000	23
O	1.989753104	2.136775169	2.994514499	CORE	24 O O	0.0000	24
O	0.349143558	4.980249772	2.994956540	CORE	25 O O	0.0000	25
O	3.351662000	1.362373000	5.553988000	CORE	26 O O	0.0000	26
O	-1.003367000	4.188267000	5.553988000	CORE	27 O O	0.0000	27
O	0.628163500	1.362373000	5.553988000	CORE	28 O O	0.0000	28
O	1.989883000	4.032526000	5.664153000	CORE	29 O O	0.0000	29
O	1.989913000	0.576201000	7.777874000	CORE	30 O O	0.0000	30
O	4.983162000	0.420459800	7.888038000	CORE	31 O O	0.0000	31
O	0.628163500	3.246302000	7.888038000	CORE	32 O O	0.0000	32
O	3.351662000	3.246302000	7.888038000	CORE	33 O O	0.0000	33
O	-2.635513076	4.795959056	10.456609130	CORE	34 O O	0.0000	34
O	0.610388107	4.807049157	10.467978400	CORE	35 O O	0.0000	35
O	1.985387379	2.443085436	10.442072108	CORE	36 O O	0.0000	36
O	-0.985701377	2.291566380	10.582485474	CORE	37 O O	0.0000	37
O	1.975382752	4.002879348	12.619580007	CORE	38 O O	0.0000	38
O	3.719297010	1.552879940	12.794364283	CORE	39 O O	0.0000	39
O	-0.996986741	3.869112310	12.864346790	CORE	40 O O	0.0000	40
O	0.484278009	1.449002826	12.751348654	CORE	41 O O	0.0000	41
C	0.511995305	1.386797110	14.175292522	CORE	42 C C	0.0000	42
H	-0.145679575	0.636783928	14.630820325	CORE	43 H H	0.0000	43
H	-1.182066419	3.203863770	13.565049464	CORE	44 H H	0.0000	44
C	0.936891678	2.415098698	14.945769962	CORE	45 C C	0.0000	45
O	1.339932567	3.214924628	15.715270481	CORE	46 O O	0.0000	46
end							
end							

CHO* + H*

!BIOSYM archive 2

PBC=ON

Energy		12	-294	-294.216501			
!DATE							
PBC	5.9865	5.9865	25.4420	90.0000	90.0000	120.0000	
Cr	3.498226559	1.446660684	1.767558515	CORE	1 Cr Cr	0.0000	1
Cr	-1.002540761	4.019751314	1.767226692	CORE	2 Cr Cr	0.0000	2
Cr	0.482026877	1.447317873	1.766410536	CORE	3 Cr Cr	0.0000	3
Cr	1.989898816	0.572682518	4.249137117	CORE	4 Cr Cr	0.0000	4
Cr	-2.499932467	4.896567956	6.721013140	CORE	5 Cr Cr	0.0000	5
Cr	0.493317533	4.896567956	6.721013140	CORE	6 Cr Cr	0.0000	6
Cr	1.989942533	2.304337416	6.721013140	CORE	7 Cr Cr	0.0000	7
Cr	1.996791499	4.031053399	9.147819727	CORE	8 Cr Cr	0.0000	8
Cr	3.437446496	3.131724817	11.654933341	CORE	9 Cr Cr	0.0000	9
Cr	4.871655145	0.522225796	11.610972789	CORE	10 Cr Cr	0.0000	10
Cr	0.484811795	3.186124148	11.571418240	CORE	11 Cr Cr	0.0000	11
Zn	1.992163637	4.032276326	0.479650927	CORE	12 Zn Zn	0.0000	12
Zn	1.990450938	4.032799810	3.638772605	CORE	13 Zn Zn	0.0000	13
Zn	-1.003122425	2.304551706	4.845217579	CORE	14 Zn Zn	0.0000	14
Zn	-1.003275237	2.301734550	8.557667878	CORE	15 Zn Zn	0.0000	15
Zn	1.927834595	0.578835605	9.738975839	CORE	16 Zn Zn	0.0000	16
Zn	1.851867712	0.796569143	13.247545150	CORE	17 Zn Zn	0.0000	17
O	4.984267129	0.689435064	0.807859397	CORE	18 O O	0.0000	18
O	0.396702582	3.112034346	0.808069901	CORE	19 O O	0.0000	19
O	3.586366626	3.111399540	0.806944846	CORE	20 O O	0.0000	20
O	1.990255362	0.576431620	0.858931161	CORE	21 O O	0.0000	21
O	-1.003189741	2.304687019	2.874907092	CORE	22 O O	0.0000	22
O	-2.355137781	4.981261550	2.993727277	CORE	23 O O	0.0000	23
O	1.989227574	2.137117774	2.994191649	CORE	24 O O	0.0000	24
O	0.348995751	4.980265839	2.994789619	CORE	25 O O	0.0000	25
O	3.351661755	1.362372683	5.553988600	CORE	26 O O	0.0000	26
O	-1.003367332	4.188266883	5.553988600	CORE	27 O O	0.0000	27
O	0.628163445	1.362372683	5.553988600	CORE	28 O O	0.0000	28
O	1.989882668	4.032525672	5.664152460	CORE	29 O O	0.0000	29
O	1.989912600	0.576201004	7.777873820	CORE	30 O O	0.0000	30
O	4.983162600	0.420459794	7.888037680	CORE	31 O O	0.0000	31
O	0.628163445	3.246302150	7.888037680	CORE	32 O O	0.0000	32
O	3.351661755	3.246302150	7.888037680	CORE	33 O O	0.0000	33
O	-2.646149080	4.818483031	10.492221906	CORE	34 O O	0.0000	34
O	0.591102221	4.799657804	10.408126331	CORE	35 O O	0.0000	35
O	1.965015937	2.455353005	10.436925712	CORE	36 O O	0.0000	36
O	-1.005448997	2.273065890	10.603791688	CORE	37 O O	0.0000	37
O	1.940089022	4.000408963	12.607769567	CORE	38 O O	0.0000	38
O	3.502359217	1.442716140	12.669345003	CORE	39 O O	0.0000	39
O	-0.993196875	3.883323109	12.830263243	CORE	40 O O	0.0000	40
O	-0.274873802	2.007505759	14.896645676	CORE	41 O O	0.0000	41
C	0.218102352	0.977440470	14.444180897	CORE	42 C C	0.0000	42
H	2.830917950	5.169455997	14.803856316	CORE	43 H H	0.0000	43
H	-0.896012659	3.362473473	13.666645933	CORE	44 H H	0.0000	44
end							
end							

CHO* + H*

!BIOSYM archive 2

PBC=ON

Energy		13	-293	-293.778690			
!DATE							
PBC	5.9865	5.9865	25.4420	90.0000	90.0000	120.0000	
Cr	3.499003117	1.447117112	1.762010953	CORE	1 Cr Cr	0.0000	1
Cr	-1.001847920	4.020014095	1.761949078	CORE	2 Cr Cr	0.0000	2
Cr	0.483116795	1.447436552	1.761469384	CORE	3 Cr Cr	0.0000	3
Cr	1.990654111	0.576464709	4.243704955	CORE	4 Cr Cr	0.0000	4
Cr	-2.499932467	4.896567956	6.721013140	CORE	5 Cr Cr	0.0000	5
Cr	0.493317533	4.896567956	6.721013140	CORE	6 Cr Cr	0.0000	6
Cr	1.989942533	2.304337416	6.721013140	CORE	7 Cr Cr	0.0000	7
Cr	1.982497623	4.032916248	9.148502878	CORE	8 Cr Cr	0.0000	8
Cr	3.438825763	3.167493552	11.572287749	CORE	9 Cr Cr	0.0000	9
Cr	4.986086930	0.574076784	11.622575339	CORE	10 Cr Cr	0.0000	10
Cr	0.511606486	3.128971577	11.641021564	CORE	11 Cr Cr	0.0000	11
Zn	1.991432776	4.032519042	0.480528711	CORE	12 Zn Zn	0.0000	12
Zn	1.991343273	4.032825914	3.631627870	CORE	13 Zn Zn	0.0000	13
Zn	-1.003138281	2.304227690	4.836282985	CORE	14 Zn Zn	0.0000	14
Zn	-0.998910123	2.303963199	8.538565778	CORE	15 Zn Zn	0.0000	15

Zn	1.991584008	0.550400427	9.731432376	CORE	16	Zn	Zn	0.0000	16
Zn	2.422541449	0.492164039	13.381341879	CORE	17	Zn	Zn	0.0000	17
O	4.984256182	0.690253701	0.801840222	CORE	18	O	O	0.0000	18
O	0.395975795	3.111911085	0.801066379	CORE	19	O	O	0.0000	19
O	3.586435800	3.111655828	0.802282553	CORE	20	O	O	0.0000	20
O	1.991167591	0.576564543	0.851476119	CORE	21	O	O	0.0000	21
O	-1.002244120	2.304865944	2.871826845	CORE	22	O	O	0.0000	22
O	-2.354036450	4.981305657	2.993690267	CORE	23	O	O	0.0000	23
O	1.990504679	2.136962732	2.993743256	CORE	24	O	O	0.0000	24
O	0.349824869	4.980627635	2.993876533	CORE	25	O	O	0.0000	25
O	3.351661755	1.362372683	5.553988600	CORE	26	O	O	0.0000	26
O	-1.003367332	4.188266883	5.553988600	CORE	27	O	O	0.0000	27
O	0.628163445	1.362372683	5.553988600	CORE	28	O	O	0.0000	28
O	1.989882668	4.032525672	5.664152460	CORE	29	O	O	0.0000	29
O	1.989912600	0.576201004	7.777873820	CORE	30	O	O	0.0000	30
O	4.983162600	0.420459794	7.888037680	CORE	31	O	O	0.0000	31
O	0.628163445	3.246302150	7.888037680	CORE	32	O	O	0.0000	32
O	3.351661755	3.246302150	7.888037680	CORE	33	O	O	0.0000	33
O	-2.631843989	4.825671234	10.450851485	CORE	34	O	O	0.0000	34
O	0.619512840	4.794101772	10.472157139	CORE	35	O	O	0.0000	35
O	1.966607506	2.437046651	10.455830903	CORE	36	O	O	0.0000	36
O	-0.980332662	2.304021679	10.579468117	CORE	37	O	O	0.0000	37
O	1.973692296	4.025310875	12.617346666	CORE	38	O	O	0.0000	38
O	3.675911668	1.570538899	12.695122800	CORE	39	O	O	0.0000	39
O	-1.030900443	3.920607699	12.799530818	CORE	40	O	O	0.0000	40
O	0.924665114	1.081563535	14.413187111	CORE	41	O	O	0.0000	41
C	0.120047209	1.599849695	13.578022611	CORE	42	C	C	0.0000	42
H	-0.771525414	1.988007730	14.134194864	CORE	43	H	H	0.0000	43
H	-1.253502691	3.350694845	13.567607974	CORE	44	H	H	0.0000	44
end									
end									

CHO* + H* + CO*

'BIOSYM archive 2

PBC=ON

	Energy	14	-309	-309.560165					
'DATE									
PBC	5.9865	5.9865	25.4420	90.0000	90.0000	120.0000			
Cr	3.496016539	1.446758605	1.765586030	CORE	1	Cr	Cr	0.0000	1
Cr	-1.004725996	4.019931971	1.765547166	CORE	2	Cr	Cr	0.0000	2
Cr	0.480213312	1.447095594	1.764870907	CORE	3	Cr	Cr	0.0000	3
Cr	1.989406388	0.576300315	4.248522797	CORE	4	Cr	Cr	0.0000	4
Cr	-2.499933000	4.896568000	6.721013000	CORE	5	Cr	Cr	0.0000	5
Cr	0.493317500	4.896568000	6.721013000	CORE	6	Cr	Cr	0.0000	6
Cr	1.989943000	2.304338000	6.721013000	CORE	7	Cr	Cr	0.0000	7
Cr	1.995205435	4.037603201	9.146374613	CORE	8	Cr	Cr	0.0000	8
Cr	3.460267071	3.175992705	11.626952222	CORE	9	Cr	Cr	0.0000	9
Cr	4.920437371	0.576986183	11.608607080	CORE	10	Cr	Cr	0.0000	10
Cr	0.536604590	3.179157348	11.591543048	CORE	11	Cr	Cr	0.0000	11
Zn	1.989374429	4.032013754	0.494748389	CORE	12	Zn	Zn	0.0000	12
Zn	1.989199359	4.032385963	3.640645005	CORE	13	Zn	Zn	0.0000	13
Zn	-1.002584772	2.304143085	4.843891522	CORE	14	Zn	Zn	0.0000	14
Zn	-1.001746974	2.307470207	8.547770665	CORE	15	Zn	Zn	0.0000	15
Zn	1.958328940	0.571856272	9.751705186	CORE	16	Zn	Zn	0.0000	16
Zn	2.671289572	0.485392277	13.913687739	CORE	17	Zn	Zn	0.0000	17
O	4.982152079	0.691150753	0.803218366	CORE	18	O	O	0.0000	18
O	0.392600030	3.110761996	0.803083640	CORE	19	O	O	0.0000	19
O	3.585406685	3.110750399	0.802223455	CORE	20	O	O	0.0000	20
O	1.988140497	0.576400039	0.854120852	CORE	21	O	O	0.0000	21
O	-1.005129297	2.304728534	2.873070358	CORE	22	O	O	0.0000	22
O	-2.356807637	4.981325378	2.992550871	CORE	23	O	O	0.0000	23
O	1.987434692	2.137314242	2.992407122	CORE	24	O	O	0.0000	24
O	0.347991036	4.979966489	2.992434732	CORE	25	O	O	0.0000	25
O	3.351662000	1.362373000	5.553988000	CORE	26	O	O	0.0000	26
O	-1.003367000	4.188267000	5.553988000	CORE	27	O	O	0.0000	27
O	0.628163500	1.362373000	5.553988000	CORE	28	O	O	0.0000	28
O	1.989883000	4.032526000	5.664153000	CORE	29	O	O	0.0000	29
O	1.989913000	0.576201000	7.777874000	CORE	30	O	O	0.0000	30
O	4.983162000	0.420459800	7.888038000	CORE	31	O	O	0.0000	31
O	0.628163500	3.246302000	7.888038000	CORE	32	O	O	0.0000	32
O	3.351662000	3.246302000	7.888038000	CORE	33	O	O	0.0000	33
O	-2.649710339	4.828508380	10.459851626	CORE	34	O	O	0.0000	34
O	0.605691154	4.804891891	10.449195115	CORE	35	O	O	0.0000	35
O	1.997941810	2.468125928	10.444469451	CORE	36	O	O	0.0000	36
O	-0.989283650	2.320169986	10.582549499	CORE	37	O	O	0.0000	37
O	1.960180291	4.048688684	12.625678868	CORE	38	O	O	0.0000	38
O	3.672081071	1.557844381	12.751679363	CORE	39	O	O	0.0000	39
O	-0.947192291	3.883247253	12.855326285	CORE	40	O	O	0.0000	40
O	0.403963038	1.442028444	12.810661379	CORE	41	O	O	0.0000	41
C	0.758363240	0.933134901	13.928484360	CORE	42	C	C	0.0000	42
H	-0.083563618	0.437573402	14.468602171	CORE	43	H	H	0.0000	43
H	-1.131607123	3.145284188	13.481307947	CORE	44	H	H	0.0000	44
C	0.818002019	4.618729023	15.255500946	CORE	45	C	C	0.0000	45
O	1.206010483	3.876396694	16.041782486	CORE	46	O	O	0.0000	46
end									
end									

CO*

'BIOSYM archive 2

PBC=ON

	Energy	15	-286	-286.572347					
'DATE									
PBC	5.9865	5.9865	25.4420	90.0000	90.0000	120.0000			
Cr	3.498533145	1.446281092	1.769204130	CORE	1	Cr	Cr	0.0000	1
Cr	-1.002551953	4.018629000	1.768837383	CORE	2	Cr	Cr	0.0000	2
Cr	0.481925138	1.446817627	1.768142035	CORE	3	Cr	Cr	0.0000	3
Cr	1.989960662	0.575836216	4.252836560	CORE	4	Cr	Cr	0.0000	4
Cr	-2.499932467	4.896567956	6.721013140	CORE	5	Cr	Cr	0.0000	5
Cr	0.493317533	4.896567956	6.721013140	CORE	6	Cr	Cr	0.0000	6
Cr	1.989942533	2.304337416	6.721013140	CORE	7	Cr	Cr	0.0000	7
Cr	1.991850651	4.032439615	9.153046949	CORE	8	Cr	Cr	0.0000	8
Cr	3.425753374	3.198754822	11.689086621	CORE	9	Cr	Cr	0.0000	9
Cr	4.840397934	0.575524465	11.581152509	CORE	10	Cr	Cr	0.0000	10
Cr	0.421389070	3.286281775	11.578947836	CORE	11	Cr	Cr	0.0000	11
Zn	1.991890499	4.032353861	0.495779640	CORE	12	Zn	Zn	0.0000	12
Zn	1.990322863	4.031543792	3.647631016	CORE	13	Zn	Zn	0.0000	13
Zn	-1.002906295	2.303902962	4.852949903	CORE	14	Zn	Zn	0.0000	14
Zn	-1.005556360	2.305394138	8.565918678	CORE	15	Zn	Zn	0.0000	15
Zn	1.892928843	0.632364746	9.746917701	CORE	16	Zn	Zn	0.0000	16
Zn	2.136707519	0.476091839	13.282221733	CORE	17	Zn	Zn	0.0000	17
O	4.984476023	0.691650820	0.806383277	CORE	18	O	O	0.0000	18
O	0.395001651	3.110731312	0.807864374	CORE	19	O	O	0.0000	19
O	3.587997513	3.110364307	0.806647127	CORE	20	O	O	0.0000	20
O	1.990407601	0.575645077	0.860703425	CORE	21	O	O	0.0000	21
O	-1.003092371	2.303971145	2.875455963	CORE	22	O	O	0.0000	22
O	-2.355473989	4.980041554	2.991032944	CORE	23	O	O	0.0000	23
O	1.989402015	2.136883329	2.991401774	CORE	24	O	O	0.0000	24
O	0.349543227	4.979013139	2.992107073	CORE	25	O	O	0.0000	25
O	3.351661755	1.362372683	5.553988600	CORE	26	O	O	0.0000	26
O	-1.003367332	4.188266883	5.553988600	CORE	27	O	O	0.0000	27
O	0.628163445	1.362372683	5.553988600	CORE	28	O	O	0.0000	28
O	1.989882668	4.032525672	5.664152460	CORE	29	O	O	0.0000	29
O	1.989912600	0.576201004	7.777873820	CORE	30	O	O	0.0000	30

O 4.983162600 0.420459794 7.888037680 CORE 31 O O 0.0000 31
O 0.628163445 3.246302150 7.888037680 CORE 32 O O 0.0000 32
O 3.351661755 3.246302150 7.888037680 CORE 33 O O 0.0000 33
O -2.680755464 4.854936305 10.479894348 CORE 34 O O 0.0000 34
O 0.582169961 4.843168705 10.377688686 CORE 35 O O 0.0000 35
O 1.935317082 2.483813037 10.473885582 CORE 36 O O 0.0000 36
O -1.034306157 2.319102665 10.595073000 CORE 37 O O 0.0000 37
O 1.901636202 4.080531340 12.618947370 CORE 38 O O 0.0000 38
O 3.568198029 1.506551854 12.721241991 CORE 39 O O 0.0000 39
O -1.020408802 3.901544724 12.730819712 CORE 40 O O 0.0000 40
O 0.018526588 1.694951488 15.280434262 CORE 41 O O 0.0000 41
C 0.716460288 1.293693434 14.464058828 CORE 42 C C 0.0000 42
end
end

CO* + H* + H*

!BIOSYM archive 2
PBC=ON

Energy 16 -294 -294.339938
!DATE
PBC 5.9865 5.9865 25.4420 90.0000 90.0000 120.0000
Cr 3.497022712 1.446544208 1.754538230 CORE 1 Cr Cr 0.0000 1
Cr -1.002914533 4.020874964 1.754448838 CORE 2 Cr Cr 0.0000 2
Cr 0.482702491 1.446834327 1.753903389 CORE 3 Cr Cr 0.0000 3
Cr 1.989830021 0.576225592 4.235523225 CORE 4 Cr Cr 0.0000 4
Cr -2.499932467 4.896567956 6.721013140 CORE 5 Cr Cr 0.0000 5
Cr 0.493317533 4.896567956 6.721013140 CORE 6 Cr Cr 0.0000 6
Cr 1.989942533 2.304337416 6.721013140 CORE 7 Cr Cr 0.0000 7
Cr 1.987656699 4.035132675 9.152626205 CORE 8 Cr Cr 0.0000 8
Cr 3.488823215 3.093811276 11.598617388 CORE 9 Cr Cr 0.0000 9
Cr 4.946364035 0.593314816 11.617947561 CORE 10 Cr Cr 0.0000 10
Cr 0.474156058 3.084522022 11.588339108 CORE 11 Cr Cr 0.0000 11
Zn 1.991693531 4.032433813 0.475791219 CORE 12 Zn Zn 0.0000 12
Zn 1.989965501 4.032477306 3.618425668 CORE 13 Zn Zn 0.0000 13
Zn -1.003607301 2.304725496 4.819157165 CORE 14 Zn Zn 0.0000 14
Zn -1.003438586 2.302362400 8.467549293 CORE 15 Zn Zn 0.0000 15
Zn 1.980935661 0.539559982 9.728115111 CORE 16 Zn Zn 0.0000 16
Zn 1.650818883 0.885190030 12.890109311 CORE 17 Zn Zn 0.0000 17
O 4.983612826 0.689872652 0.794887672 CORE 18 O O 0.0000 18
O 0.395940124 3.112171535 0.795017464 CORE 19 O O 0.0000 19
O 3.585767756 3.111717323 0.794110018 CORE 20 O O 0.0000 20
O 1.989807255 0.576632209 0.841441713 CORE 21 O O 0.0000 21
O -1.003476269 2.304824867 2.866535749 CORE 22 O O 0.0000 22
O -2.354936257 4.981497659 2.994122169 CORE 23 O O 0.0000 23
O 1.989116739 2.136554108 2.994395305 CORE 24 O O 0.0000 24
O 0.348396160 4.980738780 2.994645633 CORE 25 O O 0.0000 25
O 3.351661755 1.362372683 5.553988600 CORE 26 O O 0.0000 26
O -1.003367332 4.188266883 5.553988600 CORE 27 O O 0.0000 27
O 0.628163445 1.362372683 5.553988600 CORE 28 O O 0.0000 28
O 1.989882668 4.032525672 5.664152460 CORE 29 O O 0.0000 29
O 1.989912600 0.576201004 7.777873820 CORE 30 O O 0.0000 30
O 4.983162600 0.420459794 7.888037680 CORE 31 O O 0.0000 31
O 0.628163445 3.246302150 7.888037680 CORE 32 O O 0.0000 32
O 3.351661755 3.246302150 7.888037680 CORE 33 O O 0.0000 33
O -2.636670217 4.794890501 10.488207879 CORE 34 O O 0.0000 34
O 0.614314735 4.796691150 10.458310742 CORE 35 O O 0.0000 35
O 1.988241591 2.447648798 10.441116611 CORE 36 O O 0.0000 36
O -1.003915520 2.271904079 10.567518015 CORE 37 O O 0.0000 37
O 1.976519565 4.001131303 12.687058562 CORE 38 O O 0.0000 38
O 3.530059489 1.477389286 12.698094127 CORE 39 O O 0.0000 39
O -0.018455521 3.910860238 12.797223716 CORE 40 O O 0.0000 40
O 0.143683889 1.802359700 15.511291085 CORE 41 O O 0.0000 41
C 0.911034522 1.134518225 14.953054702 CORE 42 C C 0.0000 42
H 1.955080798 4.002064001 13.658146740 CORE 43 H H 0.0000 43
H -1.095931012 3.423463254 13.641728581 CORE 44 H H 0.0000 44
end
end

H* + H*

!BIOSYM archive 2
PBC=ON

Energy 17 -279 -279.364085
!DATE
PBC 5.9865 5.9865 25.4420 90.0000 90.0000 120.0000
Cr 3.497532062 1.446054402 1.754263812 CORE 1 Cr Cr 0.0000 1
Cr -1.002389718 4.020534768 1.754236442 CORE 2 Cr Cr 0.0000 2
Cr 0.483327512 1.446545266 1.753780038 CORE 3 Cr Cr 0.0000 3
Cr 1.990163731 0.576215009 4.235277909 CORE 4 Cr Cr 0.0000 4
Cr -2.499932467 4.896567956 6.721013140 CORE 5 Cr Cr 0.0000 5
Cr 0.493317533 4.896567956 6.721013140 CORE 6 Cr Cr 0.0000 6
Cr 1.989942533 2.304337416 6.721013140 CORE 7 Cr Cr 0.0000 7
Cr 1.992209811 4.026558540 9.153932140 CORE 8 Cr Cr 0.0000 8
Cr 3.573855691 3.187055957 11.597754200 CORE 9 Cr Cr 0.0000 9
Cr 5.060577301 0.616532746 11.595029592 CORE 10 Cr Cr 0.0000 10
Cr 0.482580516 3.168650854 11.634780532 CORE 11 Cr Cr 0.0000 11
Zn 1.992218176 4.032171018 0.478489661 CORE 12 Zn Zn 0.0000 12
Zn 1.990493037 4.032492109 3.618130448 CORE 13 Zn Zn 0.0000 13
Zn -1.003770159 2.304524666 4.818826031 CORE 14 Zn Zn 0.0000 14
Zn -0.999499166 2.303766478 8.473500330 CORE 15 Zn Zn 0.0000 15
Zn 2.036052172 0.588584952 9.720226869 CORE 16 Zn Zn 0.0000 16
Zn 1.548842923 0.715254161 12.761299657 CORE 17 Zn Zn 0.0000 17
O 4.984288864 0.689713180 0.793974107 CORE 18 O O 0.0000 18
O 0.396557462 3.111861897 0.794402004 CORE 19 O O 0.0000 19
O 3.586863360 3.111054081 0.793262158 CORE 20 O O 0.0000 20
O 1.990398963 0.576158585 0.840462204 CORE 21 O O 0.0000 21
O -1.002962014 2.304442887 2.866394573 CORE 22 O O 0.0000 22
O -2.354414354 4.981136304 2.994139695 CORE 23 O O 0.0000 23
O 1.989742025 2.136396038 2.994160502 CORE 24 O O 0.0000 24
O 0.348721511 4.980427801 2.994550141 CORE 25 O O 0.0000 25
O 3.351661755 1.362372683 5.553988600 CORE 26 O O 0.0000 26
O -1.003367332 4.188266883 5.553988600 CORE 27 O O 0.0000 27
O 0.628163445 1.362372683 5.553988600 CORE 28 O O 0.0000 28
O 1.989882668 4.032525672 5.664152460 CORE 29 O O 0.0000 29
O 1.989912600 0.576201004 7.777873820 CORE 30 O O 0.0000 30
O 4.983162600 0.420459794 7.888037680 CORE 31 O O 0.0000 31
O 0.628163445 3.246302150 7.888037680 CORE 32 O O 0.0000 32
O 3.351661755 3.246302150 7.888037680 CORE 33 O O 0.0000 33
O -2.608354716 4.811365909 10.439376728 CORE 34 O O 0.0000 34
O 0.653887379 4.827612963 10.470657531 CORE 35 O O 0.0000 35
O 2.028343022 2.458856953 10.484117566 CORE 36 O O 0.0000 36
O -0.953098476 2.302981570 10.571069004 CORE 37 O O 0.0000 37
O 2.035342408 4.042408448 12.682396444 CORE 38 O O 0.0000 38
O 3.612518787 1.499107888 12.794107262 CORE 39 O O 0.0000 39
O -0.994633420 3.964041706 12.697667454 CORE 40 O O 0.0000 40
H 2.047369878 4.048160608 13.653589552 CORE 41 H H 0.0000 41
H 4.006371145 1.813124734 13.632287935 CORE 42 H H 0.0000 42
end
end

H* + COOH*

!BIOSYM archive 2
PBC=ON

Energy	18	-302	-302.867545						
!DATE									
PBC	5.9865	5.9865	25.4420	90.0000	90.0000	120.0000			
Cr	0.482220173	1.446720242	1.748256091	CORE	1	Cr Cr	0.0000	1	
Cr	-1.004420293	4.021468324	1.748202140	CORE	2	Cr Cr	0.0000	2	
Cr	3.495416533	1.446854672	1.748148762	CORE	3	Cr Cr	0.0000	3	
Cr	1.989493136	0.576381198	4.230292228	CORE	4	Cr Cr	0.0000	4	
Cr	-2.499933000	4.896568000	6.721013000	CORE	5	Cr Cr	0.0000	5	
Cr	0.493317500	4.896568000	6.721013000	CORE	6	Cr Cr	0.0000	6	
Cr	1.989943000	2.304338000	6.721013000	CORE	7	Cr Cr	0.0000	7	
Cr	1.990613457	4.019677560	9.140163594	CORE	8	Cr Cr	0.0000	8	
Cr	4.960847803	0.592777956	11.559300436	CORE	9	Cr Cr	0.0000	9	
Cr	3.524622021	3.180008630	11.612303265	CORE	10	Cr Cr	0.0000	10	
Cr	0.447346838	3.170812026	11.584039113	CORE	11	Cr Cr	0.0000	11	
Zn	1.988205806	4.033706580	0.455581482	CORE	12	Zn Zn	0.0000	12	
Zn	1.988786304	4.032830451	3.604706486	CORE	13	Zn Zn	0.0000	13	
Zn	-1.003303513	2.304683774	4.808157763	CORE	14	Zn Zn	0.0000	14	
Zn	-1.005991342	2.302988896	8.450402631	CORE	15	Zn Zn	0.0000	15	
Zn	1.980781275	0.589950465	9.735128622	CORE	16	Zn Zn	0.0000	16	
Zn	2.134061718	0.323324144	13.617783860	CORE	17	Zn Zn	0.0000	17	
O	3.581781444	3.113600507	0.791681054	CORE	18	O O	0.0000	18	
O	4.982257680	0.688900766	0.791147430	CORE	19	O O	0.0000	19	
O	0.395449834	3.113018571	0.791470202	CORE	20	O O	0.0000	20	
O	1.988855712	0.576727262	0.835393005	CORE	21	O O	0.0000	21	
O	-1.004639848	2.304987082	2.862554571	CORE	22	O O	0.0000	22	
O	-2.354960799	4.981979470	2.994212407	CORE	23	O O	0.0000	23	
O	1.988353712	2.135864180	2.994159854	CORE	24	O O	0.0000	24	
O	0.346787334	4.981197848	2.993725494	CORE	25	O O	0.0000	25	
O	3.351662000	1.362373000	5.553988000	CORE	26	O O	0.0000	26	
O	-1.003367000	4.188267000	5.553988000	CORE	27	O O	0.0000	27	
O	0.628163500	1.362373000	5.553988000	CORE	28	O O	0.0000	28	
O	1.989883000	4.032526000	5.664153000	CORE	29	O O	0.0000	29	
O	1.989913000	0.576201000	7.777874000	CORE	30	O O	0.0000	30	
O	4.983162000	0.420459800	7.888038000	CORE	31	O O	0.0000	31	
O	0.628163500	3.246302000	7.888038000	CORE	32	O O	0.0000	32	
O	3.351662000	3.246302000	7.888038000	CORE	33	O O	0.0000	33	
O	-2.653210183	4.812900807	10.462655812	CORE	34	O O	0.0000	34	
O	2.002383243	2.461355112	10.478332975	CORE	35	O O	0.0000	35	
O	0.624341183	4.811589879	10.450216325	CORE	36	O O	0.0000	36	
O	-1.022462967	2.295856633	10.546068632	CORE	37	O O	0.0000	37	
O	1.982872069	4.033033141	12.676214939	CORE	38	O O	0.0000	38	
O	0.381004245	1.472203596	12.715399879	CORE	39	O O	0.0000	39	
O	-0.974571880	3.878783892	12.694118586	CORE	40	O O	0.0000	40	
O	3.610309599	1.473767509	12.861074690	CORE	41	O O	0.0000	41	
H	4.202799932	1.740341040	13.625280252	CORE	42	H H	0.0000	42	
H	2.003923703	4.029878371	13.649864164	CORE	43	H H	0.0000	43	
O	-0.467186600	1.480352053	14.839057960	CORE	44	O O	0.0000	44	
C	0.482906050	1.261313452	14.102161325	CORE	45	C C	0.0000	45	
end									
end									

O*

!BIOSYM archive 2									
PBC--ON									
Energy	19	-278	-278.825642						
!DATE									
PBC	5.9865	5.9865	25.4420	90.0000	90.0000	120.0000			
Cr	0.480133255	1.447675598	1.778646109	CORE	1	Cr Cr	0.0000	1	
Cr	-1.004021622	4.019373037	1.780027847	CORE	2	Cr Cr	0.0000	2	
Cr	3.497391907	1.447186261	1.7800060146	CORE	3	Cr Cr	0.0000	3	
Cr	1.989343380	0.576450960	4.263716846	CORE	4	Cr Cr	0.0000	4	
Cr	-2.499932467	4.896567956	6.721013140	CORE	5	Cr Cr	0.0000	5	
Cr	0.493317533	4.896567956	6.721013140	CORE	6	Cr Cr	0.0000	6	
Cr	1.989942533	2.304337416	6.721013140	CORE	7	Cr Cr	0.0000	7	
Cr	1.997373979	4.035751329	9.180156608	CORE	8	Cr Cr	0.0000	8	
Cr	5.004490646	0.597658953	11.671012085	CORE	9	Cr Cr	0.0000	9	
Cr	3.518736524	3.170439504	11.670193804	CORE	10	Cr Cr	0.0000	10	
Cr	0.502376053	3.169715449	11.672801236	CORE	11	Cr Cr	0.0000	11	
Zn	1.990693177	4.032013225	0.489320336	CORE	12	Zn Zn	0.0000	12	
Zn	1.988552290	4.032976506	3.667117999	CORE	13	Zn Zn	0.0000	13	
Zn	-1.003841162	2.304531309	4.877870639	CORE	14	Zn Zn	0.0000	14	
Zn	-1.000874849	2.305069013	8.571389750	CORE	15	Zn Zn	0.0000	15	
Zn	2.003818122	0.582226022	9.777515875	CORE	16	Zn Zn	0.0000	16	
Zn	2.014462062	0.585010954	12.971694365	CORE	17	Zn Zn	0.0000	17	
O	3.585992105	3.111062736	0.818183605	CORE	18	O O	0.0000	18	
O	4.983812938	0.690397743	0.819595270	CORE	19	O O	0.0000	19	
O	0.394695353	3.110764350	0.819817867	CORE	20	O O	0.0000	20	
O	1.989010947	0.576545438	0.872764659	CORE	21	O O	0.0000	21	
O	-1.004335993	2.304785597	2.882115422	CORE	22	O O	0.0000	22	
O	-2.356875971	4.981549347	2.991017714	CORE	23	O O	0.0000	23	
O	1.987667782	2.137688344	2.991012331	CORE	24	O O	0.0000	24	
O	0.348411699	4.980042895	2.991236269	CORE	25	O O	0.0000	25	
O	3.351661755	1.362372683	5.553988600	CORE	26	O O	0.0000	26	
O	-1.003367332	4.108326683	5.553988600	CORE	27	O O	0.0000	27	
O	0.628163445	1.362372683	5.553988600	CORE	28	O O	0.0000	28	
O	1.989882668	4.032525672	5.664152460	CORE	29	O O	0.0000	29	
O	1.989912600	0.576201004	7.777873820	CORE	30	O O	0.0000	30	
O	4.983162600	0.420459794	7.888037680	CORE	31	O O	0.0000	31	
O	0.628163445	3.246302150	7.888037680	CORE	32	O O	0.0000	32	
O	3.351661755	3.246302150	7.888037680	CORE	33	O O	0.0000	33	
O	-2.630063096	4.817948374	10.453044837	CORE	34	O O	0.0000	34	
O	2.009240125	2.477744432	10.458564578	CORE	35	O O	0.0000	35	
O	0.654153454	4.822529741	10.460196349	CORE	36	O O	0.0000	36	
O	-0.982711945	2.312310473	10.568659346	CORE	37	O O	0.0000	37	
O	2.011472561	4.041139272	12.579570358	CORE	38	O O	0.0000	38	
O	0.417936875	1.503537137	12.631401493	CORE	39	O O	0.0000	39	
O	-0.982409085	3.927249738	12.632994780	CORE	40	O O	0.0000	40	
O	3.608916214	1.506474364	12.634486471	CORE	41	O O	0.0000	41	
end									
end									

OH*

!BIOSYM archive 2									
PBC--ON									
Energy	20	-283	-283.783828						
!DATE									
PBC	5.9865	5.9865	25.4420	90.0000	90.0000	120.0000			
Cr	0.480114637	1.447933342	1.777639439	CORE	1	Cr Cr	0.0000	1	
Cr	-1.004121892	4.019687368	1.778869577	CORE	2	Cr Cr	0.0000	2	
Cr	3.497210431	1.447395597	1.778894482	CORE	3	Cr Cr	0.0000	3	
Cr	1.989339845	0.576556038	4.264262872	CORE	4	Cr Cr	0.0000	4	
Cr	-2.499932467	4.896567956	6.721013140	CORE	5	Cr Cr	0.0000	5	
Cr	0.493317533	4.896567956	6.721013140	CORE	6	Cr Cr	0.0000	6	
Cr	1.989942533	2.304337416	6.721013140	CORE	7	Cr Cr	0.0000	7	
Cr	1.989725008	4.031406222	9.176853425	CORE	8	Cr Cr	0.0000	8	
Cr	5.052856848	0.580507991	11.628146821	CORE	9	Cr Cr	0.0000	9	
Cr	3.528347727	3.219602603	11.627769811	CORE	10	Cr Cr	0.0000	10	
Cr	0.512738068	3.174927324	11.691824528	CORE	11	Cr Cr	0.0000	11	
Zn	1.990586441	4.032477388	0.494333007	CORE	12	Zn Zn	0.0000	12	
Zn	1.988472162	4.033127526	3.665242628	CORE	13	Zn Zn	0.0000	13	
Zn	-1.003835612	2.304489181	4.874693890	CORE	14	Zn Zn	0.0000	14	
Zn	-1.000338706	2.305231192	8.574849790	CORE	15	Zn Zn	0.0000	15	
Zn	2.028639339	0.596767907	9.763487133	CORE	16	Zn Zn	0.0000	16	

Zn	1.940271241	0.538984913	13.013987168	CORE	17 Zn Zn	0.0000	17
O	3.586479741	3.111115354	0.816004542	CORE	18 O O	0.0000	18
O	4.983709640	0.691300933	0.817302703	CORE	19 O O	0.0000	19
O	0.394217154	3.110993167	0.817833434	CORE	20 O O	0.0000	20
O	1.988853315	0.576803732	0.870850228	CORE	21 O O	0.0000	21
O	-1.004487325	2.305056032	2.881304690	CORE	22 O O	0.0000	22
O	-2.357086035	4.981660324	2.991079051	CORE	23 O O	0.0000	23
O	1.987596440	2.138022955	2.990982445	CORE	24 O O	0.0000	24
O	0.348386066	4.980148066	2.991085590	CORE	25 O O	0.0000	25
O	3.351661755	1.362372683	5.553988600	CORE	26 O O	0.0000	26
O	-1.003367332	4.188266883	5.553988600	CORE	27 O O	0.0000	27
O	0.628163445	1.362372683	5.553988600	CORE	28 O O	0.0000	28
O	1.989882668	4.032525672	5.664152460	CORE	29 O O	0.0000	29
O	1.989912600	0.576201004	7.777873820	CORE	30 O O	0.0000	30
O	4.983162600	0.420459794	7.888037680	CORE	31 O O	0.0000	31
O	0.628163445	3.246302150	7.888037680	CORE	32 O O	0.0000	32
O	3.351661755	3.246302150	7.888037680	CORE	33 O O	0.0000	33
O	-2.611138179	4.828129778	10.429302088	CORE	34 O O	0.0000	34
O	2.020283678	2.467408040	10.470091843	CORE	35 O O	0.0000	35
O	0.650066534	4.837195976	10.472544613	CORE	36 O O	0.0000	36
O	-0.980174583	2.313508316	10.576836114	CORE	37 O O	0.0000	37
O	2.035866153	4.054699350	12.569619001	CORE	38 O O	0.0000	38
O	0.395771543	1.522201228	12.728811575	CORE	39 O O	0.0000	39
O	-0.978043203	3.893880275	12.733085436	CORE	40 O O	0.0000	40
O	3.640477976	1.524589003	12.841634234	CORE	41 O O	0.0000	41
H	4.169126303	1.831911379	13.608479947	CORE	42 H H	0.0000	42

end
end

OH*+ H*

!BIOSYM archive 2

PBC=ON

Energy 21 -288 -288.075494

!DATE

PBC	5.9865	5.9865	25.4420	90.0000	90.0000	120.0000		
Cr	0.483075727	1.445643719	1.745021769	CORE	1 Cr Cr	0.0000	1	
Cr	-1.003874285	4.021195170	1.745347702	CORE	2 Cr Cr	0.0000	2	
Cr	3.495629343	1.445530063	1.745086294	CORE	3 Cr Cr	0.0000	3	
Cr	1.989518200	0.575986620	4.226757466	CORE	4 Cr Cr	0.0000	4	
Cr	-2.499933000	4.896568000	6.721013000	CORE	5 Cr Cr	0.0000	5	
Cr	0.493317500	4.896568000	6.721013000	CORE	6 Cr Cr	0.0000	6	
Cr	1.989943000	2.304338000	6.721013000	CORE	7 Cr Cr	0.0000	7	
Cr	1.991887190	4.030033551	9.145895252	CORE	8 Cr Cr	0.0000	8	
Cr	5.051135940	0.614712133	11.581377017	CORE	9 Cr Cr	0.0000	9	
Cr	3.563437314	3.189313030	11.579692624	CORE	10 Cr Cr	0.0000	10	
Cr	0.486605115	3.151954766	11.637185430	CORE	11 Cr Cr	0.0000	11	
Zn	1.989970302	4.032100570	0.468351256	CORE	12 Zn Zn	0.0000	12	
Zn	1.988991510	4.032232440	3.598948815	CORE	13 Zn Zn	0.0000	13	
Zn	-1.004044243	2.304080562	4.801781643	CORE	14 Zn Zn	0.0000	14	
Zn	-1.000655861	2.304444370	8.460019868	CORE	15 Zn Zn	0.0000	15	
Zn	2.037028436	0.595434722	9.709569394	CORE	16 Zn Zn	0.0000	16	
Zn	1.923234274	0.520083366	12.895337000	CORE	17 Zn Zn	0.0000	17	
O	3.584409558	3.111377956	0.784888695	CORE	18 O O	0.0000	18	
O	4.982908771	0.688973317	0.785318969	CORE	19 O O	0.0000	19	
O	0.395159045	3.111619965	0.785598880	CORE	20 O O	0.0000	20	
O	1.989361130	0.575927231	0.828510048	CORE	21 O O	0.0000	21	
O	-1.004166373	2.304093747	2.860107801	CORE	22 O O	0.0000	22	
O	-2.354816486	4.981239530	2.993542334	CORE	23 O O	0.0000	23	
O	1.988734374	2.135411187	2.993238214	CORE	24 O O	0.0000	24	
O	0.347026819	4.980529053	2.993358532	CORE	25 O O	0.0000	25	
O	3.351662000	1.362373000	5.553988000	CORE	26 O O	0.0000	26	
O	-1.003367000	4.188267000	5.553988000	CORE	27 O O	0.0000	27	
O	0.628163500	1.362373000	5.553988000	CORE	28 O O	0.0000	28	
O	1.989883000	4.032526000	5.664153000	CORE	29 O O	0.0000	29	
O	1.989913000	0.576201000	7.777874000	CORE	30 O O	0.0000	30	
O	4.983162000	0.420459800	7.888038000	CORE	31 O O	0.0000	31	
O	0.628163500	3.246302000	7.888038000	CORE	32 O O	0.0000	32	
O	3.351662000	3.246302000	7.888038000	CORE	33 O O	0.0000	33	
O	-2.606088685	4.823932061	10.450099541	CORE	34 O O	0.0000	34	
O	2.026904192	2.462400555	10.488874397	CORE	35 O O	0.0000	35	
O	0.653262209	4.836045918	10.494002174	CORE	36 O O	0.0000	36	
O	-0.972755126	2.310132684	10.548358176	CORE	37 O O	0.0000	37	
O	2.034738272	4.045216765	12.679074610	CORE	38 O O	0.0000	38	
O	0.371520881	1.520729430	12.746751391	CORE	39 O O	0.0000	39	
O	-0.985218705	3.860248233	12.751398678	CORE	40 O O	0.0000	40	
O	3.636021377	1.514211421	12.823072195	CORE	41 O O	0.0000	41	
H	4.187037229	1.835609321	13.569617030	CORE	42 H H	0.0000	42	
H	2.058537852	4.056318052	13.650351601	CORE	43 H H	0.0000	43	

end
end

OH* + H* + CO*

!BIOSYM archive 2

PBC=ON

Energy 22 -303 -303.155057

!DATE

PBC	5.9865	5.9865	25.4420	90.0000	90.0000	120.0000		
Cr	0.483943564	1.446071507	1.759309404	CORE	1 Cr Cr	0.0000	1	
Cr	-1.001764481	4.019393120	1.759284729	CORE	2 Cr Cr	0.0000	2	
Cr	3.498631829	1.445721481	1.759398887	CORE	3 Cr Cr	0.0000	3	
Cr	1.990515801	0.575949864	4.240311310	CORE	4 Cr Cr	0.0000	4	
Cr	-2.499933000	4.896568000	6.721013000	CORE	5 Cr Cr	0.0000	5	
Cr	0.493317500	4.896568000	6.721013000	CORE	6 Cr Cr	0.0000	6	
Cr	1.989943000	2.304338000	6.721013000	CORE	7 Cr Cr	0.0000	7	
Cr	1.985967040	4.031393940	9.153640972	CORE	8 Cr Cr	0.0000	8	
Cr	5.038937994	0.617054568	11.576932465	CORE	9 Cr Cr	0.0000	9	
Cr	3.549218925	3.197673784	11.577733600	CORE	10 Cr Cr	0.0000	10	
Cr	0.472028351	3.156658473	11.636309305	CORE	11 Cr Cr	0.0000	11	
Zn	1.992130432	4.031476524	0.484768339	CORE	12 Zn Zn	0.0000	12	
Zn	1.991130831	4.031995697	3.626568287	CORE	13 Zn Zn	0.0000	13	
Zn	-1.003437313	2.303468697	4.828239621	CORE	14 Zn Zn	0.0000	14	
Zn	-1.002860707	2.306498905	8.476194412	CORE	15 Zn Zn	0.0000	15	
Zn	2.024234695	0.598755488	9.740288782	CORE	16 Zn Zn	0.0000	16	
Zn	1.904131350	0.527017521	13.231691524	CORE	17 Zn Zn	0.0000	17	
O	3.587537799	3.110600636	0.797807241	CORE	18 O O	0.0000	18	
O	4.984917916	0.689136296	0.798757451	CORE	19 O O	0.0000	19	
O	0.396341644	3.111283057	0.799178827	CORE	20 O O	0.0000	20	
O	1.991457131	0.575176576	0.847214667	CORE	21 O O	0.0000	21	
O	-1.002388582	2.303709732	2.869948574	CORE	22 O O	0.0000	22	
O	-2.353874019	4.980346511	2.995099738	CORE	23 O O	0.0000	23	
O	1.990718185	2.136437866	2.995185530	CORE	24 O O	0.0000	24	
O	0.349599517	4.979749289	2.995738145	CORE	25 O O	0.0000	25	
O	3.351662000	1.362373000	5.553988000	CORE	26 O O	0.0000	26	
O	-1.003367000	4.188267000	5.553988000	CORE	27 O O	0.0000	27	
O	0.628163500	1.362373000	5.553988000	CORE	28 O O	0.0000	28	
O	1.989883000	4.032526000	5.664153000	CORE	29 O O	0.0000	29	
O	1.989913000	0.576201000	7.777874000	CORE	30 O O	0.0000	30	
O	4.983162000	0.420459800	7.888038000	CORE	31 O O	0.0000	31	
O	0.628163500	3.246302000	7.888038000	CORE	32 O O	0.0000	32	
O	3.351662000	3.246302000	7.888038000	CORE	33 O O	0.0000	33	
O	-2.623208463	4.825853843	10.441601187	CORE	34 O O	0.0000	34	
O	2.014532760	2.473804317	10.477412229	CORE	35 O O	0.0000	35	
O	0.649846171	4.834272540	10.477489530	CORE	36 O O	0.0000	36	

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O -0.987773282 2.314337911 10.545519263 CORE 37 O O 0.0000 37
O 2.019568095 4.051786804 12.671982328 CORE 38 O O 0.0000 38
O 0.367021668 1.510698065 12.725734468 CORE 39 O O 0.0000 39
O -1.005816597 3.887816926 12.726170322 CORE 40 O O 0.0000 40
O 3.622054383 1.519950468 12.808208040 CORE 41 O O 0.0000 41
H 4.213700667 1.862029046 13.515995876 CORE 42 H H 0.0000 42
H 2.043596931 4.072899346 13.642514154 CORE 43 H H 0.0000 43
O 1.317698771 0.176199238 16.363499067 CORE 44 O O 0.0000 44
C 1.848769337 0.480353369 15.385962997 CORE 45 C C 0.0000 45
end
end

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TS CH₂O* + H* + CO* to CH₃CO* + OH*

!BIOSYM archive 2

PBC=ON

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Energy 23 -312 -312.935976
!DATE
PBC 5.9865 5.9865 25.4420 90.0000 90.0000 120.0000
Cr 0.531441763 1.405537835 1.793816762 CORE 1 Cr Cr 0.0000 1
Cr 3.549244208 1.405532112 1.793913919 CORE 2 Cr Cr 0.0000 2
Cr -0.952972062 3.977311751 1.794870339 CORE 3 Cr Cr 0.0000 3
Cr 2.043422783 0.533843754 4.276905941 CORE 4 Cr Cr 0.0000 4
Cr -2.433584059 4.846527728 6.734802594 CORE 5 Cr Cr 0.0000 5
Cr 0.558420749 4.846475794 6.734141134 CORE 6 Cr Cr 0.0000 6
Cr 2.055728133 2.253322375 6.733624000 CORE 7 Cr Cr 0.0000 7
Cr 2.073048901 3.966637604 9.183088249 CORE 8 Cr Cr 0.0000 8
Cr 5.117438543 0.483901118 11.636537723 CORE 9 Cr Cr 0.0000 9
Cr 3.603169138 3.138012483 11.630975027 CORE 10 Cr Cr 0.0000 10
Cr 0.608840186 3.103343186 11.675906677 CORE 11 Cr Cr 0.0000 11
Zn 2.039247545 3.989662756 0.506796025 CORE 12 Zn Zn 0.0000 12
Zn 2.042271329 3.990726134 3.683914453 CORE 13 Zn Zn 0.0000 13
Zn -0.947239646 2.260113356 4.893768180 CORE 14 Zn Zn 0.0000 14
Zn -0.925699880 2.244323744 8.590208837 CORE 15 Zn Zn 0.0000 15
Zn 2.102213415 0.523558903 9.786004555 CORE 16 Zn Zn 0.0000 16
Zn 2.097984991 0.365965302 13.385250067 CORE 17 Zn Zn 0.0000 17
O 3.635645289 3.068821619 0.832887629 CORE 18 O O 0.0000 18
O 5.033933058 0.648238737 0.833367443 CORE 19 O O 0.0000 19
O 0.443836626 3.067756210 0.831781000 CORE 20 O O 0.0000 20
O 2.040196313 0.534668741 0.887205971 CORE 21 O O 0.0000 21
O -0.952834026 2.262692711 2.897987902 CORE 22 O O 0.0000 22
O -2.305399226 4.939668695 3.007253317 CORE 23 O O 0.0000 23
O 2.039764294 2.096451006 3.006342490 CORE 24 O O 0.0000 24
O 0.402094336 4.937418480 3.005432502 CORE 25 O O 0.0000 25
O 3.406761437 1.309657057 5.564165476 CORE 26 O O 0.0000 26
O -0.940470149 4.151068479 5.562816904 CORE 27 O O 0.0000 27
O 0.684870502 1.317553073 5.574952855 CORE 28 O O 0.0000 28
O 2.053662853 3.984019874 5.684175282 CORE 29 O O 0.0000 29
O 2.059209220 0.524724583 7.786320653 CORE 30 O O 0.0000 30
O 5.050378905 0.355394815 7.910833839 CORE 31 O O 0.0000 31
O 0.704614011 3.198620799 7.911317091 CORE 32 O O 0.0000 32
O 3.429234789 3.188059970 7.895950152 CORE 33 O O 0.0000 33
O -2.533027653 4.749771938 10.440984765 CORE 34 O O 0.0000 34
O 0.732346342 4.758333715 10.475335277 CORE 35 O O 0.0000 35
O 2.105835663 2.400284732 10.467017454 CORE 36 O O 0.0000 36
O -0.895391140 2.225194105 10.590719719 CORE 37 O O 0.0000 37
O 2.116215322 3.972432527 12.610701365 CORE 38 O O 0.0000 38
O -0.880737693 3.818245847 12.704367260 CORE 39 O O 0.0000 39
O 0.497650499 1.427822612 12.718343220 CORE 40 O O 0.0000 40
O 3.713758408 1.427813706 12.844481816 CORE 41 O O 0.0000 41
O 2.468417635 0.331611748 16.716936072 CORE 42 O O 0.0000 42
C 0.766683389 1.297363941 14.548195242 CORE 43 C C 0.0000 43
C 1.530441601 0.873705250 16.308478881 CORE 44 C C 0.0000 44
H 4.230198695 1.811810281 13.583334229 CORE 45 H H 0.0000 45
H 0.756363219 2.370353221 14.747254521 CORE 46 H H 0.0000 46
H -0.173481380 0.792419131 14.796436074 CORE 47 H H 0.0000 47
end
end

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TS CH₂O* + H* to CH₃O*

!BIOSYM archive 2

PBC=ON

```

Energy 24 0 -298.175330
!DATE
PBC 5.9865 5.9865 25.4420 90.0000 90.0000 120.0000
Cr 3.498732145 1.425880831 1.777278571 CORE 1 Cr Cr 0.0000 1
Cr -1.002567732 3.999423248 1.777819793 CORE 2 Cr Cr 0.0000 2
Cr 0.483009007 1.425967426 1.775258950 CORE 3 Cr Cr 0.0000 3
Cr 1.993090135 0.560501908 4.268753413 CORE 4 Cr Cr 0.0000 4
Cr -2.518379529 4.845870892 6.741906195 CORE 5 Cr Cr 0.0000 5
Cr 0.474851086 4.884228429 6.721544283 CORE 6 Cr Cr 0.0000 6
Cr 2.004730590 2.311177882 6.722520206 CORE 7 Cr Cr 0.0000 7
Cr 1.997025456 4.058920463 9.155599103 CORE 8 Cr Cr 0.0000 8
Cr 3.498487267 3.251578712 11.648828350 CORE 9 Cr Cr 0.0000 9
Cr 4.993773188 0.594241645 11.590209855 CORE 10 Cr Cr 0.0000 10
Cr 0.505926840 3.246054145 11.641237161 CORE 11 Cr Cr 0.0000 11
Zn 1.987518519 4.010712173 0.491271342 CORE 12 Zn Zn 0.0000 12
Zn 1.993571876 4.014314012 3.644229211 CORE 13 Zn Zn 0.0000 13
Zn -0.973184738 2.278018353 4.856345227 CORE 14 Zn Zn 0.0000 14
Zn -0.994055914 2.327417950 8.573178925 CORE 15 Zn Zn 0.0000 15
Zn 1.995317778 0.637543260 9.739192167 CORE 16 Zn Zn 0.0000 16
Zn 2.114172734 0.509536300 13.063874245 CORE 17 Zn Zn 0.0000 17
O 4.983357877 0.668793535 0.815663290 CORE 18 O O 0.0000 18
O 0.392486780 3.089642235 0.812546847 CORE 19 O O 0.0000 19
O 3.584101293 3.091559148 0.818350817 CORE 20 O O 0.0000 20
O 1.991125093 0.555218634 0.868046136 CORE 21 O O 0.0000 21
O -0.999423229 2.283022795 2.878575114 CORE 22 O O 0.0000 22
O -2.351236719 4.962880680 3.002158694 CORE 23 O O 0.0000 23
O 1.989875434 2.116402633 2.998436198 CORE 24 O O 0.0000 24
O 0.348626215 4.959553309 2.998944381 CORE 25 O O 0.0000 25
O 3.376060895 1.381575396 5.550293402 CORE 26 O O 0.0000 26
O -1.020662618 4.151659962 5.567756406 CORE 27 O O 0.0000 27
O 0.647120223 1.346674640 5.568820298 CORE 28 O O 0.0000 28
O 1.975314857 4.034756673 5.658228017 CORE 29 O O 0.0000 29
O 2.034055860 0.587649785 7.786812783 CORE 30 O O 0.0000 30
O 0.530033335 0.470746497 7.877284394 CORE 31 O O 0.0000 31
O 0.638800418 3.240779603 7.894747418 CORE 32 O O 0.0000 32
O 3.362281090 3.275680359 7.876220521 CORE 33 O O 0.0000 33
O -2.626965844 4.867356195 10.439972180 CORE 34 O O 0.0000 34
O 0.635744759 4.866808667 10.447394787 CORE 35 O O 0.0000 35
O 2.002244951 2.493571153 10.476125819 CORE 36 O O 0.0000 36
O -0.989759800 2.341234336 10.588093101 CORE 37 O O 0.0000 37
O 1.993915727 4.106623337 12.610725038 CORE 38 O O 0.0000 38
O 3.645455893 1.586840735 12.860881232 CORE 39 O O 0.0000 39
O -0.989808940 3.906147840 12.739747152 CORE 40 O O 0.0000 40
O 0.426906082 1.513799626 12.849797920 CORE 41 O O 0.0000 41
C -0.105967540 1.586424558 14.177454567 CORE 42 C C 0.0000 42
H 4.346505223 1.729167844 13.672981240 CORE 43 H H 0.0000 43
O 0.344102416 2.425263008 14.739392298 CORE 44 H H 0.0000 44
H -0.066476621 0.587004314 14.654747083 CORE 45 H H 0.0000 45
end
end

```

TS CH₂O* + CO* to CH₃CO* + O*

Cr	1.994074213	4.022862149	9.157602064	CORE	8	Cr	Cr	0.0000	8
Cr	3.445919800	3.134026655	11.662545409	CORE	9	Cr	Cr	0.0000	9
Cr	4.922151303	0.533946846	11.632889302	CORE	10	Cr	Cr	0.0000	10
Cr	0.475444486	3.167241195	11.590050798	CORE	11	Cr	Cr	0.0000	11
Zn	1.990481569	4.033616524	0.495318122	CORE	12	Zn	Zn	0.0000	12
Zn	1.988203294	4.035119179	3.646822114	CORE	13	Zn	Zn	0.0000	13
Zn	-1.003852448	2.306063591	4.853556352	CORE	14	Zn	Zn	0.0000	14
Zn	-1.005079127	2.301468977	8.568031356	CORE	15	Zn	Zn	0.0000	15
Zn	1.949821441	0.566450956	9.732073609	CORE	16	Zn	Zn	0.0000	16
Zn	2.118493144	0.465087667	12.923624127	CORE	17	Zn	Zn	0.0000	17
O	4.982775606	0.692301480	0.812136438	CORE	18	O	O	0.0000	18
O	0.393863195	3.112905978	0.812301826	CORE	19	O	O	0.0000	19
O	3.585968214	3.112349530	0.810981017	CORE	20	O	O	0.0000	20
O	1.988500788	0.578289628	0.863765236	CORE	21	O	O	0.0000	21
O	-1.004835069	2.306300336	2.878706687	CORE	22	O	O	0.0000	22
O	-2.356979872	4.983434426	2.996313513	CORE	23	O	O	0.0000	23
O	1.987158890	2.138740821	2.997085745	CORE	24	O	O	0.0000	24
O	0.346755404	4.982316811	2.997035232	CORE	25	O	O	0.0000	25
O	3.351662000	1.362373000	5.553988000	CORE	26	O	O	0.0000	26
O	-1.003367000	4.188267000	5.553988000	CORE	27	O	O	0.0000	27
O	0.628163500	1.362373000	5.553988000	CORE	28	O	O	0.0000	28
O	1.989883000	4.032526000	5.664153000	CORE	29	O	O	0.0000	29
O	1.989913000	0.576201000	7.777874000	CORE	30	O	O	0.0000	30
O	4.983162000	0.420459800	7.888038000	CORE	31	O	O	0.0000	31
O	0.628163500	3.246302000	7.888038000	CORE	32	O	O	0.0000	32
O	3.351662000	3.246302000	7.888038000	CORE	33	O	O	0.0000	33
O	-2.643218958	4.809998548	10.486336558	CORE	34	O	O	0.0000	34
O	0.601161055	4.799664022	10.442345909	CORE	35	O	O	0.0000	35
O	1.964817370	2.438619535	10.449325831	CORE	36	O	O	0.0000	36
O	-1.019765331	2.270581252	10.580937614	CORE	37	O	O	0.0000	37
O	1.928974367	3.998637732	12.629128404	CORE	38	O	O	0.0000	38
O	3.611633979	1.498821750	12.749815969	CORE	39	O	O	0.0000	39
O	-1.025266512	3.813057043	12.795415005	CORE	40	O	O	0.0000	40
O	0.385640674	1.467935815	12.874159250	CORE	41	O	O	0.0000	41
C	-0.053497394	1.892798507	14.167855270	CORE	42	C	C	0.0000	42
H	5.213908870	1.188762650	14.623737299	CORE	43	H	H	0.0000	43
H	-0.636024704	2.924491759	13.891223591	CORE	44	H	H	0.0000	44
O	0.984774803	2.193350045	15.084212509	CORE	45	C	C	0.0000	45
O	1.451896998	2.617521669	16.072091761	CORE	46	O	O	0.0000	46

end
end

TS CHO* + H* to CH₃O*

BIOSYM archive 2									
PBC=ON									
Energy		28	-293	-293.604122					
!DATE									
PBC	5.9865	5.9865	25.4420	90.0000	90.0000	120.0000			
Cr	3.529749507	1.461078691	1.741901915	CORE	1	Cr	Cr	0.0000	1
Cr	-0.970106871	4.035923303	1.742246806	CORE	2	Cr	Cr	0.0000	2
Cr	0.515975164	1.461630575	1.740600127	CORE	3	Cr	Cr	0.0000	3
Cr	2.021367585	0.590961904	4.231974331	CORE	4	Cr	Cr	0.0000	4
Cr	-2.510246467	4.875922742	6.696249894	CORE	5	Cr	Cr	0.0000	5
Cr	0.483842325	4.907354982	6.690771372	CORE	6	Cr	Cr	0.0000	6
Cr	1.999138079	2.316078131	6.667205070	CORE	7	Cr	Cr	0.0000	7
Cr	1.993267037	4.073908919	9.118097213	CORE	8	Cr	Cr	0.0000	8
Cr	3.438077940	3.160726192	11.564413972	CORE	9	Cr	Cr	0.0000	9
Cr	4.953284285	0.566991311	11.631341063	CORE	10	Cr	Cr	0.0000	10
Cr	0.505664049	3.176975512	11.583690489	CORE	11	Cr	Cr	0.0000	11
Zn	2.024696419	4.048397136	0.445556775	CORE	12	Zn	Zn	0.0000	12
Zn	2.022592766	4.048838531	3.593723464	CORE	13	Zn	Zn	0.0000	13
Zn	-0.968101033	2.305587945	4.805658033	CORE	14	Zn	Zn	0.0000	14
Zn	-0.992327070	2.342664777	8.526129357	CORE	15	Zn	Zn	0.0000	15
Zn	1.972584820	0.584616120	9.698878176	CORE	16	Zn	Zn	0.0000	16
Zn	1.993618895	0.693139317	13.014777037	CORE	17	Zn	Zn	0.0000	17
O	5.016305560	0.703744676	0.782405079	CORE	18	O	O	0.0000	18
O	0.430675020	3.128333280	0.784110335	CORE	19	O	O	0.0000	19
O	3.616972749	3.127272367	0.783624318	CORE	20	O	O	0.0000	20
O	2.023250187	0.591301084	0.830578569	CORE	21	O	O	0.0000	21
O	-0.969632664	2.317811781	2.848563278	CORE	22	O	O	0.0000	22
O	-2.321021730	4.997710803	2.976879858	CORE	23	O	O	0.0000	23
O	2.022568750	2.149499124	2.979712814	CORE	24	O	O	0.0000	24
O	0.378756116	4.997413125	2.978887539	CORE	25	O	O	0.0000	25
O	3.377548424	1.397072046	5.533961078	CORE	26	O	O	0.0000	26
O	-1.008248662	4.178121140	5.529529286	CORE	27	O	O	0.0000	27
O	0.653286913	1.368472479	5.538945875	CORE	28	O	O	0.0000	28
O	1.987694429	4.054234658	5.634904363	CORE	29	O	O	0.0000	29
O	2.028197463	0.605869643	7.763914245	CORE	30	O	O	0.0000	30
O	5.024140554	0.481983161	7.869289323	CORE	31	O	O	0.0000	31
O	0.638373950	3.262980710	7.864857703	CORE	32	O	O	0.0000	32
O	3.362635461	3.291580277	7.859872906	CORE	33	O	O	0.0000	33
O	-2.626874292	4.851148688	10.458283051	CORE	34	O	O	0.0000	34
O	0.615428188	4.825776477	10.434790599	CORE	35	O	O	0.0000	35
O	1.960825977	2.470533970	10.411343448	CORE	36	O	O	0.0000	36
O	-0.984145221	2.303744470	10.574061002	CORE	37	O	O	0.0000	37
O	1.965918706	4.012568746	12.589166637	CORE	38	O	O	0.0000	38
O	3.568704017	1.537202614	12.650733275	CORE	39	O	O	0.0000	39
O	-1.042022786	3.940752291	12.764534553	CORE	40	O	O	0.0000	40
O	0.813485989	0.975679173	14.616704095	CORE	41	O	O	0.0000	41
C	0.031912563	1.418051679	13.729896470	CORE	42	C	C	0.0000	42
H	-0.928679952	1.844078165	14.114386696	CORE	43	H	H	0.0000	43
H	-1.169372790	3.501543884	13.629838137	CORE	44	H	H	0.0000	44
end									
end									

end
end

TS CHO* + H* + CO* to CHOCO* + H*

BIOSYM archive 2									
PBC=ON									
Energy		29	-308	-308.796138					
!DATE									
PBC	5.9865	5.9865	25.4420	90.0000	90.0000	120.0000			
Cr	3.498337387	1.447807342	1.766473869	CORE	1	Cr	Cr	0.0000	1
Cr	-1.002241731	4.020775573	1.765713980	CORE	2	Cr	Cr	0.0000	2
Cr	0.482439764	1.448442566	1.765207134	CORE	3	Cr	Cr	0.0000	3
Cr	1.989406000	0.576300300	4.248523000	CORE	4	Cr	Cr	0.0000	4
Cr	-2.499933000	4.896568000	6.721013000	CORE	5	Cr	Cr	0.0000	5
Cr	0.493317500	4.896568000	6.721013000	CORE	6	Cr	Cr	0.0000	6
Cr	1.989601719	2.301615400	6.693909655	CORE	7	Cr	Cr	0.0000	7
Cr	1.993303341	4.027489138	9.141358305	CORE	8	Cr	Cr	0.0000	8
Cr	3.448480420	3.161192430	11.622853288	CORE	9	Cr	Cr	0.0000	9
Cr	4.942211810	0.558294831	11.599779268	CORE	10	Cr	Cr	0.0000	10
Cr	0.532562221	3.166683140	11.595639242	CORE	11	Cr	Cr	0.0000	11
Zn	1.992485156	4.033504047	0.479734388	CORE	12	Zn	Zn	0.0000	12
Zn	1.990514134	4.034682805	3.636340894	CORE	13	Zn	Zn	0.0000	13
Zn	-1.003197782	2.306698859	4.842821439	CORE	14	Zn	Zn	0.0000	14
Zn	-1.002193608	2.307630618	8.549019512	CORE	15	Zn	Zn	0.0000	15
Zn	1.965281386	0.558219573	9.746125659	CORE	16	Zn	Zn	0.0000	16
Zn	2.708032087	0.365672094	13.788231050	CORE	17	Zn	Zn	0.0000	17
O	4.984496571	0.690791014	0.806554220	CORE	18	O	O	0.0000	18
O	0.396924793	3.113084125	0.806851781	CORE	19	O	O	0.0000	19
O	3.586772200	3.112414560	0.805716395	CORE	20	O	O	0.0000	20
O	1.990560320	0.577600669	0.857668998	CORE	21	O	O	0.0000	21
O	-1.002864384	2.305630652	2.874372877	CORE	22	O	O	0.0000	22

O	-2.354954046	4.982317783	2.993834362	CORE	23	O	O	0.0000	23
O	1.989374058	2.138017879	2.995306639	CORE	24	O	O	0.0000	24
O	0.348800866	4.981437082	2.994898982	CORE	25	O	O	0.0000	25
O	3.351662000	1.362373000	5.553988000	CORE	26	O	O	0.0000	26
O	-1.003367000	4.188267000	5.553988000	CORE	27	O	O	0.0000	27
O	0.628163500	1.362373000	5.553988000	CORE	28	O	O	0.0000	28
O	1.989883000	4.032526000	5.664153000	CORE	29	O	O	0.0000	29
O	1.989913000	0.576201000	7.777874000	CORE	30	O	O	0.0000	30
O	4.983162000	0.420459800	7.888038000	CORE	31	O	O	0.0000	31
O	0.628163500	3.246302000	7.888038000	CORE	32	O	O	0.0000	32
O	3.351662000	3.246302000	7.888038000	CORE	33	O	O	0.0000	33
O	-2.641278261	4.809253002	10.45539867	CORE	34	O	O	0.0000	34
O	0.605954898	4.791765225	10.446320380	CORE	35	O	O	0.0000	35
O	1.991147381	2.454301389	10.445462924	CORE	36	O	O	0.0000	36
O	-0.990925021	2.311037637	10.587116609	CORE	37	O	O	0.0000	37
O	1.955779612	4.038366785	12.613976384	CORE	38	O	O	0.0000	38
O	3.664746128	1.531257501	12.738142725	CORE	39	O	O	0.0000	39
O	-0.958530300	3.889268793	12.800806237	CORE	40	O	O	0.0000	40
O	0.408997642	1.402967733	12.836463181	CORE	41	O	O	0.0000	41
O	0.448044391	1.194870156	14.106052457	CORE	42	C	C	0.0000	42
H	5.493997789	0.747235263	14.525297894	CORE	43	H	H	0.0000	43
H	-1.136965328	3.182056569	13.539598572	CORE	44	H	H	0.0000	44
C	1.948921661	0.534883243	15.55722517	CORE	45	C	C	0.0000	45
O	1.492668392	0.570677365	16.629921015	CORE	46	O	O	0.0000	46

end
end

TS CO* + H* + H* to CHO* + H*

!BIOSYM archive 2

PBC=ON

	Energy		30	-293	-293.751260				
!DATE									
PBC	5.9865	5.9865	25.4420	90.0000	90.0000	120.0000			
Cr	3.499619927	1.457052917		1.787925813	CORE	1	Cr	Cr	0.0000 1
Cr	-1.001153606	4.031193979		1.788612359	CORE	2	Cr	Cr	0.0000 2
Cr	0.483756067	1.457541078		1.787046483	CORE	3	Cr	Cr	0.0000 3
Cr	1.990844942	0.589179378		4.270937630	CORE	4	Cr	Cr	0.0000 4
Cr	-2.500184788	4.910326509		6.747397443	CORE	5	Cr	Cr	0.0000 5
Cr	0.493204915	4.910344595		6.748032103	CORE	6	Cr	Cr	0.0000 6
Cr	1.989969144	2.318023127		6.749985100	CORE	7	Cr	Cr	0.0000 7
Cr	1.990931177	4.055127407		9.178766609	CORE	8	Cr	Cr	0.0000 8
Cr	3.470722486	3.176624495		11.654039385	CORE	9	Cr	Cr	0.0000 9
Cr	4.905379185	0.615222118		11.602495057	CORE	10	Cr	Cr	0.0000 10
Cr	0.495924641	3.177459315		11.650228130	CORE	11	Cr	Cr	0.0000 11
Zn	1.993522963	4.040544885		0.495693224	CORE	12	Zn	Zn	0.0000 12
Zn	1.991495307	4.044774765		3.652302041	CORE	13	Zn	Zn	0.0000 13
Zn	-1.002658835	2.316387462		4.858562861	CORE	14	Zn	Zn	0.0000 14
Zn	-1.000962641	2.322008189		8.546143603	CORE	15	Zn	Zn	0.0000 15
Zn	1.964296804	0.603733522		9.761401546	CORE	16	Zn	Zn	0.0000 16
Zn	1.709784068	0.93666905		13.027253505	CORE	17	Zn	Zn	0.0000 17
O	4.985545244	0.697418112		0.830409307	CORE	18	O	O	0.0000 18
O	0.398200854	3.122175887		0.829129966	CORE	19	O	O	0.0000 19
O	3.587666848	3.121457810		0.827908640	CORE	20	O	O	0.0000 20
O	1.991846037	0.587163458		0.878854583	CORE	21	O	O	0.0000 21
O	-1.001642508	2.315349093		2.897723471	CORE	22	O	O	0.0000 22
O	-2.352968144	4.993030227		3.021764765	CORE	23	O	O	0.0000 23
O	1.990976185	2.148239389		3.021043116	CORE	24	O	O	0.0000 24
O	0.349349907	4.992364167		3.022654525	CORE	25	O	O	0.0000 25
O	3.352062571	1.375322021		5.583784216	CORE	26	O	O	0.0000 26
O	-1.003245408	4.201298889		5.581077711	CORE	27	O	O	0.0000 27
O	0.628437148	1.375305566		5.583206752	CORE	28	O	O	0.0000 28
O	1.990121519	4.045636616		5.691980113	CORE	29	O	O	0.0000 29
O	1.989726966	0.590461483		7.807990036	CORE	30	O	O	0.0000 30
O	4.983093893	0.434799211		7.918892437	CORE	31	O	O	0.0000 31
O	0.627815848	3.260724234		7.916185971	CORE	32	O	O	0.0000 32
O	3.351441272	3.260740689		7.916763436	CORE	33	O	O	0.0000 33
O	-2.638599015	4.858052980		10.497228379	CORE	34	O	O	0.0000 34
O	0.608025707	4.839301293		10.463482043	CORE	35	O	O	0.0000 35
O	1.980200560	2.492213783		10.486347679	CORE	36	O	O	0.0000 36
O	-0.989208705	2.336096344		10.614003439	CORE	37	O	O	0.0000 37
O	1.995506020	4.085627492		12.692300863	CORE	38	O	O	0.0000 38
O	3.521853013	1.514216011		12.706541371	CORE	39	O	O	0.0000 39
O	-1.000685095	3.952826477		12.836815365	CORE	40	O	O	0.0000 40
O	-0.220035187	1.158231807		15.356922568	CORE	41	O	O	0.0000 41
C	0.004284469	0.496917127		14.400924091	CORE	42	C	C	0.0000 42
H	2.427000104	4.675157363		13.778188707	CORE	43	H	H	0.0000 43
H	-1.047678753	3.482096758		13.692223346	CORE	44	H	H	0.0000 44

end
end

TS OH* + H* + CO* to H* + COOH*

!BIOSYM archive 2

PBC=ON

	Energy		31	-302	-302.756477				
!DATE									
PBC	5.9865	5.9865	25.4420	90.0000	90.0000	120.0000			
Cr	0.481969539	1.449034596		1.748079717	CORE	1	Cr	Cr	0.0000 1
Cr	-1.004842567	4.023822691		1.746497568	CORE	2	Cr	Cr	0.0000 2
Cr	3.494598712	1.449063317		1.747930130	CORE	3	Cr	Cr	0.0000 3
Cr	1.989493000	0.576381200		4.230292000	CORE	4	Cr	Cr	0.0000 4
Cr	-2.499933000	4.896568000		6.721013000	CORE	5	Cr	Cr	0.0000 5
Cr	0.493317500	4.896568000		6.721013000	CORE	6	Cr	Cr	0.0000 6
Cr	1.990040850	2.298644722		6.672719094	CORE	7	Cr	Cr	0.0000 7
Cr	1.987046670	4.024962865		9.128875769	CORE	8	Cr	Cr	0.0000 8
Cr	5.008695228	0.597861968		11.566813930	CORE	9	Cr	Cr	0.0000 9
Cr	3.535063638	3.184300138		11.580922058	CORE	10	Cr	Cr	0.0000 10
Cr	0.462620966	3.152141793		11.603494930	CORE	11	Cr	Cr	0.0000 11
Zn	1.988310195	4.037515198		0.460079481	CORE	12	Zn	Zn	0.0000 12
Zn	1.988521884	4.036906100		3.602059922	CORE	13	Zn	Zn	0.0000 13
Zn	-1.003667850	2.308453109		4.804647761	CORE	14	Zn	Zn	0.0000 14
Zn	-1.004369212	2.306504884		8.449131435	CORE	15	Zn	Zn	0.0000 15
Zn	2.008575508	0.594006229		9.727568738	CORE	16	Zn	Zn	0.0000 16
Zn	2.042197791	0.410984163		13.375989105	CORE	17	Zn	Zn	0.0000 17
O	3.581602754	3.116343713		0.790232682	CORE	18	O	O	0.0000 18
O	4.981889066	0.692935364		0.788214244	CORE	19	O	O	0.0000 19
O	0.395527637	3.116089300		0.790704169	CORE	20	O	O	0.0000 20
O	1.988267899	0.579289857		0.833093240	CORE	21	O	O	0.0000 21
O	-1.005131769	2.206834155		2.861208858	CORE	22	O	O	0.0000 22
O	-2.354698886	4.984579831		2.994178933	CORE	23	O	O	0.0000 23
O	1.987859261	2.137396682		2.996925187	CORE	24	O	O	0.0000 24
O	0.345816971	4.983636110		2.993615502	CORE	25	O	O	0.0000 25
O	3.351662000	1.362373000		5.553988000	CORE	26	O	O	0.0000 26
O	-1.003367000	4.188267000		5.553988000	CORE	27	O	O	0.0000 27
O	0.628163500	1.362373000		5.553988000	CORE	28	O	O	0.0000 28
O	1.989883000	4.032526000		5.664153000	CORE	29	O	O	0.0000 29
O	1.989913000	0.576201000		7.777874000	CORE	30	O	O	0.0000 30
O	4.983162000	0.420459800		7.888038000	CORE	31	O	O	0.0000 31
O	0.628163500	3.246302000		7.888038000	CORE	32	O	O	0.0000 32
O	3.351662000	3.246302000		7.888038000	CORE	33	O	O	0.0000 33
O	-2.636538548	4.813889351		10.448277907	CORE	34	O	O	0.0000 34
O	2.008733668	2.467548720		10.470277306	CORE	35	O	O	0.0000 35
O	0.636961567	4.820800501		10.469981975	CORE	36	O	O	0.0000 36
O	-1.006123655	2.297088197		10.542945243	CORE	37	O	O	0.0000 37

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O      2.003480956    4.033302063    12.673672689 CORE   38   O   O   0.0000   38
O      0.405712311    1.469637725    12.695740437 CORE   39   O   O   0.0000   39
O     -0.992066759    3.848808949    12.721220245 CORE   40   O   O   0.0000   40
O      3.620602821    1.493836552    12.844225155 CORE   41   O   O   0.0000   41
H      4.165621723    1.835461215    13.590847346 CORE   42   H   H   0.0000   42
H      2.032331015    4.023892750    13.645906275 CORE   43   H   H   0.0000   43
O     -0.372043206    1.549921572    15.082946234 CORE   44   O   O   0.0000   44
C      0.571750016    1.257714159    14.435499723 CORE   45   C   C   0.0000   45
end
end

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Completed surface

!BIOSYM archive 2

PBC=ON

Energy 32 -271 -271.237914

!DATE

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PBC      5.9865    5.9865    25.4420    90.0000    90.0000    120.0000
Cr      3.498011840    1.446760399    1.765329078 CORE   1   Cr Cr  0.0000   1
Cr     -1.002793578    4.019743460    1.765310716 CORE   2   Cr Cr  0.0000   2
Cr      0.481816589    1.447238429    1.764436840 CORE   3   Cr Cr  0.0000   3
Cr      1.990029880    0.576404612    4.247460184 CORE   4   Cr Cr  0.0000   4
Cr     -2.499933000    4.896568000    6.721013000 CORE   5   Cr Cr  0.0000   5
Cr      0.493317500    4.896568000    6.721013000 CORE   6   Cr Cr  0.0000   6
Cr      1.989943000    2.304338000    6.721013000 CORE   7   Cr Cr  0.0000   7
Cr      1.991222980    4.033352802    9.151160420 CORE   8   Cr Cr  0.0000   8
Cr      3.415444458    3.214271078    11.703477859 CORE   9   Cr Cr  0.0000   9
Cr      4.877943590    0.596005567    11.570379343 CORE  10   Cr Cr  0.0000  10
Cr      0.427063942    3.255722006    11.571806738 CORE  11   Cr Cr  0.0000  11
Zn      1.991045836    4.032129621    0.480216742 CORE  12   Zn Zn  0.0000  12
Zn      1.990811126    4.032771539    3.637418035 CORE  13   Zn Zn  0.0000  13
Zn     -1.002884028    2.304384171    4.843515932 CORE  14   Zn Zn  0.0000  14
Zn     -1.007687060    2.307216451    8.551464017 CORE  15   Zn Zn  0.0000  15
Zn      1.906478611    0.628374086    9.737402555 CORE  16   Zn Zn  0.0000  16
Zn      2.563921595    0.248888118    13.240001274 CORE  17   Zn Zn  0.0000  17
O       4.983674625    0.689801453    0.805510918 CORE  18   O   O   0.0000  18
O       0.395516100    3.111671101    0.805392545 CORE  19   O   O   0.0000  19
O       3.585861931    3.111413497    0.805275011 CORE  20   O   O   0.0000  20
O       1.990057931    0.576427793    0.856530449 CORE  21   O   O   0.0000  21
O     -1.003400759    2.304652255    2.873803317 CORE  22   O   O   0.0000  22
O     -2.355028617    4.981283213    2.993160228 CORE  23   O   O   0.0000  23
O       1.989260366    2.137082526    2.993200251 CORE  24   O   O   0.0000  24
O       0.349103539    4.980254469    2.993873414 CORE  25   O   O   0.0000  25
O       3.351662000    1.362373000    5.553988000 CORE  26   O   O   0.0000  26
O     -1.003367000    4.188267000    5.553988000 CORE  27   O   O   0.0000  27
O       0.628163500    1.362373000    5.553988000 CORE  28   O   O   0.0000  28
O       1.989883000    4.032526000    5.664153000 CORE  29   O   O   0.0000  29
O       1.989913000    0.576201000    7.777874000 CORE  30   O   O   0.0000  30
O       4.983162000    0.420459800    7.888038000 CORE  31   O   O   0.0000  31
O       0.628163500    3.246302000    7.888038000 CORE  32   O   O   0.0000  32
O       3.351662000    3.246302000    7.888038000 CORE  33   O   O   0.0000  33
O     -2.673115946    4.854286589    10.481543595 CORE  34   O   O   0.0000  34
O       0.581125704    4.849516318    10.394900328 CORE  35   O   O   0.0000  35
O       1.943569918    2.480625359    10.482818771 CORE  36   O   O   0.0000  36
O     -1.045761605    2.333250770    10.588152192 CORE  37   O   O   0.0000  37
O       1.876277476    4.102665769    12.617171230 CORE  38   O   O   0.0000  38
O       3.667434100    1.580287439    12.801859283 CORE  39   O   O   0.0000  39
O     -1.030113651    3.812074754    12.804009017 CORE  40   O   O   0.0000  40
end
end

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➤ SAPO-34 surface

TS CH₃CH₂CO* to HS + C₂H₄* + CO*

!BIOSYM archive 2

PBC=ON

	Energy		0	-284	-284.291646				
!DATE									
PBC	9.3040	9.3040	9.3040	94.5972	94.5972	94.5972			
Al	2.353654000	8.064435000	0.968225600	CORE	1	Al	Al	0.0000	1
P	5.378220168	8.233684169	0.958793555	CORE	2	P	P	0.0000	2
Si	7.449683829	0.795847672	6.010161408	CORE	3	Si	Si	0.0000	3
Al	7.853212126	0.814894836	2.980626259	CORE	4	Al	Al	0.0000	4
P	0.039694036	7.916560320	3.204253205	CORE	5	P	P	0.0000	5
Al	7.677390018	6.167327823	1.243880899	CORE	6	Al	Al	0.0000	6
Al	-0.373087212	7.918367025	6.227962880	CORE	7	Al	Al	0.0000	7
Al	-0.173064549	2.518016193	7.952720158	CORE	8	Al	Al	0.0000	8
P	2.073265003	0.450186783	8.339972554	CORE	9	P	P	0.0000	9
P	-0.024426407	5.548168502	8.214782254	CORE	10	P	P	0.0000	10
Al	5.132253448	0.620295659	8.279047404	CORE	11	Al	Al	0.0000	11
O	1.196852801	6.199631988	8.883418305	CORE	12	O	O	0.0000	12
O	6.278052536	2.501092384	0.408378541	CORE	13	O	O	0.0000	13
O	7.844339779	2.550401946	9.141487314	CORE	14	O	O	0.0000	14
O	2.975131891	0.451076542	0.408555528	CORE	15	O	O	0.0000	15
O	6.256978621	7.013140838	0.676356397	CORE	16	O	O	0.0000	16
O	4.005677941	7.738697241	1.458818992	CORE	17	O	O	0.0000	17
O	7.152273332	4.527689197	1.577331421	CORE	18	O	O	0.0000	18
O	8.134938796	2.304179950	2.105202250	CORE	19	O	O	0.0000	19
O	1.318224990	7.849069846	2.361075883	CORE	20	O	O	0.0000	20
O	6.006173135	9.084377281	2.057878783	CORE	21	O	O	0.0000	21
O	8.344949223	6.837894966	2.728639332	CORE	22	O	O	0.0000	22
O	0.136664328	0.033388631	3.062975010	CORE	23	O	O	0.0000	23
O	7.035526273	1.181890158	4.464175120	CORE	24	O	O	0.0000	24
O	0.425777858	7.652856923	4.660616300	CORE	25	O	O	0.0000	25
O	7.359785082	8.580590337	6.014048278	CORE	26	O	O	0.0000	26
O	8.571274056	1.868534570	6.480232289	CORE	27	O	O	0.0000	27
O	1.471502403	-0.409289437	7.228863540	CORE	28	O	O	0.0000	28
O	6.109272189	0.872260488	6.907840174	CORE	29	O	O	0.0000	29
O	-0.488192791	6.344748403	7.000339171	CORE	30	O	O	0.0000	30
O	0.398014232	4.160852625	7.750434544	CORE	31	O	O	0.0000	31
O	3.447217914	0.954177999	7.872187857	CORE	32	O	O	0.0000	32
O	1.179656072	1.645800105	8.661870644	CORE	33	O	O	0.0000	33
O	4.467599386	8.229740003	8.902183459	CORE	34	O	O	0.0000	34
O	-1.169013387	5.476496583	9.232052997	CORE	35	O	O	0.0000	35
P	7.543085144	3.159452100	0.985349363	CORE	36	P	P	0.0000	36
O	5.272184468	6.126174736	6.087392578	CORE	37	O	O	0.0000	37
C	5.163545123	5.264591033	5.353688862	CORE	38	C	C	0.0000	38
H	3.896589334	1.789375655	5.124850799	CORE	39	H	H	0.0000	39
C	3.954640371	3.627683785	4.051949009	CORE	40	C	C	0.0000	40
H	4.268718234	4.154818631	3.153819927	CORE	41	H	H	0.0000	41
H	3.153002108	4.084936738	4.625373266	CORE	42	H	H	0.0000	42
C	4.369904473	2.292046968	4.285283015	CORE	43	C	C	0.0000	43
H	4.250055274	1.755958427	3.322866967	CORE	44	H	H	0.0000	44
H	5.501235699	2.131502550	4.352108383	CORE	45	H	H	0.0000	45
end									
end									

TS CH₃CH₂CO* to HS + CH₂CH₂CO*

!BIOSYM archive 2

PBC=ON

	Energy		1	-284	-284.384351				
!DATE									
PBC	9.3040	9.3040	9.3040	94.5972	94.5972	94.5972			
Al	2.353654000	8.064435000	0.968225600	CORE	1	Al	Al	0.0000	1
P	5.352820641	8.230075954	0.988616451	CORE	2	P	P	0.0000	2
Si	7.403265698	0.816895058	6.027694422	CORE	3	Si	Si	0.0000	3
Al	7.790604028	0.824240751	2.998132236	CORE	4	Al	Al	0.0000	4
P	0.009861904	7.943801513	3.207068916	CORE	5	P	P	0.0000	5
Al	7.662616924	6.171873773	1.252004690	CORE	6	Al	Al	0.0000	6
Al	-0.417731172	7.934818606	6.195577994	CORE	7	Al	Al	0.0000	7
Al	-0.197469402	2.543099933	7.943356514	CORE	8	Al	Al	0.0000	8
P	2.038572173	0.457205195	8.312309716	CORE	9	P	P	0.0000	9
P	-0.061670869	5.569036913	8.211006325	CORE	10	P	P	0.0000	10
Al	5.085486183	0.619617943	8.295229538	CORE	11	Al	Al	0.0000	11
O	1.167981721	6.198419193	8.886851814	CORE	12	O	O	0.0000	12
O	6.246914052	2.523213679	0.394503781	CORE	13	O	O	0.0000	13
O	7.836117102	2.524663828	9.153889291	CORE	14	O	O	0.0000	14
O	2.955677885	0.442568415	0.367042552	CORE	15	O	O	0.0000	15
O	6.251891646	7.033598755	0.691830729	CORE	16	O	O	0.0000	16
O	3.985430631	7.707705751	1.467282352	CORE	17	O	O	0.0000	17
O	7.140798559	4.532185297	1.575665780	CORE	18	O	O	0.0000	18
O	8.072580741	2.299450096	2.116672163	CORE	19	O	O	0.0000	19
O	1.273361981	7.930992607	2.343524293	CORE	20	O	O	0.0000	20
O	5.944764804	9.073448640	2.117044621	CORE	21	O	O	0.0000	21
O	8.331744179	6.858065205	2.721625044	CORE	22	O	O	0.0000	22
O	0.063865095	0.049853320	3.124207768	CORE	23	O	O	0.0000	23
O	6.903729576	1.281571246	4.476922985	CORE	24	O	O	0.0000	24
O	0.414726089	7.651468961	4.653082139	CORE	25	O	O	0.0000	25
O	7.331679837	8.627271233	5.885863906	CORE	26	O	O	0.0000	26
O	8.515213457	1.894100174	6.475072470	CORE	27	O	O	0.0000	27
O	1.406185877	-0.375462180	7.198753437	CORE	28	O	O	0.0000	28
O	6.076640603	0.847778024	6.926201015	CORE	29	O	O	0.0000	29
O	-0.550986933	6.39086545	7.029311277	CORE	30	O	O	0.0000	30
O	0.348690443	4.189796977	7.706200411	CORE	31	O	O	0.0000	31
O	3.417551078	0.945736421	7.836524016	CORE	32	O	O	0.0000	32
O	1.162970040	1.666860677	8.637186070	CORE	33	O	O	0.0000	33
O	4.444677508	8.246186578	8.946189899	CORE	34	O	O	0.0000	34
O	-1.190775664	5.461894892	9.238527474	CORE	35	O	O	0.0000	35
P	7.515099800	3.163294010	0.982629600	CORE	36	P	P	0.0000	36
O	6.310511227	4.387875534	5.212989663	CORE	37	O	O	0.0000	37
C	5.278056137	4.012676382	4.819036239	CORE	38	C	C	0.0000	38
H	4.089580640	1.798226762	5.120809967	CORE	39	H	H	0.0000	39
C	3.931401519	3.892637911	4.434982675	CORE	40	C	C	0.0000	40
H	3.691724949	4.371928514	3.483933098	CORE	41	H	H	0.0000	41
H	3.183673320	4.097013479	5.204477311	CORE	42	H	H	0.0000	42
C	4.505879685	2.415901057	4.328303143	CORE	43	C	C	0.0000	43
H	4.349765237	2.035363706	3.319339880	CORE	44	H	H	0.0000	44
H	5.857983609	1.975885857	4.431953167	CORE	45	H	H	0.0000	45
end									
end									

TS CH₃CO* to HS CH₃CO*

!BIOSYM archive 2

PBC=ON

	Energy		2	-268	-268.446750				
!DATE									
PBC	9.3040	9.3040	9.3040	94.5972	94.5972	94.5972			
Al	2.353654000	8.064435000	0.968225600	CORE	1	Al	Al	0.0000	1
P	5.354133667	8.231901826	0.899667111	CORE	2	P	P	0.0000	2
Si	7.366096323	0.808743526	5.966554328	CORE	3	Si	Si	0.0000	3
Al	7.779224973	0.825026443	2.974421585	CORE	4	Al	Al	0.0000	4
P	-0.016771453	7.942539964	3.168255227	CORE	5	P	P	0.0000	5
Al	7.625750698	6.172795737	1.186894248	CORE	6	Al	Al	0.0000	6

Al	-0.400094982	7.922487557	6.199789682	CORE	7	Al	Al	0.0000	7
Al	-0.251493370	2.522245996	7.906303215	CORE	8	Al	Al	0.0000	8
P	2.047107777	0.447741621	8.265746485	CORE	9	P	P	0.0000	9
P	-0.031589481	5.538106744	8.210968239	CORE	10	P	P	0.0000	10
Al	5.090270150	0.620000535	8.265933209	CORE	11	Al	Al	0.0000	11
O	1.186427018	6.146865252	8.925473470	CORE	12	O	O	0.0000	12
O	6.268494394	2.473774084	0.397317036	CORE	13	O	O	0.0000	13
O	7.834478120	2.525913668	9.158492451	CORE	14	O	O	0.0000	14
O	2.947759194	0.424141855	0.314433472	CORE	15	O	O	0.0000	15
O	6.201515194	6.996541970	0.589220810	CORE	16	O	O	0.0000	16
O	3.997832627	7.768104453	1.471642389	CORE	17	O	O	0.0000	17
S	7.104655517	4.538285595	5.323239096	CORE	18	O	O	0.0000	18
O	8.084557259	2.339846285	2.144093733	CORE	19	O	O	0.0000	19
O	1.277848405	7.928099216	2.343252885	CORE	20	O	O	0.0000	20
O	6.050267153	9.086903249	1.943430822	CORE	21	O	O	0.0000	21
O	8.302946526	6.878106737	2.645931528	CORE	22	O	O	0.0000	22
O	0.078157229	0.062301238	3.086626662	CORE	23	O	O	0.0000	23
O	6.909684556	1.123898479	4.429497408	CORE	24	O	O	0.0000	24
O	0.353137313	7.623831346	4.617806988	CORE	25	O	O	0.0000	25
O	7.344899648	8.627089673	6.069687656	CORE	26	O	O	0.0000	26
O	8.438952377	1.949471606	6.419685696	CORE	27	O	O	0.0000	27
O	1.540589634	-0.396410409	7.094129408	CORE	28	O	O	0.0000	28
O	6.015727704	0.891064644	6.863041065	CORE	29	O	O	0.0000	29
O	-0.458991820	6.371832979	7.011442453	CORE	30	O	O	0.0000	30
O	0.376921776	4.151217018	7.721408377	CORE	31	O	O	0.0000	31
O	3.413470289	1.036875048	7.855723419	CORE	32	O	O	0.0000	32
O	1.091594168	1.595982742	8.567418341	CORE	33	O	O	0.0000	33
O	4.384844109	8.215368882	8.841090126	CORE	34	O	O	0.0000	34
O	-1.203507220	5.455037434	9.192020989	CORE	35	O	O	0.0000	35
P	7.512828604	3.158363938	0.988169006	CORE	36	P	P	0.0000	36
O	2.618670813	1.354227071	4.368327399	CORE	37	O	O	0.0000	37
C	3.329858590	2.177857056	4.678915484	CORE	38	C	C	0.0000	38
H	5.246714803	2.834213995	4.856823914	CORE	39	H	H	0.0000	39
C	4.224008110	3.224507131	5.020073821	CORE	40	C	C	0.0000	40
H	4.007996055	4.086076579	4.373764087	CORE	41	H	H	0.0000	41
H	4.061731205	3.474257208	6.076553563	CORE	42	H	H	0.0000	42
end									
end									

TS CH₃OH₂⁺ to CH₃S H₂O⁺

!BIOSYM archive 2

PBC=ON

DATE	Energy		-266		-266.609484					
PBC	9.3040	9.3040	9.3040	94.5972	94.5972	94.5972				
Al	2.353654000	8.064435000	0.968225600	CORE	1	Al	Al	0.0000	1	
P	5.325444183	8.235894135	1.142422492	CORE	2	P	P	0.0000	2	
Si	7.446154914	0.676590391	6.151292565	CORE	3	Si	Si	0.0000	3	
Al	7.749766577	0.806628210	3.125216411	CORE	4	Al	Al	0.0000	4	
P	0.033090148	8.037779593	3.190140345	CORE	5	P	P	0.0000	5	
Al	7.679413199	6.257905644	1.227938094	CORE	6	Al	Al	0.0000	6	
Al	-0.269847541	7.897539688	6.196341558	CORE	7	Al	Al	0.0000	7	
Al	-0.177083806	2.493765945	8.146476843	CORE	8	Al	Al	0.0000	8	
P	2.131361672	0.460984305	8.307358285	CORE	9	P	P	0.0000	9	
P	-0.018187087	5.529968344	8.209073700	CORE	10	P	P	0.0000	10	
Al	5.141692424	0.647005528	8.373722976	CORE	11	Al	Al	0.0000	11	
O	1.179574983	6.138186158	8.950921014	CORE	12	O	O	0.0000	12	
O	6.369610653	2.745031878	0.230371855	CORE	13	O	O	0.0000	13	
O	8.832592004	3.325930410	0.306932788	CORE	14	O	O	0.0000	14	
O	3.090752004	0.422278654	0.322966234	CORE	15	O	O	0.0000	15	
O	6.245783990	7.098927122	0.705489915	CORE	16	O	O	0.0000	16	
O	3.957709570	7.663954608	1.537408397	CORE	17	O	O	0.0000	17	
O	7.174527976	4.636505788	1.627639512	CORE	18	O	O	0.0000	18	
O	7.751087866	2.322590135	2.283364017	CORE	19	O	O	0.0000	19	
O	1.279337000	8.064708718	2.318595895	CORE	20	O	O	0.0000	20	
O	5.908885749	8.955307907	2.355444541	CORE	21	O	O	0.0000	21	
O	8.373649035	6.952648256	2.679393686	CORE	22	O	O	0.0000	22	
O	0.080081345	0.139737741	3.135375332	CORE	23	O	O	0.0000	23	
O	7.003848667	1.188642246	4.641524357	CORE	24	O	O	0.0000	24	
O	0.483158482	7.710044746	4.612831867	CORE	25	O	O	0.0000	25	
O	7.457885313	8.534032309	6.014187498	CORE	26	O	O	0.0000	26	
O	8.412812670	1.803746316	6.771892049	CORE	27	O	O	0.0000	27	
O	1.549588829	-0.359920873	7.161638274	CORE	28	O	O	0.0000	28	
O	6.074509314	0.535641526	6.969322111	CORE	29	O	O	0.0000	29	
O	-0.326130555	6.320152231	6.945589266	CORE	30	O	O	0.0000	30	
O	0.367195658	4.116437492	7.794601949	CORE	31	O	O	0.0000	31	
O	3.490809939	1.033013741	7.823117896	CORE	32	O	O	0.0000	32	
O	1.251504631	1.638888978	8.685305707	CORE	33	O	O	0.0000	33	
O	4.414799139	8.387239374	9.205934752	CORE	34	O	O	0.0000	34	
O	-1.244765497	5.530872192	9.131842160	CORE	35	O	O	0.0000	35	
P	7.533310581	3.246256981	1.098299767	CORE	36	P	P	0.0000	36	
H	2.953630237	3.298592938	5.253079371	CORE	37	H	H	0.0000	37	
O	3.167419403	2.351734982	5.225736631	CORE	38	O	O	0.0000	38	
S	3.183922679	2.034568146	6.158907374	CORE	39	H	H	0.0000	39	
C	4.981974084	1.921924912	4.682368582	CORE	40	C	C	0.0000	40	
H	5.423452886	2.719942707	5.251001580	CORE	41	H	H	0.0000	41	
H	4.850122195	2.057079965	3.616351940	CORE	42	H	H	0.0000	42	
H	4.837082869	0.949919329	5.108849473	CORE	43	H	H	0.0000	43	
end										
end										

TS CH₃OHCH₃⁺ to HS + CH₃OCH₃⁺

!BIOSYM archive 2

PBC=ON

DATE	9.3040		9.3040		9.3040		94.5972		94.5972		94.5972							
PBC	9.3040	9.3040	9.3040	94.5972	94.5972	94.5972												
Al	2.353654000	8.064435000	0.968225600	CORE	1	Al	Al	0.0000	1									
P	5.375223603	8.240280116	0.849061427	CORE	2	P	P	0.0000	2									
Si	7.373517583	0.795400388	5.925066353	CORE	3	Si	Si	0.0000	3									
Al	7.836208938	0.819621286	2.917894583	CORE	4	Al	Al	0.0000	4									
P	0.002679380	7.925715242	3.156638372	CORE	5	P	P	0.0000	5									
Al	7.636207536	6.172644128	1.163266147	CORE	6	Al	Al	0.0000	6									
Al	-0.431031199	7.903780092	6.206739833	CORE	7	Al	Al	0.0000	7									
Al	-0.245957805	2.502526752	7.862013835	CORE	8	Al	Al	0.0000	8									
P	2.020779273	0.432885914	8.298031646	CORE	9	P	P	0.0000	9									
O	-0.008832826	5.522431600	8.199054289	CORE	10	P	P	0.0000	10									
Al	5.088869411	0.623566801	8.213942971	CORE	11	Al	Al	0.0000	11									
O	1.203835727	6.152824161	8.909420175	CORE	12	O	O	0.0000	12									
O	6.234795994	2.466442921	0.383116817	CORE	13	O	O	0.0000	13									
O	7.781604629	2.521871318	9.061615230	CORE	14	O	O	0.0000	14									
O	2.920406071	0.438726321	0.372536537	CORE	15	O	O	0.0000	15									
O	6.210669144	6.991001098	0.557622001	CORE	16	O	O	0.0000	16									
O	4.017638990	7.790573207	1.438784081	CORE	17	O	O	0.0000	17									
O	7.104842091	4.532362162	1.489969955	CORE	18	O	O	0.0000	18									
O	8.114776687	2.335509495	2.069087955	CORE	19	O	O	0.0000	19									
O	1.317311772	7.839629733	2.362486615	CORE	20	O	O	0.0000	20									
O	6.086885044	9.103932463	1.876914951	CORE	21	O	O	0.0000	21									
O	8.303793081	6.84729829	2.633083299	CORE	22	O	O	0.0000	22									
O	0.140953466	0.060582587	3.012350657	CORE	23	O	O	0.0000	23									
O	6.955785367	1.074312901	4.370440058	CORE	24	O	O	0.0000	24									
O	0.331532245	7.636439511	4.621020740	CORE	25	O	O	0.0000	25									
O	7.306948925	8.590574088	6.077150418	CORE	26	O	O	0.0000	26									

H	5.443311817	4.546250399	5.061735293	CORE	39	H	H	0.0000	39
C	6.183959690	3.753155897	5.192461556	CORE	40	C	C	0.0000	40
H	7.190131225	4.139305160	5.003904876	CORE	41	H	H	0.0000	41
H	6.129124696	3.350491476	6.199343591	CORE	42	H	H	0.0000	42
H	2.463479330	0.721077324	4.588326531	CORE	43	H	H	0.0000	43
H	4.090472768	-0.000395006	4.376673257	CORE	44	H	H	0.0000	44
C	3.498049990	0.918408674	4.311627708	CORE	45	C	C	0.0000	45
H	3.525652706	1.305044592	3.293084683	CORE	46	H	H	0.0000	46
O	4.039534511	1.942431314	5.167116501	CORE	47	O	O	0.0000	47
H	4.208071459	1.537137566	6.032654543	CORE	48	H	H	0.0000	48
end									
end									

TS CHOS + CH₃OH* to HS + HCOOCH₃*

!BIOSYM archive 2

PBC=ON

Energy	7	-281	-281.222012						
!DATE									
PBC	9.3040	9.3040	9.3040	94.5972	94.5972	94.5972			
Al	2.353654000	8.064435000	0.968225600	CORE	1	Al	Al	0.0000	1
P	5.406409712	8.118869340	0.935533281	CORE	2	P	P	0.0000	2
Si	7.457346928	0.750022227	5.989549557	CORE	3	Si	Si	0.0000	3
Al	7.866146388	0.727747176	2.956720895	CORE	4	Al	Al	0.0000	4
P	0.042029649	7.852107524	3.207032624	CORE	5	P	P	0.0000	5
Al	7.674967645	6.068365702	1.228894517	CORE	6	Al	Al	0.0000	6
Al	-0.335202344	7.852220053	6.194942564	CORE	7	Al	Al	0.0000	7
Al	-0.139053626	2.493286818	7.862821199	CORE	8	Al	Al	0.0000	8
P	2.129533573	0.394875111	8.230343164	CORE	9	P	P	0.0000	9
P	-0.017879828	5.505444438	8.226401029	CORE	10	P	P	0.0000	10
Al	5.193660176	0.484328543	8.301840222	CORE	11	Al	Al	0.0000	11
O	1.192856796	6.136871494	8.929668693	CORE	12	O	O	0.0000	12
O	6.403535223	2.366131703	0.376260123	CORE	13	O	O	0.0000	13
O	7.967545575	2.396602072	9.134628148	CORE	14	O	O	0.0000	14
O	2.935729508	0.409029042	0.307782499	CORE	15	O	O	0.0000	15
O	6.191927041	6.832032078	0.688316365	CORE	16	O	O	0.0000	16
O	4.006960875	7.771655220	1.462955550	CORE	17	O	O	0.0000	17
O	7.246938024	4.409087667	1.534581761	CORE	18	O	O	0.0000	18
O	8.214730150	2.207233802	2.116517843	CORE	19	O	O	0.0000	19
O	1.314078448	7.879919289	2.358330929	CORE	20	O	O	0.0000	20
O	6.122062535	8.959841735	1.986240468	CORE	21	O	O	0.0000	21
O	8.350124739	6.811299915	2.666725331	CORE	22	O	O	0.0000	22
O	0.128610786	-0.026867372	3.198271815	CORE	23	O	O	0.0000	23
O	6.913776786	1.048188107	4.424844319	CORE	24	O	O	0.0000	24
O	0.428424532	7.488946425	4.640076367	CORE	25	O	O	0.0000	25
O	7.407615491	8.572408421	6.023801709	CORE	26	O	O	0.0000	26
O	8.507729098	1.904234753	6.386881600	CORE	27	O	O	0.0000	27
O	1.584372200	-0.455327840	7.082199286	CORE	28	O	O	0.0000	28
O	6.093146010	0.831801468	6.870838463	CORE	29	O	O	0.0000	29
O	-0.490729829	6.343559299	7.048558187	CORE	30	O	O	0.0000	30
O	0.415001066	4.140614106	7.703434582	CORE	31	O	O	0.0000	31
O	3.542017870	0.861801707	7.840541464	CORE	32	O	O	0.0000	32
O	1.259765355	1.622161373	8.454536815	CORE	33	O	O	0.0000	33
O	4.551982139	8.085210371	8.847494008	CORE	34	O	O	0.0000	34
O	-1.177582385	5.382512510	9.216059463	CORE	35	O	O	0.0000	35
P	7.647121209	3.044806260	0.969312924	CORE	36	P	P	0.0000	36
O	4.803160902	1.902557927	3.082858303	CORE	37	O	O	0.0000	37
C	5.033430879	1.495228747	4.152754185	CORE	38	C	C	0.0000	38
H	4.690091910	0.722289059	4.831606206	CORE	39	H	H	0.0000	39
H	5.257571840	2.411345256	6.256963373	CORE	40	H	H	0.0000	40
O	5.060343729	2.922633550	5.439964457	CORE	41	O	O	0.0000	41
C	3.818804978	3.684282003	5.560800936	CORE	42	C	C	0.0000	42
H	2.995088235	3.054307849	5.902957222	CORE	43	H	H	0.0000	43
H	3.991551389	4.497024924	6.269424110	CORE	44	H	H	0.0000	44
H	3.612124911	4.092277160	4.572934615	CORE	45	H	H	0.0000	45
end									
end									

TS HS + CH₃CH₂CO* to HS + C₂H₅* + CO*

!BIOSYM archive 2

PBC=ON

Energy	8	-283	-283.779165						
!DATE									
PBC	9.3040	9.3040	9.3040	94.5972	94.5972	94.5972			
Al	2.353654000	8.064435000	0.968225600	CORE	1	Al	Al	0.0000	1
P	5.394437126	8.186302937	1.014446131	CORE	2	P	P	0.0000	2
Si	7.502894142	0.772427796	6.092694302	CORE	3	Si	Si	0.0000	3
Al	7.894946422	0.746385431	2.958072156	CORE	4	Al	Al	0.0000	4
P	0.077499774	7.869829214	3.237069404	CORE	5	P	P	0.0000	5
Al	7.701953624	6.125173920	1.293962687	CORE	6	Al	Al	0.0000	6
Al	-0.344497206	7.895738591	6.210360186	CORE	7	Al	Al	0.0000	7
Al	-0.110431412	2.537265204	7.969655591	CORE	8	Al	Al	0.0000	8
P	2.097300959	0.438433316	8.328408977	CORE	9	P	P	0.0000	9
P	-0.044036007	5.561526922	8.228371524	CORE	10	P	P	0.0000	10
O	5.161142279	0.572600699	8.304032903	CORE	11	Al	Al	0.0000	11
O	1.187682322	6.213924744	8.872999320	CORE	12	O	O	0.0000	12
O	6.333518395	2.489701301	0.382375303	CORE	13	O	O	0.0000	13
O	7.934733466	2.477983706	9.184004740	CORE	14	O	O	0.0000	14
O	2.953627632	0.445719720	0.402106542	CORE	15	O	O	0.0000	15
O	6.271110019	6.965262706	0.755182165	CORE	16	O	O	0.0000	16
O	3.999874278	7.717000677	1.445464475	CORE	17	O	O	0.0000	17
O	7.223136829	4.476178423	1.600131723	CORE	18	O	O	0.0000	18
O	8.139859217	2.237849181	2.121016583	CORE	19	O	O	0.0000	19
O	1.325460796	7.833074059	2.359599720	CORE	20	O	O	0.0000	20
O	5.986537024	9.008998018	2.167208918	CORE	21	O	O	0.0000	21
O	8.373886518	6.803239879	2.768890394	CORE	22	O	O	0.0000	22
O	0.151933484	-0.010646924	3.143977520	CORE	23	O	O	0.0000	23
O	7.027939933	1.240592455	4.484981377	CORE	24	O	O	0.0000	24
O	0.493822510	7.589478775	4.680293667	CORE	25	O	O	0.0000	25
O	7.417655980	8.604621468	5.860583752	CORE	26	O	O	0.0000	26
O	-0.711327343	1.868506538	6.508043661	CORE	27	O	O	0.0000	27
O	1.429404810	-0.391824850	7.233342802	CORE	28	O	O	0.0000	28
O	6.151614464	0.797246781	6.928281498	CORE	29	O	O	0.0000	29
O	-0.560146867	6.378925425	7.050162020	CORE	30	O	O	0.0000	30
O	0.382770673	4.190387944	7.717769380	CORE	31	O	O	0.0000	31
O	3.494019860	0.850402459	7.850872746	CORE	32	O	O	0.0000	32
O	1.281473634	1.695666945	8.621533029	CORE	33	O	O	0.0000	33
O	4.572241822	8.212389016	8.970926761	CORE	34	O	O	0.0000	34
O	-0.408082621	6.254207483	0.037449117	CORE	35	O	O	0.0000	35
P	7.592030525	3.119493398	0.992298198	CORE	36	P	P	0.0000	36
O	5.585350402	4.959779600	5.309147018	CORE	37	O	O	0.0000	37
C	4.516408728	4.675108236	4.923910525	CORE	38	C	C	0.0000	38
H	3.892478185	1.972305793	5.146248587	CORE	39	H	H	0.0000	39
C	3.303802564	3.964525064	4.433878512	CORE	40	C	C	0.0000	40
H	2.974375092	4.461273796	3.512605460	CORE	41	H	H	0.0000	41
H	2.506513149	4.103226103	5.178189056	CORE	42	H	H	0.0000	42
C	3.954521434	2.654234397	4.310543423	CORE	43	C	C	0.0000	43
H	4.237036725	2.318834300	3.321879299	CORE	44	H	H	0.0000	44
H	6.250410234	1.845226840	4.429796049	CORE	45	H	H	0.0000	45
end									
end									

TS HS + CO* to CHOS

O	8.097444315	2.255633853	2.114555727	CORE	19	O	O	0.0000	19
O	1.271408800	7.868551494	2.328065174	CORE	20	O	O	0.0000	20
O	6.010044889	9.012737529	2.033366603	CORE	21	O	O	0.0000	21
O	8.314842553	6.810027823	2.690546226	CORE	22	O	O	0.0000	22
O	0.080986309	-0.005953878	3.119545132	CORE	23	O	O	0.0000	23
O	6.914039010	1.161072608	4.440954296	CORE	24	O	O	0.0000	24
O	0.410747680	7.563868260	4.629181220	CORE	25	O	O	0.0000	25
O	7.365204170	8.577527009	5.915231644	CORE	26	O	O	0.0000	26
O	8.482827150	1.888836449	6.429663010	CORE	27	O	O	0.0000	27
O	1.464180538	-0.446390905	7.168600587	CORE	28	O	O	0.0000	28
O	6.088970705	0.783095091	6.906660739	CORE	29	O	O	0.0000	29
O	-0.521625493	6.53138366	7.004428144	CORE	30	O	O	0.0000	30
O	0.374906754	4.142766639	7.727410044	CORE	31	O	O	0.0000	31
O	3.438122560	0.917322537	7.828814002	CORE	32	O	O	0.0000	32
O	1.158612934	1.612192876	8.573174028	CORE	33	O	O	0.0000	33
O	4.430724771	8.162853598	8.893963201	CORE	34	O	O	0.0000	34
O	-1.196120486	5.429864065	9.213366055	CORE	35	O	O	0.0000	35
P	7.534070135	3.096362687	0.966139089	CORE	36	P	P	0.0000	36
O	5.073386280	5.853311723	6.268860135	CORE	37	O	O	0.0000	37
C	4.572055194	5.272683602	5.401705658	CORE	38	C	C	0.0000	38
H	5.041262020	2.285239553	5.266610884	CORE	39	H	H	0.0000	39
C	4.089366979	4.498513984	4.409900596	CORE	40	C	C	0.0000	40
H	4.247019170	4.887325064	3.406023764	CORE	41	H	H	0.0000	41
C	3.122012382	4.044394969	4.612664448	CORE	42	H	H	0.0000	42
C	5.561082103	2.728224825	4.432877258	CORE	43	C	C	0.0000	43
H	5.234296848	2.510277175	3.427848396	CORE	44	H	H	0.0000	44
H	6.380316779	3.407760581	4.590286704	CORE	45	H	H	0.0000	45
end									
end									

TS CH₃S + CO* to CH₃CO*

!BIOSYM archive 2

PBC=ON

Energy 12 -267 -267.422516

!DATE

PBC	9.3040	9.3040	9.3040	94.5972	94.5972	94.5972			
Al	2.353654000	8.064435000	0.968225600	CORE	1	Al	Al	0.0000	1
P	5.392226981	8.195986859	0.947357239	CORE	2	P	P	0.0000	2
Si	7.461529624	0.765647625	6.001987917	CORE	3	Si	Si	0.0000	3
Al	7.878615101	0.771540419	2.974281921	CORE	4	Al	Al	0.0000	4
P	0.051912752	7.892245447	3.211279018	CORE	5	P	P	0.0000	5
Al	7.673901952	6.130379156	1.235358802	CORE	6	Al	Al	0.0000	6
Al	-0.342971535	7.881101017	6.214734427	CORE	7	Al	Al	0.0000	7
Al	-0.159759353	2.501191055	7.902759656	CORE	8	Al	Al	0.0000	8
P	2.104435569	0.430487597	8.286742684	CORE	9	P	P	0.0000	9
P	-0.018789232	5.523533962	8.225701097	CORE	10	P	P	0.0000	10
Al	5.164510219	0.573932127	8.287295219	CORE	11	Al	Al	0.0000	11
O	1.196800446	6.159186841	8.918895971	CORE	12	O	O	0.0000	12
O	6.332891443	2.429577757	0.422072354	CORE	13	O	O	0.0000	13
O	7.898580235	2.450917970	9.136042649	CORE	14	O	O	0.0000	14
O	2.962742235	0.435122417	0.361692238	CORE	15	O	O	0.0000	15
O	6.223324851	6.940895710	0.689004547	CORE	16	O	O	0.0000	16
O	4.007002447	7.783902997	1.474741295	CORE	17	O	O	0.0000	17
O	7.208521521	4.475569933	1.555988269	CORE	18	O	O	0.0000	18
O	8.177075373	2.272304898	2.133210422	CORE	19	O	O	0.0000	19
O	1.327126559	7.880120933	2.366217829	CORE	20	O	O	0.0000	20
O	6.068155892	9.048120523	2.019521775	CORE	21	O	O	0.0000	21
O	8.351419760	6.847179530	2.691612333	CORE	22	O	O	0.0000	22
O	0.158194468	0.023431729	3.145071013	CORE	23	O	O	0.0000	23
O	6.977254182	1.098507316	4.442079018	CORE	24	O	O	0.0000	24
O	0.437854920	7.570809456	4.652560600	CORE	25	O	O	0.0000	25
O	7.400593194	8.575196347	6.012848821	CORE	26	O	O	0.0000	26
O	8.552447098	1.885797073	6.418254446	CORE	27	O	O	0.0000	27
O	1.536387009	-0.425300161	7.155584638	CORE	28	O	O	0.0000	28
O	6.121219332	0.844618674	6.898742708	CORE	29	O	O	0.0000	29
O	-0.474930719	6.343630504	7.028195164	CORE	30	O	O	0.0000	30
O	0.399798617	4.145439998	7.736759437	CORE	31	O	O	0.0000	31
O	3.493902923	0.929259568	7.860254718	CORE	32	O	O	0.0000	32
O	1.210434104	1.630543433	8.570573242	CORE	33	O	O	0.0000	33
O	4.503438981	8.177932127	8.878480541	CORE	34	O	O	0.0000	34
O	-1.175550847	5.435216401	9.225887376	CORE	35	O	O	0.0000	35
P	7.596828019	3.103986733	0.984328628	CORE	36	P	P	0.0000	36
O	2.220877919	3.191801139	4.208614620	CORE	37	O	O	0.0000	37
C	3.219021474	2.662932854	4.098393904	CORE	38	C	C	0.0000	38
H	4.816745309	1.076016159	3.543781978	CORE	39	H	H	0.0000	39
C	5.038569383	1.893998862	4.212924289	CORE	40	C	C	0.0000	40
H	5.495495351	2.792585134	3.821230337	CORE	41	H	H	0.0000	41
H	4.943538577	1.749384794	5.281785277	CORE	42	H	H	0.0000	42
end									
end									

TS CH₃S + CH₃OH* to CH₃OHCH₃*

!BIOSYM archive 2

PBC=ON

Energy 13 -283 -283.744949

!DATE

PBC	9.3040	9.3040	9.3040	94.5972	94.5972	94.5972			
Al	2.353654000	8.064435000	0.968225600	CORE	1	Al	Al	0.0000	1
P	5.375328086	8.211439168	0.898068184	CORE	2	P	P	0.0000	2
Si	7.387870770	0.755890748	5.982190383	CORE	3	Si	Si	0.0000	3
Al	7.853661440	0.780879511	2.957371814	CORE	4	Al	Al	0.0000	4
P	0.015981018	7.908759497	3.189590112	CORE	5	P	P	0.0000	5
Al	7.624226807	6.149655950	1.183078104	CORE	6	Al	Al	0.0000	6
Al	-0.337955226	7.886083171	6.210706168	CORE	7	Al	Al	0.0000	7
Al	-0.245017192	2.496562830	7.846735961	CORE	8	Al	Al	0.0000	8
P	2.061389566	0.424217982	8.264047402	CORE	9	P	P	0.0000	9
P	-0.015669495	5.510285406	8.230024159	CORE	10	P	P	0.0000	10
Al	5.112848007	0.599324513	8.284500949	CORE	11	Al	Al	0.0000	11
O	1.201181673	6.104287967	8.963605501	CORE	12	O	O	0.0000	12
O	6.309581459	2.412699493	0.447559287	CORE	13	O	O	0.0000	13
O	7.858987617	2.444344625	9.131040612	CORE	14	O	O	0.0000	14
O	2.883472350	0.414660467	0.338456796	CORE	15	O	O	0.0000	15
O	6.158621287	6.927462821	0.618714954	CORE	16	O	O	0.0000	16
O	4.006073301	7.849425212	1.512496079	CORE	17	O	O	0.0000	17
O	7.175619991	4.497486301	1.530423676	CORE	18	O	O	0.0000	18
O	8.153729866	2.31380192	2.163793479	CORE	19	O	O	0.0000	19
O	1.316386030	7.921284241	2.375071426	CORE	20	O	O	0.0000	20
O	6.150955929	9.054616495	1.903464420	CORE	21	O	O	0.0000	21
O	8.305264088	6.906323439	2.621172412	CORE	22	O	O	0.0000	22
O	0.158881042	0.064486740	3.157999943	CORE	23	O	O	0.0000	23
O	6.878911021	0.973158782	4.403599363	CORE	24	O	O	0.0000	24
O	0.374611021	7.536531091	4.622897413	CORE	25	O	O	0.0000	25
O	7.413326643	8.608478962	6.066952180	CORE	26	O	O	0.0000	26
O	8.421016389	1.952464686	6.348929388	CORE	27	O	O	0.0000	27
O	1.617240602	-0.448190906	7.088237334	CORE	28	O	O	0.0000	28
O	6.059007028	0.815835381	6.886057252	CORE	29	O	O	0.0000	29
O	-0.427409663	6.351496957	7.034528434	CORE	30	O	O	0.0000	30
O	0.377058264	4.124969048	7.739005715	CORE	31	O	O	0.0000	31
O	3.439018098	1.009532087	7.944483776	CORE	32	O	O	0.0000	32
O	1.074998091	1.555406929	8.513229394	CORE	33	O	O	0.0000	33
O	4.421223183	8.180851307	8.833490334	CORE	34	O	O	0.0000	34
O	-1.199714757	5.443126409	9.199784976	CORE	35	O	O	0.0000	35
P	7.565375994	3.114466235	0.990689684	CORE	36	P	P	0.0000	36

O	2.897945023	1.838318773	3.920928887	CORE	37	O	O	0.0000	37
H	2.431634698	1.177259272	3.382773551	CORE	38	H	H	0.0000	38
C	2.603877849	3.170651469	3.384978172	CORE	39	C	C	0.0000	39
H	3.418908479	3.499865998	2.734941969	CORE	40	H	H	0.0000	40
H	2.498769873	3.838888930	4.239543839	CORE	41	H	H	0.0000	41
H	1.670554435	3.127728197	2.822996260	CORE	42	H	H	0.0000	42
H	5.042939751	1.672591547	3.090500025	CORE	43	H	H	0.0000	43
C	4.832279799	1.382730460	4.106961736	CORE	44	C	C	0.0000	44
H	4.907157569	2.093884853	4.908899127	CORE	45	H	H	0.0000	45
H	4.604382840	0.354143640	4.336155161	CORE	46	H	H	0.0000	46
end									
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CH₃CH₂CO* + CO*

!BIOSYM archive 2

PBC=ON

Energy 14 -299 -299.812043

!DATE

PBC	9.3040	9.3040	9.3040	94.5972	94.5972	94.5972			
Al	2.353654000	8.064435000	0.968225600	CORE	1	Al	Al	0.0000	1
P	5.394325152	8.030723536	1.149852412	CORE	2	P	P	0.0000	2
Si	7.512854398	0.647539869	6.132018834	CORE	3	Si	Si	0.0000	3
Al	7.749060176	0.569823015	3.123414209	CORE	4	Al	Al	0.0000	4
P	0.139960893	7.860843147	3.106931354	CORE	5	P	P	0.0000	5
Al	7.741152904	6.015301365	1.057836468	CORE	6	Al	Al	0.0000	6
Al	0.005938607	7.835211837	6.143385956	CORE	7	Al	Al	0.0000	7
Al	-0.089611077	2.396517579	8.051896487	CORE	8	Al	Al	0.0000	8
P	2.370195179	0.306654704	8.053287054	CORE	9	P	P	0.0000	9
P	-0.016465858	5.395532480	8.195585397	CORE	10	P	P	0.0000	10
Al	5.404477541	0.455824382	8.294573448	CORE	11	Al	Al	0.0000	11
O	1.673667953	6.764901616	0.020781086	CORE	12	O	O	0.0000	12
O	6.093533829	1.807441833	9.196975686	CORE	13	O	O	0.0000	13
O	-0.021270472	3.160029341	0.443821843	CORE	14	O	O	0.0000	14
O	2.963665358	0.310363975	0.125519323	CORE	15	O	O	0.0000	15
O	6.234817661	6.821516647	0.723667372	CORE	16	O	O	0.0000	16
O	3.962427188	7.537203515	1.391180799	CORE	17	O	O	0.0000	17
O	7.440867705	4.380359711	1.613070826	CORE	18	O	O	0.0000	18
O	7.902793177	1.985128649	2.126379435	CORE	19	O	O	0.0000	19
O	1.499978416	8.168334716	2.478093308	CORE	20	O	O	0.0000	20
O	5.951268242	8.604034812	2.451658746	CORE	21	O	O	0.0000	21
O	-0.600259101	6.787392641	2.298636460	CORE	22	O	O	0.0000	22
O	0.079713163	-0.120750760	3.172005900	CORE	23	O	O	0.0000	23
O	7.162230449	1.075599181	4.619484552	CORE	24	O	O	0.0000	24
O	0.426659532	7.293064233	4.507041343	CORE	25	O	O	0.0000	25
O	8.642253945	-0.523636238	6.196764403	CORE	26	O	O	0.0000	26
O	8.071898114	1.986895751	6.868233339	CORE	27	O	O	0.0000	27
O	1.428577614	8.646912234	6.841275194	CORE	28	O	O	0.0000	28
O	6.177068421	0.085199653	6.837019723	CORE	29	O	O	0.0000	29
O	-0.064842138	6.286524687	6.967772427	CORE	30	O	O	0.0000	30
O	0.542197041	4.033802347	7.746341725	CORE	31	O	O	0.0000	31
O	3.746834179	0.950047907	7.994708711	CORE	32	O	O	0.0000	32
O	1.346830098	1.423272796	8.038117195	CORE	33	O	O	0.0000	33
O	5.386865709	9.087513944	0.055832833	CORE	34	O	O	0.0000	34
O	7.875663729	5.223663314	8.772201334	CORE	35	O	O	0.0000	35
P	7.859077258	3.017878252	1.021874559	CORE	36	P	P	0.0000	36
O	5.657016110	4.249506241	5.212511400	CORE	37	O	O	0.0000	37
C	6.786507175	4.439234452	5.181528936	CORE	38	C	C	0.0000	38
H	0.367907131	4.508369459	3.906019490	CORE	39	H	H	0.0000	39
C	1.165703876	3.773815649	3.98960316	CORE	40	C	C	0.0000	40
H	1.656152005	3.622557650	3.027905022	CORE	41	H	H	0.0000	41
H	0.741175474	2.830379476	4.335396353	CORE	42	H	H	0.0000	42
H	3.005219507	3.471575577	5.210796744	CORE	43	H	H	0.0000	43
C	2.845236824	5.434468999	4.807433685	CORE	44	C	C	0.0000	44
O	3.398573231	6.400571803	4.586339885	CORE	45	O	O	0.0000	45
C	2.191559325	4.203358497	5.081484627	CORE	46	C	C	0.0000	46
H	1.692012090	4.322497475	6.063702116	CORE	47	H	H	0.0000	47
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CH₃CH₂CO*

!BIOSYM archive 2

PBC=ON

Energy 15 -285 -285.664306

!DATE

PBC	9.3040	9.3040	9.3040	94.5972	94.5972	94.5972			
Al	2.353654000	8.064435000	0.968225600	CORE	1	Al	Al	0.0000	1
P	5.372006189	8.138591759	0.863173964	CORE	2	P	P	0.0000	2
Si	7.412645786	0.705528466	5.958090811	CORE	3	Si	Si	0.0000	3
Al	7.841251992	0.718622111	2.925852071	CORE	4	Al	Al	0.0000	4
P	0.014669868	7.827817127	3.153859391	CORE	5	P	P	0.0000	5
Al	7.641314326	6.076117807	1.162262346	CORE	6	Al	Al	0.0000	6
Al	-0.388957590	7.819618907	6.218133776	CORE	7	Al	Al	0.0000	7
Al	-0.221875030	2.440407509	7.874743766	CORE	8	Al	Al	0.0000	8
P	2.066143748	8.680992977	8.274830885	CORE	9	P	P	0.0000	9
P	-0.003545671	5.466574721	8.201404324	CORE	10	P	P	0.0000	10
Al	5.113460138	0.530791616	8.226790616	CORE	11	Al	Al	0.0000	11
O	1.183274701	6.153896439	8.900300996	CORE	12	O	O	0.0000	12
O	6.278229184	2.369273910	0.380557424	CORE	13	O	O	0.0000	13
O	7.829691785	2.446839408	9.100803042	CORE	14	O	O	0.0000	14
O	2.960169598	0.421234009	0.378345074	CORE	15	O	O	0.0000	15
O	6.191202745	6.874487266	0.575705344	CORE	16	O	O	0.0000	16
O	4.007017222	7.701338215	1.453244147	CORE	17	O	O	0.0000	17
O	7.124615561	4.437203207	1.508738791	CORE	18	O	O	0.0000	18
O	8.129130935	2.237592665	2.091961378	CORE	19	O	O	0.0000	19
O	1.332536853	7.742853678	2.361999994	CORE	20	O	O	0.0000	20
O	6.102202506	8.989089494	1.884443682	CORE	21	O	O	0.0000	21
O	8.318240877	6.768674282	2.637112398	CORE	22	O	O	0.0000	22
O	0.149002637	-0.045254121	3.009482120	CORE	23	O	O	0.0000	23
O	7.014288124	0.929435922	4.401990236	CORE	24	O	O	0.0000	24
O	0.354896720	7.527547387	4.618993187	CORE	25	O	O	0.0000	25
O	7.349289660	8.503484691	6.152829010	CORE	26	O	O	0.0000	26
O	8.501224874	1.849075498	6.382226088	CORE	27	O	O	0.0000	27
O	1.541315202	-0.557549589	7.174807740	CORE	28	O	O	0.0000	28
O	6.071060174	0.825860566	6.857186551	CORE	29	O	O	0.0000	29
O	-0.426077835	6.219485870	6.943606089	CORE	30	O	O	0.0000	30
O	0.441997870	4.069051087	7.779609471	CORE	31	O	O	0.0000	31
O	3.432396289	0.910061091	7.837618744	CORE	32	O	O	0.0000	32
O	1.118194070	1.526267190	8.540031918	CORE	33	O	O	0.0000	33
O	4.403668081	8.105098197	8.792543805	CORE	34	O	O	0.0000	34
O	-1.191864622	5.404334558	9.167467255	CORE	35	O	O	0.0000	35
P	7.529643398	3.057489667	0.948617485	CORE	36	P	P	0.0000	36
O	3.714290036	6.669628483	5.516320023	CORE	37	O	O	0.0000	37
C	3.637304616	5.703411946	4.927802644	CORE	38	C	C	0.0000	38
H	4.044563719	3.198014313	6.028471725	CORE	39	H	H	0.0000	39
C	3.598870147	4.442918161	4.257281019	CORE	40	C	C	0.0000	40
H	3.985214112	4.617312569	3.240113455	CORE	41	H	H	0.0000	41
H	2.534987560	4.168088945	4.181954100	CORE	42	H	H	0.0000	42
C	4.432962089	3.359855959	5.023089222	CORE	43	C	C	0.0000	43
H	4.323002686	2.442784741	4.444065669	CORE	44	H	H	0.0000	44
H	5.488967395	3.626811498	5.054655049	CORE	45	H	H	0.0000	45
end									
end									

CH₃CO*

'BIOSYM archive 2

PBC=ON

Energy		16	-268	-268.513099				
'DATE								
PBC		9.3040	9.3040	9.3040	94.5972	94.5972	94.5972	
Al	2.353654000		8.064435000		0.968225600	CORE	1 Al Al 0.0000 1	
P	5.409494705		8.188732709		0.952731542	CORE	2 P P 0.0000 2	
Si	7.439158275		0.772948684		5.980189738	CORE	3 Si Si 0.0000 3	
Al	7.866701083		0.778166046		3.005643233	CORE	4 Al Al 0.0000 4	
P	0.066682745		7.912774246		3.224919077	CORE	5 P P 0.0000 5	
Al	7.683591788		6.130715240		1.243721192	CORE	6 Al Al 0.0000 6	
Al	-0.357008745		7.897044371		6.234132928	CORE	7 Al Al 0.0000 7	
Al	-0.163484536		2.487814100		7.913675434	CORE	8 Al Al 0.0000 8	
P	2.124308353		0.434362524		8.291723051	CORE	9 P P 0.0000 9	
P	-0.016896958		5.517758178		8.226515807	CORE	10 P P 0.0000 10	
Al	5.200565875		0.572067435		8.311443201	CORE	11 Al Al 0.0000 11	
O	1.196341969		6.141791409		8.937964390	CORE	12 O O 0.0000 12	
O	6.358219119		2.421408477		0.453311394	CORE	13 O O 0.0000 13	
O	7.915480182		2.440591036		9.153934964	CORE	14 O O 0.0000 14	
O	2.967029713		0.437795398		0.364645721	CORE	15 O O 0.0000 15	
O	6.214964696		6.913134933		0.698704278	CORE	16 O O 0.0000 16	
O	4.013232408		7.803058460		1.476449753	CORE	17 O O 0.0000 17	
O	7.247662397		4.472243518		1.581179396	CORE	18 O O 0.0000 18	
O	8.223766514		2.263646811		2.147686333	CORE	19 O O 0.0000 19	
O	1.360943508		7.920152472		2.399460208	CORE	20 O O 0.0000 20	
O	6.117438390		9.026059422		2.009346801	CORE	21 O O 0.0000 21	
O	8.393256391		6.854194232		2.684500586	CORE	22 O O 0.0000 22	
O	0.170697117		0.038645450		3.162831296	CORE	23 O O 0.0000 23	
O	6.993444934		1.101109609		4.447559825	CORE	24 O O 0.0000 24	
O	0.439532213		7.592308729		4.672142405	CORE	25 O O 0.0000 25	
O	7.377180634		8.570856320		6.073453050	CORE	26 O O 0.0000 26	
O	8.559978764		1.863210427		6.436154369	CORE	27 O O 0.0000 27	
O	1.570506572		-0.418693716		7.148308055	CORE	28 O O 0.0000 28	
O	6.086316982		0.868680869		6.880634084	CORE	29 O O 0.0000 29	
O	-0.440646920		6.341782955		7.021763967	CORE	30 O O 0.0000 30	
O	0.397906882		4.135463274		7.741273292	CORE	31 O O 0.0000 31	
O	3.520496059		0.934490377		7.880174343	CORE	32 O O 0.0000 32	
O	1.238427677		1.643412775		8.560233286	CORE	33 O O 0.0000 33	
O	4.529220135		8.169232135		8.879140849	CORE	34 O O 0.0000 34	
O	-1.186351408		5.443883752		9.210596889	CORE	35 O O 0.0000 35	
P	7.623861833		3.096658995		1.015253604	CORE	36 P P 0.0000 36	
O	1.905569098		3.170160583		4.338633821	CORE	37 O O 0.0000 37	
C	2.851976483		2.556675743		4.466637596	CORE	38 C C 0.0000 38	
H	3.965873496		0.902878932		4.008254071	CORE	39 H H 0.0000 39	
C	4.047354454		1.817855216		4.609728825	CORE	40 C C 0.0000 40	
H	4.899710766		2.418395369		4.257019372	CORE	41 H H 0.0000 41	
H	4.217107480		1.557381268		5.670219338	CORE	42 H H 0.0000 42	
end								
end								

CH₃OH*

'BIOSYM archive 2

PBC=ON

Energy		17	-267	-267.612942				
IDATE								
PBC	9.3040	9.3040	9.3040	94.5972	94.5972	94.5972		
Al	2.353654000		8.064435000		0.968225600	CORE	1 Al Al	0.0000 1
P	5.400091090		8.323351210		0.896458674	CORE	2 P P	0.0000 2
Si	7.448806889		0.753716057		6.031405184	CORE	3 Si Si	0.0000 3
Al	7.847258586		0.880500233		2.994322913	CORE	4 Al Al	0.0000 4
P	0.079667946		8.077155665		3.101027603	CORE	5 P P	0.0000 5
Al	7.676166061		6.267787102		1.000211420	CORE	6 Al Al	0.0000 6
Al	-0.287306643		7.945454956		6.194942825	CORE	7 Al Al	0.0000 7
Al	-0.208561459		2.514444755		7.872181166	CORE	8 Al Al	0.0000 8
P	2.125407448		0.460275229		8.115666817	CORE	9 P P	0.0000 9
P	0.028313155		5.506255760		8.231509648	CORE	10 P P	0.0000 10
Al	5.206453877		0.711799614		8.322283157	CORE	11 Al Al	0.0000 11
O	1.759830414		6.667733967		0.128045949	CORE	12 O O	0.0000 12
O	6.373143254		2.571769789		0.442391767	CORE	13 O O	0.0000 13
O	7.995019330		2.472224269		9.235751313	CORE	14 O O	0.0000 14
O	2.060317270		-0.621598175		9.196393299	CORE	15 O O	0.0000 15
O	6.149113673		7.019468039		0.631535633	CORE	16 O O	0.0000 16
O	4.015293994		7.977337010		1.480293589	CORE	17 O O	0.0000 17
O	7.290602200		4.650118101		1.504210376	CORE	18 O O	0.0000 18
O	8.099602049		2.450185226		2.267071629	CORE	19 O O	0.0000 19
O	1.533130335		8.240821525		2.548448263	CORE	20 O O	0.0000 20
O	6.920762502		-0.113349709		1.894680773	CORE	21 O O	0.0000 21
O	-0.702398398		7.069736639		2.269700412	CORE	22 O O	0.0000 22
O	0.184263168		0.189599575		3.071214783	CORE	23 O O	0.0000 23
O	7.018761116		0.859007852		4.475415819	CORE	24 O O	0.0000 24
O	0.241773687		7.585382088		4.539281729	CORE	25 O O	0.0000 25
O	7.449732587		8.594151315		6.341976008	CORE	26 O O	0.0000 26
O	8.505543677		1.943426375		6.379650650	CORE	27 O O	0.0000 27
O	1.782652290		-0.174388330		6.714120886	CORE	28 O O	0.0000 28
O	6.113022105		0.926835293		6.917075171	CORE	29 O O	0.0000 29
O	0.117611381		6.522725025		7.105208398	CORE	30 O O	0.0000 30
O	0.418748532		4.142148002		7.689690679	CORE	31 O O	0.0000 31
O	3.510744200		1.067983000		7.974234757	CORE	32 O O	0.0000 32
O	1.128318208		1.536580735		8.472696647	CORE	33 O O	0.0000 33
O	4.470297845		8.285652437		8.825196374	CORE	34 O O	0.0000 34
O	7.897857340		5.501864392		8.782205637	CORE	35 O O	0.0000 35
P	7.629842038		3.229329772		1.039680035	CORE	36 P P	0.0000 36
H	3.171927635		-0.339381362		3.962513077	CORE	37 H H	0.0000 37
O	3.473294099		0.147132331		4.778908330	CORE	38 O O	0.0000 38
H	2.804100953		0.003732780		5.547592387	CORE	39 H H	0.0000 39
C	3.681242397		1.597757310		4.499936266	CORE	40 C C	0.0000 40
H	4.640001746		1.661434047		3.994053823	CORE	41 H H	0.0000 41
H	3.726905551		2.077502043		5.472688423	CORE	42 H H	0.0000 42
H	2.839879591		1.955652402		3.908053141	CORE	43 H H	0.0000 43
end								
end								

CH₃OHCH₃*

'BIOSYM archive 2

PBC=ON

Energy		18	-284	-284.274737				
DATE								
PBC		9.3040	9.3040	9.3040	94.5972	94.5972	94.5972	
Al	2.353654000		8.064435000		0.968225600	CORE	1 Al Al	0.0000 1
P	5.383305822		8.246966219		0.856523710	CORE	2 P P	0.0000 2
Si	7.435253549		0.820107653		5.925811387	CORE	3 Si Si	0.0000 3
Al	7.839111301		0.819046575		2.905894034	CORE	4 Al Al	0.0000 4
P	0.023077295		7.938814397		3.167958549	CORE	5 P P	0.0000 5
Al	7.656614267		6.184896242		1.188168466	CORE	6 Al Al	0.0000 6
Al	-0.408685538		7.918668804		6.215591039	CORE	7 Al Al	0.0000 7
Al	-0.188224622		2.527355651		7.861753817	CORE	8 Al Al	0.0000 8
P	2.046791849		0.442552615		8.322968003	CORE	9 P P	0.0000 9
P	-0.005966015		5.549359305		8.195008831	CORE	10 P P	0.0000 10
Al	5.135475073		0.638983530		8.202470272	CORE	11 Al Al	0.0000 11
O	1.209559813		6.199325124		8.877694604	CORE	12 O O	0.0000 12
O	6.290328229		2.491542607		0.370192236	CORE	13 O O	0.0000 13

O	7.833198622	2.574026689	9.049828514	CORE	14	O	O	0.0000	14
O	2.906299667	0.467045091	0.422754360	CORE	15	O	O	0.0000	15
O	6.236772605	7.004894451	0.582500172	CORE	16	O	O	0.0000	16
O	4.019735321	7.791402228	1.416100410	CORE	17	O	O	0.0000	17
O	7.183137868	4.526736740	1.532061834	CORE	18	O	O	0.0000	18
O	8.208852057	2.305468672	2.012378536	CORE	19	O	O	0.0000	19
O	1.323409196	7.838553753	2.358772268	CORE	20	O	O	0.0000	20
O	6.070052011	9.107194869	1.905905977	CORE	21	O	O	0.0000	21
O	8.312588591	6.887077271	2.670992629	CORE	22	O	O	0.0000	22
O	0.173190714	0.083693240	2.994702173	CORE	23	O	O	0.0000	23
O	7.048384204	1.136446183	4.380257365	CORE	24	O	O	0.0000	24
O	0.372443116	7.679545325	4.631643315	CORE	25	O	O	0.0000	25
O	7.336798167	8.600347143	6.053615198	CORE	26	O	O	0.0000	26
O	-0.702192310	1.890167165	6.365828764	CORE	27	O	O	0.0000	27
O	1.473547740	-0.424044876	7.209036584	CORE	28	O	O	0.0000	28
O	6.119542743	0.952473563	6.858123635	CORE	29	O	O	0.0000	29
O	-0.462181747	6.341235211	6.977591554	CORE	30	O	O	0.0000	30
O	0.421921202	4.163798756	7.720254065	CORE	31	O	O	0.0000	31
O	3.422010241	0.961758330	7.895028933	CORE	32	O	O	0.0000	32
O	1.130394586	1.632370401	8.641393120	CORE	33	O	O	0.0000	33
O	4.442813060	8.231018862	8.797062457	CORE	34	O	O	0.0000	34
O	-1.150118267	5.475403075	9.212205645	CORE	35	O	O	0.0000	35
P	7.558134969	3.167305988	0.914821479	CORE	36	P	P	0.0000	36
O	2.214394211	2.993391648	2.732500173	CORE	37	O	O	0.0000	37
H	1.842743867	2.312281388	2.130331739	CORE	38	H	H	0.0000	38
C	1.378969608	3.161672010	3.977684024	CORE	39	C	C	0.0000	39
H	1.397891301	2.231042354	4.540409266	CORE	40	H	H	0.0000	40
H	0.384561663	3.403158547	3.617947226	CORE	41	H	H	0.0000	41
H	1.832503021	3.990846297	4.513220280	CORE	42	H	H	0.0000	42
H	4.092754959	2.561905594	1.954225684	CORE	43	H	H	0.0000	43
C	3.693092807	2.803443365	2.934651799	CORE	44	C	C	0.0000	44
H	4.055614154	3.767370162	3.284748417	CORE	45	H	H	0.0000	45
H	3.852773471	2.009143580	3.665337052	CORE	46	H	H	0.0000	46

end
end

CH₃COS + CH₃CO*

'BIOSYM archive 2
PBC=ON

Energy	19	-300	-300.168991						
'DATE									
PBC	9.3040	9.3040	9.3040	94.5972	94.5972	94.5972			
Al	2.353654000	8.064435000	0.968225600	CORE	1	Al	Al	0.0000	1
P	5.434920421	8.099561162	0.992830036	CORE	2	P	P	0.0000	2
Si	7.580786557	0.731870817	6.029801063	CORE	3	Si	Si	0.0000	3
Al	7.966661448	0.650104747	2.902065606	CORE	4	Al	Al	0.0000	4
P	0.116267800	7.761014485	3.230274054	CORE	5	P	P	0.0000	5
Al	7.721240404	6.032980297	1.282856156	CORE	6	Al	Al	0.0000	6
Al	-0.317640566	7.839258815	6.182353759	CORE	7	Al	Al	0.0000	7
Al	-0.016407954	2.498655489	7.928868719	CORE	8	Al	Al	0.0000	8
P	2.153644409	0.380930899	8.283511320	CORE	9	P	P	0.0000	9
P	-0.046078950	5.539890133	8.216303587	CORE	10	P	P	0.0000	10
Al	5.249682651	0.456934293	8.238022801	CORE	11	Al	Al	0.0000	11
O	1.163714083	6.221330336	8.864896863	CORE	12	O	O	0.0000	12
O	6.413655267	2.405256889	0.290128205	CORE	13	O	O	0.0000	13
O	8.017538168	2.398455449	9.119091782	CORE	14	O	O	0.0000	14
O	2.933264747	0.437267829	0.389133882	CORE	15	O	O	0.0000	15
O	6.244578468	6.821026303	0.785606265	CORE	16	O	O	0.0000	16
O	4.010643706	7.717252241	1.394634903	CORE	17	O	O	0.0000	17
O	7.3046652134	4.361916972	1.552344641	CORE	18	O	O	0.0000	18
O	8.225199242	2.113104979	2.020400783	CORE	19	O	O	0.0000	19
O	1.367482712	7.738805058	2.362171806	CORE	20	O	O	0.0000	20
O	6.054155165	8.898977244	2.146456470	CORE	21	O	O	0.0000	21
O	8.410566159	6.691646315	2.763237496	CORE	22	O	O	0.0000	22
O	0.205537300	-0.117279926	3.125386741	CORE	23	O	O	0.0000	23
O	7.160144621	1.292526598	4.423408187	CORE	24	O	O	0.0000	24
O	0.525781933	7.476675093	4.672963748	CORE	25	O	O	0.0000	25
O	7.455490887	8.551867737	5.768663965	CORE	26	O	O	0.0000	26
O	-0.627702474	1.800779146	6.486339458	CORE	27	O	O	0.0000	27
O	1.440407730	-0.447362652	7.213799667	CORE	28	O	O	0.0000	28
O	6.212367612	0.736089412	6.842602102	CORE	29	O	O	0.0000	29
O	-0.579091311	6.331242264	7.022776794	CORE	30	O	O	0.0000	30
O	0.399438168	4.172824815	7.718677393	CORE	31	O	O	0.0000	31
O	3.574214712	0.684452223	7.803481875	CORE	32	O	O	0.0000	32
O	1.425449415	1.703966793	8.508463500	CORE	33	O	O	0.0000	33
O	4.701086944	8.107431658	8.931325688	CORE	34	O	O	0.0000	34
O	-0.430424118	6.230175789	0.002239594	CORE	35	O	O	0.0000	35
P	7.670289557	3.018557060	0.914815422	CORE	36	P	P	0.0000	36
O	5.291078012	2.305213247	3.534263068	CORE	37	O	O	0.0000	37
C	6.253535540	2.487508457	4.208408936	CORE	38	C	C	0.0000	38
H	6.652503307	3.693509391	5.919989646	CORE	39	H	H	0.0000	39
C	6.775721808	3.738661915	4.834453247	CORE	40	C	C	0.0000	40
H	6.207977791	4.578291341	4.440107302	CORE	41	H	H	0.0000	41
H	7.838937205	3.854467193	4.620089734	CORE	42	H	H	0.0000	42
H	3.39322557	4.00882737	6.767214865	CORE	43	H	H	0.0000	43
C	2.337261526	3.735866421	4.986854349	CORE	44	C	C	0.0000	44
O	1.590999765	3.138578721	4.301232438	CORE	45	O	O	0.0000	45
C	3.171249277	4.385254764	5.766642704	CORE	46	C	C	0.0000	46
H	3.543363968	5.355981561	5.469163529	CORE	47	H	H	0.0000	47

end
end

CH₃COS + CH₃OH*

'BIOSYM archive 2
PBC=ON

Energy	20	-299	-299.296462						
'DATE									
PBC	9.3040	9.3040	9.3040	94.5972	94.5972	94.5972			
Al	2.353654000	8.064435000	0.968225600	CORE	1	Al	Al	0.0000	1
P	5.421350276	8.143351085	1.020882401	CORE	2	P	P	0.0000	2
Si	7.528519771	0.768116844	6.074791841	CORE	3	Si	Si	0.0000	3
Al	7.898536070	0.680091331	2.945295987	CORE	4	Al	Al	0.0000	4
P	0.096638211	7.842368519	3.232904652	CORE	5	P	P	0.0000	5
Al	7.711474605	6.090234084	1.292506408	CORE	6	Al	Al	0.0000	6
Al	-0.360870153	7.886403711	6.197696409	CORE	7	Al	Al	0.0000	7
Al	-0.047997612	2.532980115	7.971181478	CORE	8	Al	Al	0.0000	8
P	2.102420620	0.414610665	8.324586601	CORE	9	P	P	0.0000	9
P	-0.059613417	5.564467193	8.213845457	CORE	10	P	P	0.0000	10
Al	5.182430928	0.550167255	8.270364722	CORE	11	Al	Al	0.0000	11
O	1.152813865	6.252347443	8.850180202	CORE	12	O	O	0.0000	12
O	6.340205115	2.560248485	0.266339059	CORE	13	O	O	0.0000	13
O	7.986292781	2.461200235	9.175896434	CORE	14	O	O	0.0000	14
O	2.939749334	0.446887011	0.413654920	CORE	15	O	O	0.0000	15
O	6.267347669	6.903012584	0.735222381	CORE	16	O	O	0.0000	16
O	4.004231474	7.700277425	1.382384905	CORE	17	O	O	0.0000	17
O	7.286063512	4.429342042	1.621317240	CORE	18	O	O	0.0000	18
O	8.090920005	2.126572656	2.028072846	CORE	19	O	O	0.0000	19
O	1.356108717	7.808509967	2.374790595	CORE	20	O	O	0.0000	20
O	6.001690546	8.874495691	2.240513807	CORE	21	O	O	0.0000	21
O	8.395242407	6.774395994	2.761800620	CORE	22	O	O	0.0000	22
O	0.175734619	-0.035931912	3.122092547	CORE	23	O	O	0.0000	23
O	7.090328340	1.340514903	4.465671863	CORE	24	O	O	0.0000	24
O	0.497172549	7.575481281	4.683564926	CORE	25	O	O	0.0000	25

C 5.532951792 1.504974168 4.288132765 CORE 38 C C 0.0000 38
H 4.976052516 1.448380170 5.224245214 CORE 39 H H 0.0000 39

end
end

HS + C₂H₄* + CO*

!BIOSYM archive 2

PBC=ON

Energy 23 -285 -285.725594

!DATE

PBC	9.3040	9.3040	9.3040	94.5972	94.5972	94.5972			
Al	2.353654000	8.064435000	0.968225600	CORE	1	Al	Al	0.0000	1
P	5.377911807	8.192688794	0.931424101	CORE	2	P	P	0.0000	2
Si	7.478366086	0.724302012	6.106754867	CORE	3	Si	Si	0.0000	3
Al	7.897625354	0.746566092	2.899091946	CORE	4	Al	Al	0.0000	4
P	0.044887786	7.861308093	3.207060013	CORE	5	P	P	0.0000	5
Al	7.668168212	6.128098915	1.232889185	CORE	6	Al	Al	0.0000	6
Al	-0.313295261	7.857484143	6.213917737	CORE	7	Al	Al	0.0000	7
Al	-0.160014259	2.514108616	7.941475837	CORE	8	Al	Al	0.0000	8
P	2.087326351	0.423406072	8.305256515	CORE	9	P	P	0.0000	9
P	-0.019667927	5.526245314	8.225656734	CORE	10	P	P	0.0000	10
Al	5.120405576	0.585685098	8.279979038	CORE	11	Al	Al	0.0000	11
O	1.194153983	6.188594785	8.888502200	CORE	12	O	O	0.0000	12
O	6.324481547	2.429466935	0.402994546	CORE	13	O	O	0.0000	13
O	7.895625171	2.451139695	9.167780563	CORE	14	O	O	0.0000	14
O	2.967269291	0.430587046	0.374704288	CORE	15	O	O	0.0000	15
O	6.253407108	6.975349455	0.661761010	CORE	16	O	O	0.0000	16
O	4.005327110	7.737846257	1.443365772	CORE	17	O	O	0.0000	17
O	7.166825809	4.487134557	1.541219190	CORE	18	O	O	0.0000	18
O	8.118627536	2.293081361	2.162337197	CORE	19	O	O	0.0000	19
O	1.298224932	7.848400391	2.339801421	CORE	20	O	O	0.0000	20
O	6.021875318	9.049890838	2.028968843	CORE	21	O	O	0.0000	21
O	8.330749185	6.820692042	2.708518600	CORE	22	O	O	0.0000	22
O	0.135173125	-0.008461339	3.150355220	CORE	23	O	O	0.0000	23
O	7.004676058	1.073541308	4.458802768	CORE	24	O	O	0.0000	24
O	0.443619747	7.554792392	4.646689558	CORE	25	O	O	0.0000	25
O	7.421046886	8.559529322	6.005372154	CORE	26	O	O	0.0000	26
O	8.523566245	1.880097076	6.466992105	CORE	27	O	O	0.0000	27
O	1.525296847	-0.440939092	7.175388648	CORE	28	O	O	0.0000	28
O	6.089007253	0.795577905	6.879924901	CORE	29	O	O	0.0000	29
O	-0.504652074	6.324795770	7.021548273	CORE	30	O	O	0.0000	30
O	0.407006561	4.145889585	7.746024058	CORE	31	O	O	0.0000	31
O	3.459487596	0.947723122	7.871423460	CORE	32	O	O	0.0000	32
O	1.170133779	1.600697944	8.600998064	CORE	33	O	O	0.0000	33
O	4.489925015	8.192588147	8.875360568	CORE	34	O	O	0.0000	34
O	-0.414660538	6.239035249	0.003703110	CORE	35	O	O	0.0000	35
P	7.562909951	3.117325267	0.988614833	CORE	36	P	P	0.0000	36
O	5.288803910	5.676762014	6.419762017	CORE	37	O	O	0.0000	37
C	5.116019199	6.347792084	5.510473799	CORE	38	C	C	0.0000	38
H	3.649644964	1.972873167	4.864663404	CORE	39	H	H	0.0000	39
C	3.258010298	3.800691819	3.872798314	CORE	40	C	C	0.0000	40
H	3.327204099	4.379638827	2.957010524	CORE	41	H	H	0.0000	41
H	2.788871869	4.284213903	4.724829101	CORE	42	H	H	0.0000	42
C	3.721825727	2.551288530	3.946920995	CORE	43	C	C	0.0000	43
H	4.154693409	2.067791860	3.073561356	CORE	44	H	H	0.0000	44
H	6.173955422	1.574342160	4.404110383	CORE	45	H	H	0.0000	45

end
end

HS + CH₂CH₂CO*

!BIOSYM archive 2

PBC=ON

Energy 24 -285 -285.512593

!DATE

PBC	9.3040	9.3040	9.3040	94.5972	94.5972	94.5972			
Al	2.353654000	8.064435000	0.968225600	CORE	1	Al	Al	0.0000	1
P	5.403597812	8.203148519	1.024961301	CORE	2	P	P	0.0000	2
Si	7.527414462	0.762925698	6.079184552	CORE	3	Si	Si	0.0000	3
Al	7.913487624	0.746521989	2.943568560	CORE	4	Al	Al	0.0000	4
P	0.098534190	7.874326514	3.236634165	CORE	5	P	P	0.0000	5
Al	7.713454559	6.134173150	1.306326187	CORE	6	Al	Al	0.0000	6
Al	-0.349760904	7.895078130	6.220396065	CORE	7	Al	Al	0.0000	7
Al	-0.087841350	2.538439873	7.991356082	CORE	8	Al	Al	0.0000	8
P	2.100311886	0.438849360	8.346339665	CORE	9	P	P	0.0000	9
P	-0.040252907	5.564760382	8.228971624	CORE	10	P	P	0.0000	10
Al	5.175117421	0.580718284	8.271813823	CORE	11	Al	Al	0.0000	11
O	1.189708035	6.231318239	8.862909258	CORE	12	O	O	0.0000	12
O	6.329380877	2.534301220	0.325558621	CORE	13	O	O	0.0000	13
O	7.945861099	2.512630696	9.187438254	CORE	14	O	O	0.0000	14
O	2.963081993	0.456916297	0.427168350	CORE	15	O	O	0.0000	15
O	6.296065345	6.993524825	0.767249742	CORE	16	O	O	0.0000	16
O	4.006161187	7.716110865	1.422667726	CORE	17	O	O	0.0000	17
O	7.211560799	4.488628980	1.591468762	CORE	18	O	O	0.0000	18
O	8.113275434	2.232129878	2.082683442	CORE	19	O	O	0.0000	19
O	1.359183826	7.823432098	2.377243992	CORE	20	O	O	0.0000	20
O	5.966464204	9.012656986	2.202308454	CORE	21	O	O	0.0000	21
O	8.404264331	6.793503487	2.783729855	CORE	22	O	O	0.0000	22
O	0.178371787	-0.009093866	3.087736820	CORE	23	O	O	0.0000	23
O	7.162425569	1.295765100	4.482653030	CORE	24	O	O	0.0000	24
O	0.506766941	7.637909962	4.690384359	CORE	25	O	O	0.0000	25
O	7.403548113	8.574141199	5.862861659	CORE	26	O	O	0.0000	26
O	-0.673144522	1.822441778	6.554033882	CORE	27	O	O	0.0000	27
O	1.400867939	-0.389889033	7.270035542	CORE	28	O	O	0.0000	28
O	6.149389090	0.804378938	6.881329098	CORE	29	O	O	0.0000	29
O	-0.555900733	6.367469902	7.040483044	CORE	30	O	O	0.0000	30
O	0.393472188	4.192242500	7.730281941	CORE	31	O	O	0.0000	31
O	3.493745974	0.824671313	7.834686475	CORE	32	O	O	0.0000	32
O	1.312122741	1.711665799	8.651808610	CORE	33	O	O	0.0000	33
O	4.601964164	8.243550132	8.988775154	CORE	34	O	O	0.0000	34
O	-0.399175350	6.269966458	0.044357133	CORE	35	O	O	0.0000	35
P	7.582839144	3.139687794	0.969398800	CORE	36	P	P	0.0000	36
O	5.983779063	3.625276624	4.569562874	CORE	37	O	O	0.0000	37
C	4.765048873	3.566691059	4.496692854	CORE	38	C	C	0.0000	38
H	3.260613187	2.089364662	5.111750510	CORE	39	H	H	0.0000	39
C	3.503515783	4.292972256	4.493543477	CORE	40	C	C	0.0000	40
H	3.276640416	4.906904945	3.624574422	CORE	41	H	H	0.0000	41
C	3.098585621	4.669226232	5.430483478	CORE	42	H	H	0.0000	42
C	3.587520135	2.727287150	4.293064485	CORE	43	C	C	0.0000	43
H	3.404831102	2.226980461	3.297404500	CORE	44	H	H	0.0000	44
H	6.739688059	2.217349022	4.468797982	CORE	45	H	H	0.0000	45

end
end

HS + CH₃CO*

!BIOSYM archive 2

PBC=ON

Energy 25 -268 -268.832682

!DATE

PBC	9.3040	9.3040	9.3040	94.5972	94.5972	94.5972			
Al	2.353654000	8.064435000	0.968225600	CORE	1	Al	Al	0.0000	1
P	5.355912860	8.193889204	0.968627395	CORE	2	P	P	0.0000	2
Si	7.480650322	0.730855000	6.095357079	CORE	3	Si	Si	0.0000	3

Al	7.872293955	0.760741735	2.930687136	CORE	4	Al	Al	0.0000	4
P	0.028638195	7.875197300	3.198283726	CORE	5	P	P	0.0000	5
Al	7.652369856	6.141566999	1.224327462	CORE	6	Al	Al	0.0000	6
Al	-0.338692605	7.855027116	6.190752874	CORE	7	Al	Al	0.0000	7
Al	-0.154691766	2.508783278	7.962341404	CORE	8	Al	Al	0.0000	8
P	2.085325726	0.423819535	8.284943668	CORE	9	P	P	0.0000	9
P	-0.035062938	5.528674341	8.221025739	CORE	10	P	P	0.0000	10
Al	5.106791075	0.576292610	8.282896067	CORE	11	Al	Al	0.0000	11
O	1.173032055	6.188181262	8.896418975	CORE	12	O	O	0.0000	12
O	6.282323095	2.471553928	0.380451303	CORE	13	O	O	0.0000	13
O	7.877211676	2.461830034	9.172173004	CORE	14	O	O	0.0000	14
O	2.997169499	0.426375255	0.347775863	CORE	15	O	O	0.0000	15
O	6.223799961	6.975214415	0.669381476	CORE	16	O	O	0.0000	16
O	3.988795412	7.726757065	1.485349181	CORE	17	O	O	0.0000	17
O	7.145584640	4.501106845	1.546022286	CORE	18	O	O	0.0000	18
O	8.067833643	2.293275765	2.151792375	CORE	19	O	O	0.0000	19
O	1.274352115	7.870337928	2.322317650	CORE	20	O	O	0.0000	20
O	6.011985450	9.034182120	2.068011766	CORE	21	O	O	0.0000	21
O	8.313478651	6.834696562	2.695257620	CORE	22	O	O	0.0000	22
O	0.117704713	0.003716795	3.153445498	CORE	23	O	O	0.0000	23
O	7.003825096	1.156346919	4.475732131	CORE	24	O	O	0.0000	24
O	0.433554562	7.544743995	4.631458273	CORE	25	O	O	0.0000	25
O	7.403826152	8.560541003	5.929718383	CORE	26	O	O	0.0000	26
O	8.536553292	1.868968128	6.490037472	CORE	27	O	O	0.0000	27
O	1.461128051	-0.427067525	7.179205802	CORE	28	O	O	0.0000	28
O	6.121923814	0.786909910	6.922806983	CORE	29	O	O	0.0000	29
O	-0.511510036	6.324475683	7.012052399	CORE	30	O	O	0.0000	30
O	0.394865914	4.145995774	7.751581953	CORE	31	O	O	0.0000	31
O	3.456447009	0.919278886	7.803501191	CORE	32	O	O	0.0000	32
O	1.203672642	1.623677080	8.611100968	CORE	33	O	O	0.0000	33
O	4.453245263	8.203485641	8.922299784	CORE	34	O	O	0.0000	34
O	-1.190871284	5.432849415	9.221974405	CORE	35	O	O	0.0000	35
P	7.531101557	3.129434249	0.980948228	CORE	36	P	P	0.0000	36
O	2.907769587	2.485756470	4.245222722	CORE	37	O	O	0.0000	37
C	3.921495317	2.987155287	4.533475640	CORE	38	C	C	0.0000	38
H	6.335352719	1.893481257	4.453956826	CORE	39	H	H	0.0000	39
C	5.108530355	3.492694610	4.843745415	CORE	40	C	C	0.0000	40
H	5.562519853	4.211063276	4.170868512	CORE	41	H	H	0.0000	41
H	5.374728861	3.506281491	5.894566332	CORE	42	H	H	0.0000	42

end
end

HS + CH₃COOCH₃*

!BIOSYM archive 2									
PBC--ON									
Energy	26	-299	-299.989052						
!DATE									
PBC	9.3040	9.3040	9.3040	94.5972	94.5972	94.5972			
Al	2.353654000	8.064435000	0.968225600	CORE	1	Al	Al	0.0000	1
P	5.415228017	8.131018828	0.803842146	CORE	2	P	P	0.0000	2
Si	7.522192025	0.726050740	5.918352622	CORE	3	Si	Si	0.0000	3
Al	7.912695749	0.687493323	2.853723198	CORE	4	Al	Al	0.0000	4
P	0.030748444	7.808250334	3.120523039	CORE	5	P	P	0.0000	5
Al	7.647575429	6.068731287	1.133024136	CORE	6	Al	Al	0.0000	6
Al	-0.316134332	7.802582114	6.230955133	CORE	7	Al	Al	0.0000	7
Al	-0.164595491	2.501925965	7.866592479	CORE	8	Al	Al	0.0000	8
P	2.116840255	0.329158768	8.213618783	CORE	9	P	P	0.0000	9
P	0.016405579	5.474023045	8.197545177	CORE	10	P	P	0.0000	10
Al	5.137386583	0.493101803	8.260329850	CORE	11	Al	Al	0.0000	11
O	1.183483554	6.169752412	8.902856895	CORE	12	O	O	0.0000	12
O	6.540711241	2.358467703	0.214032042	CORE	13	O	O	0.0000	13
O	8.840234411	3.285099553	0.019832055	CORE	14	O	O	0.0000	14
O	2.913558731	0.407315197	0.327933293	CORE	15	O	O	0.0000	15
O	6.184836664	6.839041811	0.546314529	CORE	16	O	O	0.0000	16
O	4.036642719	7.808133702	1.398233609	CORE	17	O	O	0.0000	17
O	7.161130897	4.429847514	1.465425788	CORE	18	O	O	0.0000	18
O	8.132577036	2.269117423	2.166489328	CORE	19	O	O	0.0000	19
O	1.366871880	7.718088923	2.372788359	CORE	20	O	O	0.0000	20
O	6.190330918	9.002251261	1.777830972	CORE	21	O	O	0.0000	21
O	8.319151736	6.777812416	2.595008150	CORE	22	O	O	0.0000	22
O	0.213613921	-0.044221353	2.939341451	CORE	23	O	O	0.0000	23
O	7.131667013	0.795345481	4.374637348	CORE	24	O	O	0.0000	24
O	0.287042702	7.533028802	4.598465128	CORE	25	O	O	0.0000	25
O	7.470707012	8.628459801	6.371714627	CORE	26	O	O	0.0000	26
O	8.294788304	2.026249279	6.443983606	CORE	27	O	O	0.0000	27
O	1.723741211	-0.614884649	7.071641227	CORE	28	O	O	0.0000	28
O	5.934086170	0.771961808	6.649678885	CORE	29	O	O	0.0000	29
O	-0.450909036	6.234535598	6.961123320	CORE	30	O	O	0.0000	30
O	0.500275183	4.103267426	7.743181237	CORE	31	O	O	0.0000	31
O	3.499756797	0.910257523	7.878854747	CORE	32	O	O	0.0000	32
O	1.140697717	1.470849638	8.339345792	CORE	33	O	O	0.0000	33
O	4.507545128	8.077487332	8.702331341	CORE	34	O	O	0.0000	34
O	-1.173278358	5.373806754	9.155270622	CORE	35	O	O	0.0000	35
P	7.670076448	3.078426406	0.961947651	CORE	36	P	P	0.0000	36
P	4.476975569	2.620681233	2.731442926	CORE	37	O	O	0.0000	37
C	4.590743588	2.808329868	3.923226749	CORE	38	C	C	0.0000	38
H	4.309646551	4.833887375	4.419422057	CORE	39	H	H	0.0000	39
C	5.080789377	4.072445526	4.573008628	CORE	40	C	C	0.0000	40
H	5.982447674	4.401648682	4.055711584	CORE	41	H	H	0.0000	41
H	5.259331264	3.962385031	5.642696723	CORE	42	H	H	0.0000	42
H	3.277942212	0.063191366	5.133861794	CORE	43	H	H	0.0000	43
H	4.352005835	0.112301713	3.699314235	CORE	44	H	H	0.0000	44
C	3.608784999	0.652325519	4.284560215	CORE	45	C	C	0.0000	45
O	2.761935538	0.953861713	3.670888847	CORE	46	H	H	0.0000	46
O	4.219197591	1.849222328	4.857259105	CORE	47	O	O	0.0000	47
H	5.307291753	1.216608787	6.012769098	CORE	48	H	H	0.0000	48

end
end

HS + CO*

!BIOSYM archive 2									
PBC--ON									
Energy	27	-251	-251.922925						
!DATE									
PBC	9.3040	9.3040	9.3040	94.5972	94.5972	94.5972			
Al	2.353654000	8.064435000	0.968225600	CORE	1	Al	Al	0.0000	1
P	5.369576844	8.220311272	0.917407983	CORE	2	P	P	0.0000	2
Si	7.456136543	0.721837008	6.085563605	CORE	3	Si	Si	0.0000	3
Al	7.893261079	0.779001987	2.880899341	CORE	4	Al	Al	0.0000	4
P	0.026830481	7.885218352	3.197874772	CORE	5	P	P	0.0000	5
Al	7.650756070	6.153979678	1.219158457	CORE	6	Al	Al	0.0000	6
Al	-0.357473131	7.864493488	6.205749290	CORE	7	Al	Al	0.0000	7
Al	-0.176099748	2.509158354	7.926211412	CORE	8	Al	Al	0.0000	8
P	2.063264127	0.429575153	8.828884396	CORE	9	P	P	0.0000	9
P	-0.020430719	5.530150381	8.235723490	CORE	10	P	P	0.0000	10
Al	5.092722451	0.602463020	8.251454736	CORE	11	Al	Al	0.0000	11
O	1.206276771	6.161979159	8.906455996	CORE	12	O	O	0.0000	12
O	6.280370625	2.458752871	0.371282480	CORE	13	O	O	0.0000	13
O	7.859144712	2.439794005	9.133178749	CORE	14	O	O	0.0000	14
O	2.957825505	0.419851284	0.340175580	CORE	15	O	O	0.0000	15
O	6.236113460	6.997000494	0.643384358	CORE	16	O	O	0.0000	16
O	4.005931307	7.775715805	1.460054972	CORE	17	O	O	0.0000	17
O	7.141914980	4.513570763	1.499004581	CORE	18	O	O	0.0000	18

H	4.209506174	0.543635000	3.671039725 CORE	39	H	H	0.0000	39
H	5.254047375	1.178602165	6.034610453 CORE	40	H	H	0.0000	40
O	4.103320324	2.045516275	5.007617243 CORE	41	O	O	0.0000	41
C	3.703492406	3.427695816	5.298376629 CORE	42	C	C	0.0000	42
H	2.668129235	3.431600532	5.646049015 CORE	43	H	H	0.0000	43
H	4.372318949	3.769818376	6.085781211 CORE	44	H	H	0.0000	44
H	3.809980199	4.029841110	4.399060857 CORE	45	H	H	0.0000	45
end								
end								

HS + CH₃OH*

!BIOSYM archive 2

PBC=ON

	Energy		30	-268	-268.134838				
!DATE									
PBC	9.3040	9.3040	9.3040	94.5972	94.5972	94.5972			
Al	2.353654000	8.064435000	0.968225600 CORE	1	Al	Al	0.0000	1	
P	5.395650513	8.210800053	0.924544705 CORE	2	P	P	0.0000	2	
Si	7.484030211	0.778294989	6.010131511 CORE	3	Si	Si	0.0000	3	
Al	7.945581437	0.788879561	2.861227900 CORE	4	Al	Al	0.0000	4	
P	0.059754044	7.892196408	3.194377969 CORE	5	P	P	0.0000	5	
Al	7.672133896	6.156994340	1.212034334 CORE	6	Al	Al	0.0000	6	
Al	-0.332600757	7.892013814	6.189342668 CORE	7	Al	Al	0.0000	7	
Al	-0.128892832	2.532525249	7.875317069 CORE	8	Al	Al	0.0000	8	
P	2.094100311	0.432200203	8.303444722 CORE	9	P	P	0.0000	9	
P	-0.021069129	5.55185062	8.201685147 CORE	10	P	P	0.0000	10	
Al	5.153508084	0.590967680	8.226822154 CORE	11	Al	Al	0.0000	11	
O	1.194271047	6.201429803	8.885285535 CORE	12	O	O	0.0000	12	
O	6.342711280	2.470668625	0.333208604 CORE	13	O	O	0.0000	13	
O	7.899145785	2.503957589	9.071067908 CORE	14	O	O	0.0000	14	
O	2.966451116	0.454485477	0.392860425 CORE	15	O	O	0.0000	15	
O	6.214954087	6.950911543	0.657036189 CORE	16	O	O	0.0000	16	
O	4.013574043	7.810398371	1.467351231 CORE	17	O	O	0.0000	17	
O	7.212260013	4.499411102	1.509658657 CORE	18	O	O	0.0000	18	
O	8.190623357	2.293469299	2.047232841 CORE	19	O	O	0.0000	19	
O	1.328475307	7.839486243	2.348966125 CORE	20	O	O	0.0000	20	
O	6.094836989	9.044013522	2.002833400 CORE	21	O	O	0.0000	21	
O	8.330002399	6.873156077	2.679898570 CORE	22	O	O	0.0000	22	
O	0.194734383	0.039621894	3.110096913 CORE	23	O	O	0.0000	23	
O	7.032172840	1.158244145	4.382171637 CORE	24	O	O	0.0000	24	
O	0.446189229	7.581491805	4.634144763 CORE	25	O	O	0.0000	25	
O	7.424447868	8.605889005	5.900556555 CORE	26	O	O	0.0000	26	
O	8.563027971	1.902639957	6.397582715 CORE	27	O	O	0.0000	27	
O	1.493335790	-0.438086331	7.201939127 CORE	28	O	O	0.0000	28	
O	6.121198075	0.820416476	6.834683844 CORE	29	O	O	0.0000	29	
O	-0.496571432	6.357756288	6.998949481 CORE	30	O	O	0.0000	30	
O	0.409145630	4.178463148	7.719152677 CORE	31	O	O	0.0000	31	
O	3.474895040	0.914191877	7.853867543 CORE	32	O	O	0.0000	32	
O	1.205735643	1.640964695	8.578524704 CORE	33	O	O	0.0000	33	
O	4.511148109	8.208126099	8.868019738 CORE	34	O	O	0.0000	34	
O	-1.72721962	5.475393102	9.208301419 CORE	35	O	O	0.0000	35	
P	7.595761479	3.141327581	0.912955439 CORE	36	P	P	0.0000	36	
H	6.131432010	1.537873608	4.182962025 CORE	37	H	H	0.0000	37	
O	4.769085901	2.053675985	3.290044598 CORE	38	O	O	0.0000	38	
H	4.350280962	1.410401897	2.703986530 CORE	39	H	H	0.0000	39	
C	4.235851465	3.368524313	2.980060693 CORE	40	C	C	0.0000	40	
H	4.876239553	4.091322422	3.483501482 CORE	41	H	H	0.0000	41	
H	3.209839884	3.456370968	3.349944982 CORE	42	H	H	0.0000	42	
H	4.268502787	3.547908798	1.902155832 CORE	43	H	H	0.0000	43	
end									
end									

HS

!BIOSYM archive 2

PBC=ON

Energy		31	-237	-237.812744					
!DATE									
PBC	9.3040	9.3040	9.3040	94.5972	94.5972	94.5972			
Al	2.353654000	8.064435000	0.968225600 CORE	1	Al	Al	0.0000	1	
P	5.347888846	8.042695450	1.108108835 CORE	2	P	P	0.0000	2	
Si	7.656588351	0.517068181	6.208686709 CORE	3	Si	Si	0.0000	3	
Al	7.840058010	0.658715357	3.032827425 CORE	4	Al	Al	0.0000	4	
P	0.051723483	7.813702942	3.200514752 CORE	5	P	P	0.0000	5	
Al	7.735829415	6.108466052	1.174937830 CORE	6	Al	Al	0.0000	6	
Al	-0.126850354	7.664269271	6.181651888 CORE	7	Al	Al	0.0000	7	
Al	-0.057985034	2.290595391	8.057962036 CORE	8	Al	Al	0.0000	8	
P	2.277762052	0.327141609	8.218466936 CORE	9	P	P	0.0000	9	
P	-0.031481091	5.499436688	8.287085587 CORE	10	P	P	0.0000	10	
Al	5.269122900	0.370604701	8.362266126 CORE	11	Al	Al	0.0000	11	
O	1.215139999	6.091671697	8.961073363 CORE	12	O	O	0.0000	12	
O	6.420633822	2.320908316	0.417692780 CORE	13	O	O	0.0000	13	
O	8.903596307	2.530583099	0.092056456 CORE	14	O	O	0.0000	14	
O	3.108534790	0.420740417	0.341503557 CORE	15	O	O	0.0000	15	
O	6.136547530	6.751255719	0.923137769 CORE	16	O	O	0.0000	16	
O	3.941020588	7.688330535	1.585194461 CORE	17	O	O	0.0000	17	
O	7.599935916	4.385070165	1.195694971 CORE	18	O	O	0.0000	18	
O	7.980139796	2.254902587	2.380560910 CORE	19	O	O	0.0000	19	
O	1.232961946	7.970609737	2.267278709 CORE	20	O	O	0.0000	20	
O	5.990670391	8.913692145	2.194368867 CORE	21	O	O	0.0000	21	
O	8.397480782	6.725459814	2.686557108 CORE	22	O	O	0.0000	22	
O	0.068163937	-0.098803971	3.270744793 CORE	23	O	O	0.0000	23	
O	7.024062740	0.903004716	4.624016887 CORE	24	O	O	0.0000	24	
O	0.574469028	7.443795327	4.582646175 CORE	25	O	O	0.0000	25	
O	7.606804650	8.367634745	6.034402789 CORE	26	O	O	0.0000	26	
O	-0.644510252	1.721298729	6.538059646 CORE	27	O	O	0.0000	27	
O	1.625905193	-0.592016912	7.188295993 CORE	28	O	O	0.0000	28	
O	6.302184702	0.519459176	7.023703562 CORE	29	O	O	0.0000	29	
O	-0.187542507	6.058847466	6.876950272 CORE	30	O	O	0.0000	30	
O	0.128812426	3.997834696	8.205311456 CORE	31	O	O	0.0000	31	
O	3.677715957	0.697424808	7.734564461 CORE	32	O	O	0.0000	32	
O	1.503347097	1.619384757	8.418926945 CORE	33	O	O	0.0000	33	
O	4.571332508	8.006268677	9.024005205 CORE	34	O	O	0.0000	34	
O	8.021999167	5.861758948	9.114203146 CORE	35	O	O	0.0000	35	
P	7.725366779	2.884635215	1.000852991 CORE	36	P	P	0.0000	36	
H	6.079165613	1.103388823	4.660237920 CORE	37	H	H	0.0000	37	
end									
end									

CH₃S + CH₃CO*

!BIOSYM archive 2

PBC=ON

Energy		32	-285	-285.548529					
!DATE									
PBC	9.3040	9.3040	9.3040	94.5972	94.5972	94.5972			
Al	2.353654000	8.064435000	0.968225600 CORE	1	Al	Al	0.0000	1	
P	5.391186686	8.076623349	0.910910134 CORE	2	P	P	0.0000	2	
Si	7.479695500	0.676897170	5.989362868 CORE	3	Si	Si	0.0000	3	
Al	7.943207565	0.646265584	2.867406131 CORE	4	Al	Al	0.0000	4	
P	0.059895342	7.747276847	3.195609384 CORE	5	P	P	0.0000	5	
Al	7.655494704	6.008732800	1.222856662 CORE	6	Al	Al	0.0000	6	
Al	-0.323897824	7.781881158	6.169733557 CORE	7	Al	Al	0.0000	7	
Al	-0.151810695	2.478488572	7.829385234 CORE	8	Al	Al	0.0000	8	


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O -0.695650738 1.825522006 6.492336565 CORE 27 O O 0.0000 27
O 1.457399192 -0.459357403 7.242694490 CORE 28 O O 0.0000 28
O 6.223058712 0.668582651 6.959931315 CORE 29 O O 0.0000 29
O -0.589260545 6.329340177 7.057650412 CORE 30 O O 0.0000 30
O 0.379168865 4.162851453 7.745172723 CORE 31 O O 0.0000 31
O 3.563666199 0.728928701 7.839916024 CORE 32 O O 0.0000 32
O 1.371849888 1.684164209 8.545333982 CORE 33 O O 0.0000 33
O 4.644291807 8.118726419 9.003155346 CORE 34 O O 0.0000 34
O -0.423466981 6.222666815 0.053894923 CORE 35 O O 0.0000 35
P 7.672939572 3.015506247 1.000523914 CORE 36 P P 0.0000 36
H 2.669196815 4.166135691 4.032920247 CORE 37 H H 0.0000 37
O 3.069911469 3.914142884 4.874963097 CORE 38 O O 0.0000 38
O 2.767303284 4.592364445 5.494826440 CORE 39 H H 0.0000 39
C 5.879637624 2.115204029 4.406236912 CORE 40 C C 0.0000 40
H 6.158049578 3.034856218 4.920698902 CORE 41 H H 0.0000 41
H 5.683350414 2.315833182 3.356253608 CORE 42 H H 0.0000 42
H 5.019999921 1.649616139 4.878922084 CORE 43 H H 0.0000 43
end
end

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CH₃S + CH₃OH*

!BIOSYM archive 2

PBC=ON

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Energy 35 -284 -284.579076
!DATE
PBC 9.3040 9.3040 9.3040 94.5972 94.5972 94.5972
Al 2.353654000 8.064435000 0.968225600 CORE 1 Al Al 0.0000 1
P 5.389588826 8.139994124 0.955341809 CORE 2 P P 0.0000 2
Si 7.525675047 0.714267238 6.062737698 CORE 3 Si Si 0.0000 3
Al 7.932170170 0.702116329 2.925881800 CORE 4 Al Al 0.0000 4
P 0.054352712 7.819840112 3.217053230 CORE 5 P P 0.0000 5
Al 7.667472061 6.082918334 1.238026555 CORE 6 Al Al 0.0000 6
Al -0.272424012 7.820009434 6.189515019 CORE 7 Al Al 0.0000 7
Al -0.142236101 2.486093953 7.903364024 CORE 8 Al Al 0.0000 8
P 2.132857525 0.292406483 8.253904239 CORE 9 P P 0.0000 9
P -0.010517301 5.505400020 8.245393712 CORE 10 P P 0.0000 10
Al 5.183013415 0.522923315 8.299998410 CORE 11 Al Al 0.0000 11
O 1.212424229 6.140081522 8.918122149 CORE 12 O O 0.0000 12
O 6.372396629 2.364487667 0.435242401 CORE 13 O O 0.0000 13
O 7.924101009 2.400692437 9.137709050 CORE 14 O O 0.0000 14
O 2.948376158 0.406418670 0.333000848 CORE 15 O O 0.0000 15
O 6.204973324 6.874817471 0.695658239 CORE 16 O O 0.0000 16
O 4.002472330 7.760483799 1.488805505 CORE 17 O O 0.0000 17
O 7.236207419 4.422816849 1.560062832 CORE 18 O O 0.0000 18
O 8.212226107 2.225959076 2.145642718 CORE 19 O O 0.0000 19
O 1.287824221 7.829824016 2.325252152 CORE 20 O O 0.0000 20
O 6.098258261 8.982354687 2.023293090 CORE 21 O O 0.0000 21
O 8.308288956 6.824881281 2.694373687 CORE 22 O O 0.0000 22
O 0.173394971 -0.034406863 3.239835101 CORE 23 O O 0.0000 23
O 6.981110921 1.053432687 4.440525660 CORE 24 O O 0.0000 24
O 0.470093901 7.429349840 4.632581702 CORE 25 O O 0.0000 25
O 7.489137238 8.560814408 5.939446279 CORE 26 O O 0.0000 26
O 8.572428404 1.892475132 6.390171925 CORE 27 O O 0.0000 27
O 1.600852314 -0.471830707 7.107141889 CORE 28 O O 0.0000 28
O 6.203383243 0.753468563 6.945349037 CORE 29 O O 0.0000 29
O -0.488322936 6.325678418 7.055100705 CORE 30 O O 0.0000 30
O 0.400675018 4.129379985 7.741122745 CORE 31 O O 0.0000 31
O 3.527896421 0.895143724 7.874863575 CORE 32 O O 0.0000 32
O 1.217167126 1.580997179 8.506959225 CORE 33 O O 0.0000 33
O 4.516476661 8.125441406 8.888494750 CORE 34 O O 0.0000 34
O -0.414876937 6.214295496 0.011180533 CORE 35 O O 0.0000 35
P 7.624309794 3.055600845 0.990674419 CORE 36 P P 0.0000 36
O 2.632512113 2.527791871 4.666611837 CORE 37 O O 0.0000 37
H 1.735870934 2.225370827 4.859408751 CORE 38 H H 0.0000 38
C 2.852905477 3.782768506 5.338799014 CORE 39 C C 0.0000 39
H 3.658621739 4.290919930 4.804689165 CORE 40 H H 0.0000 40
H 3.155160172 3.631961613 6.383698190 CORE 41 H H 0.0000 41
H 1.963668468 4.420137699 5.313720358 CORE 42 H H 0.0000 42
H 5.511726274 1.933417753 3.222248723 CORE 43 H H 0.0000 43
C 5.648637569 1.689797790 4.273701625 CORE 44 C C 0.0000 44
H 5.635964094 2.594151673 4.877337437 CORE 45 H H 0.0000 45
H 4.889900115 0.988791847 4.606172139 CORE 46 H H 0.0000 46
end
end

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CH₃S

!BIOSYM archive 2

PBC=ON

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Energy 36 -254 -254.589128
!DATE
PBC 9.3040 9.3040 9.3040 94.5972 94.5972 94.5972
Al 2.353654000 8.064435000 0.968225600 CORE 1 Al Al 0.0000 1
P 5.318561396 8.183297619 1.262829162 CORE 2 P P 0.0000 2
Si 7.469131904 0.617069299 6.269490773 CORE 3 Si Si 0.0000 3
Al 7.767243876 0.725727249 3.181735791 CORE 4 Al Al 0.0000 4
P 0.051704143 7.988368931 3.234884886 CORE 5 P P 0.0000 5
Al 7.682245620 6.208117233 1.327438716 CORE 6 Al Al 0.0000 6
Al -0.211134402 7.896660559 6.197983638 CORE 7 Al Al 0.0000 7
Al -0.147903530 2.498477525 8.189178728 CORE 8 Al Al 0.0000 8
P 2.164868534 0.466513028 8.318682287 CORE 9 P P 0.0000 9
P -0.069427817 5.557324110 8.256347159 CORE 10 P P 0.0000 10
Al 5.166215782 0.583254780 8.449739305 CORE 11 Al Al 0.0000 11
O 1.175574671 6.138613182 8.944161574 CORE 12 O O 0.0000 12
O 6.441826139 2.698181033 0.263362181 CORE 13 O O 0.0000 13
O 8.909514460 3.229751346 0.396922311 CORE 14 O O 0.0000 14
O 3.029039185 0.424720392 0.353819476 CORE 15 O O 0.0000 15
O 6.224344242 7.031561608 0.842740891 CORE 16 O O 0.0000 16
O 3.925496491 7.653275590 1.611784852 CORE 17 O O 0.0000 17
O 7.239409084 4.563730323 1.696222333 CORE 18 O O 0.0000 18
O 7.755697429 2.241606356 2.354521800 CORE 19 O O 0.0000 19
O 1.231228086 8.031367826 2.286132955 CORE 20 O O 0.0000 20
O 5.893239299 8.868367433 2.508578319 CORE 21 O O 0.0000 21
O 8.358920715 6.906637594 2.786944214 CORE 22 O O 0.0000 22
O 0.089834081 0.096967651 3.221993315 CORE 23 O O 0.0000 23
O 6.897834382 1.160160860 4.721442727 CORE 24 O O 0.0000 24
O 0.570754424 7.666846033 4.635625678 CORE 25 O O 0.0000 25
O 7.548216271 8.589134641 5.861080802 CORE 26 O O 0.0000 26
O 8.369188965 1.804378884 6.835718368 CORE 27 O O 0.0000 27
O 1.545965983 -0.344631240 7.182131122 CORE 28 O O 0.0000 28
O 6.142578148 0.341222840 7.080540839 CORE 29 O O 0.0000 29
O -0.440345490 6.381112811 7.029276361 CORE 30 O O 0.0000 30
O 0.257102588 4.145098951 7.802391980 CORE 31 O O 0.0000 31
O 3.553786262 0.939200832 7.883812123 CORE 32 O O 0.0000 32
O 1.322644922 1.687678162 8.651830376 CORE 33 O O 0.0000 33
O 5.210101948 9.171871353 0.112468518 CORE 34 O O 0.0000 34
O -1.249978256 5.555634354 9.237517712 CORE 35 O O 0.0000 35
P 7.589387996 3.177366452 1.157795308 CORE 36 P P 0.0000 36
C 5.604227121 1.867254200 4.633437205 CORE 37 C C 0.0000 37
H 5.727366791 2.860174025 5.065542204 CORE 38 H H 0.0000 38
H 5.333427241 1.943882793 3.582268935 CORE 39 H H 0.0000 39
H 4.860805448 1.288505213 5.176773945 CORE 40 H H 0.0000 40
end
end

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