

## Supplementary Information

# Unraveling the Mechanisms of Ketene Generation and Transformation in Syngas-to-Olefins Conversion over ZnCrO<sub>x</sub>/SAPO-34 Catalysts

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## TOF evaluation of experimental CO conversion on the ZnCrO<sub>x</sub>/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  $H^*$  ( $\rho_H$ ) 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 conditions<sup>1</sup> 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  $H^*$  ( $\rho_H$ ) 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  $\text{H}^*$  ( $\rho_H$ ) 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.

## CH<sub>3</sub>OH and CH<sub>2</sub>CO 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 CH<sub>3</sub>OH and CH<sub>2</sub>CO, 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<sup>2,3</sup> 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  $\xi_i^{ref}$  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 simulation<sup>4</sup>:

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

The derivative of free energy to the reaction coordinate  $\xi$ ,  $\frac{\partial G_i}{\partial \xi}$  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  $\xi$  and  $\sigma_i^b$  represents the variance.

In this work, the force constant K for harmonic bias potential is set to 10.0 eV Å<sup>-2</sup> to keep the appropriate overlap of  $\xi$  between windows. The z coordinate varies from 3.0 Å to 15.0 Å during the US MD sampling process. For the CH<sub>2</sub>CO 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<sup>-2</sup>.

### ➤ Diffusion Free Energy Barrier of CH<sub>3</sub>OH and CH<sub>2</sub>CO

The diffusion free energy profile of CH<sub>3</sub>OH and CH<sub>2</sub>CO 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 CH<sub>3</sub>OH diffusion profile in the acid-free system displays a diffusion free energy barrier of ~0.6 eV. For CH<sub>2</sub>CO 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 CH<sub>2</sub>CO in the AlPO-34 zeolite with the absence of acid sites has a diffusion free barrier to ~0.4 eV.

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In conclusion, the diffusion free energy of both two key intermediates, i.e.  $\text{CH}_3\text{OH}$  and  $\text{CH}_2\text{CO}$ , 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.

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## Reference

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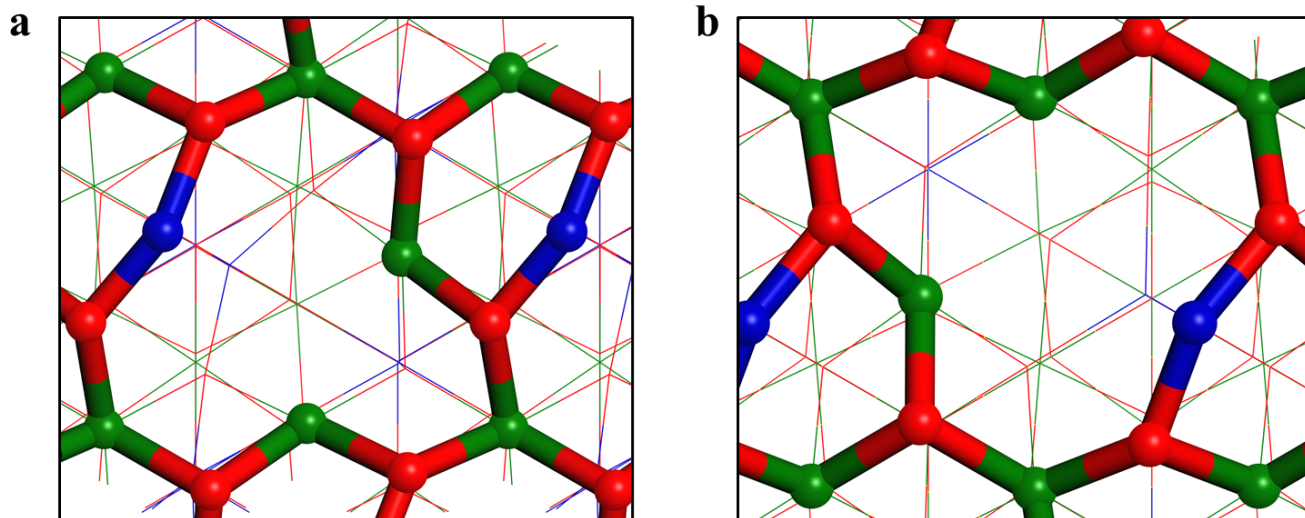


Figure S1 The structure of  $\text{ZnCrO}_x$  surface (a)  $\text{Zn}_3\text{Cr}_3\text{O}_8$  (0001) surface; (b)  $\text{ZnCr}_2\text{O}_4$  (111) surface.

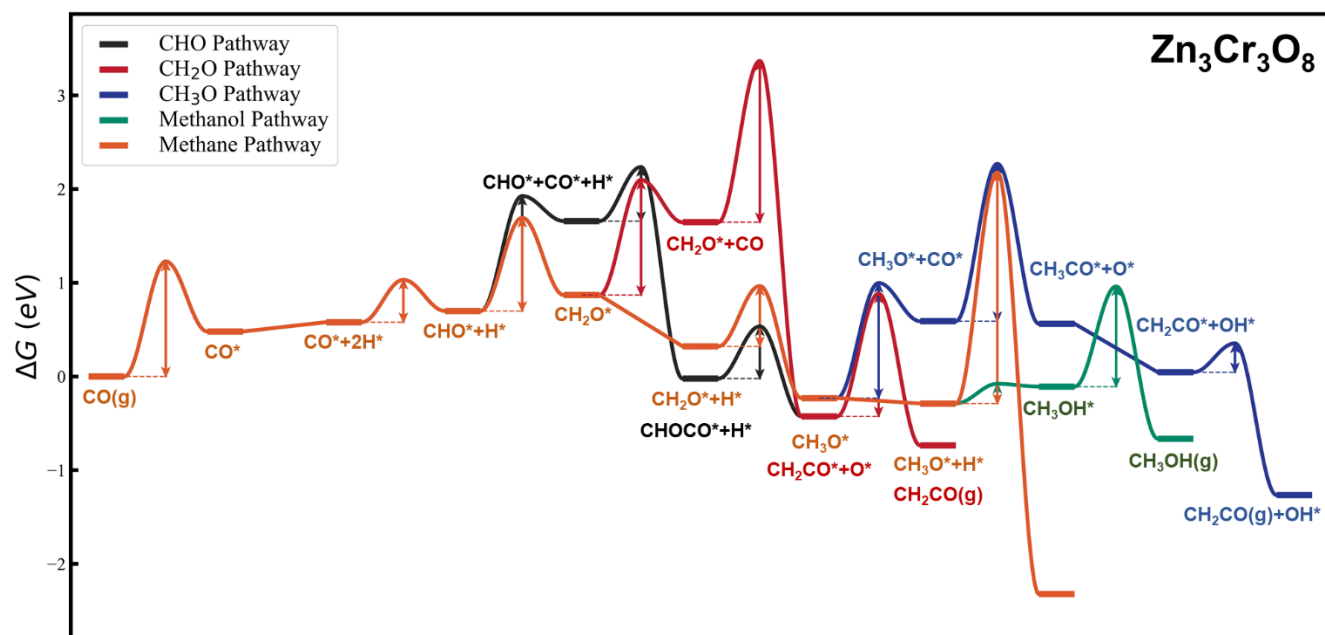


Figure S2 Gibbs free energy reaction profile of  $\text{Zn}_3\text{Cr}_3\text{O}_8$  (0001) surface catalyzed ketene, methanol and methane formation pathway (Surface adsorbed species are denoted by the symbol \*). Three ketene pathways are plotted in black, red and blue, with key C-C coupling with CO at  $\text{CHO}^*$ ,  $\text{CH}_2\text{O}^*$  and  $\text{CH}_3\text{O}^*$  respectively. The methanol and methane pathway are plotted in green and orange lines.



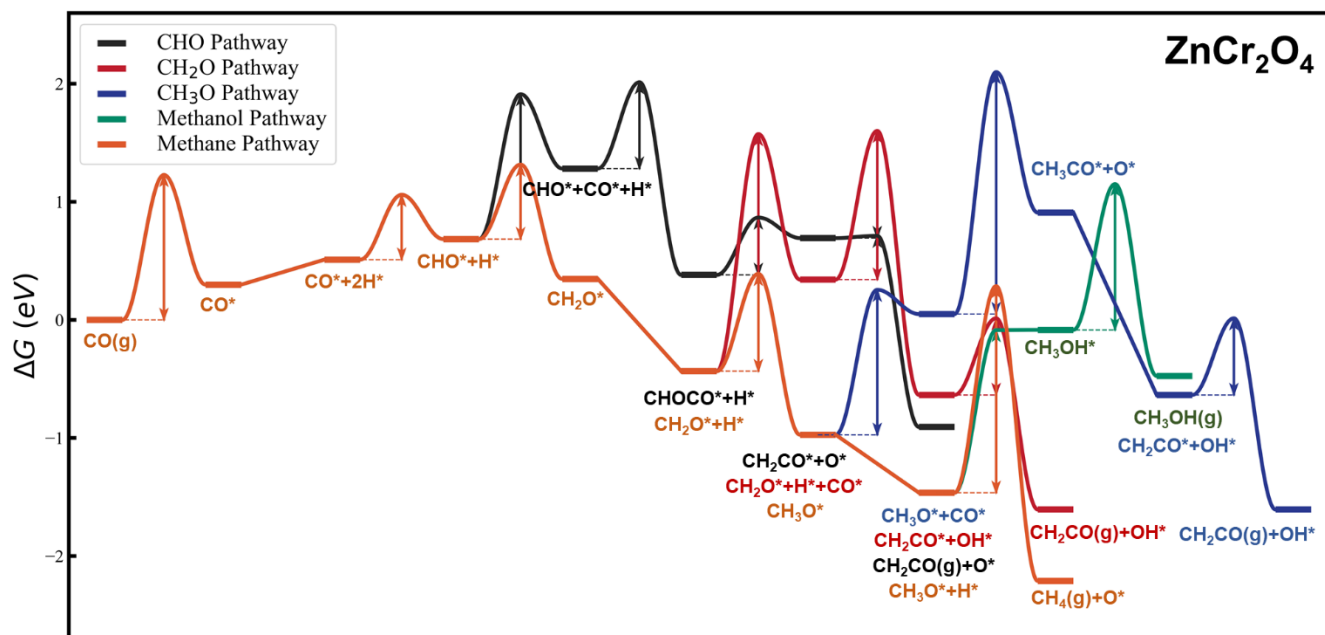


Figure S3 Gibbs free energy reaction profile of  $\text{ZnCr}_2\text{O}_4$  (111) surface catalyzed ketene, methanol and methane formation pathways (Surface adsorbed species are denoted by the symbol \*). Three ketene pathways are plotted in black, red and blue, with key C-C coupling with CO at  $\text{CHO}^*$ ,  $\text{CH}_2\text{O}^*$ ,  $\text{CH}_3\text{O}^*$  respectively. The methanol and methane pathways are plotted in green and orange lines.

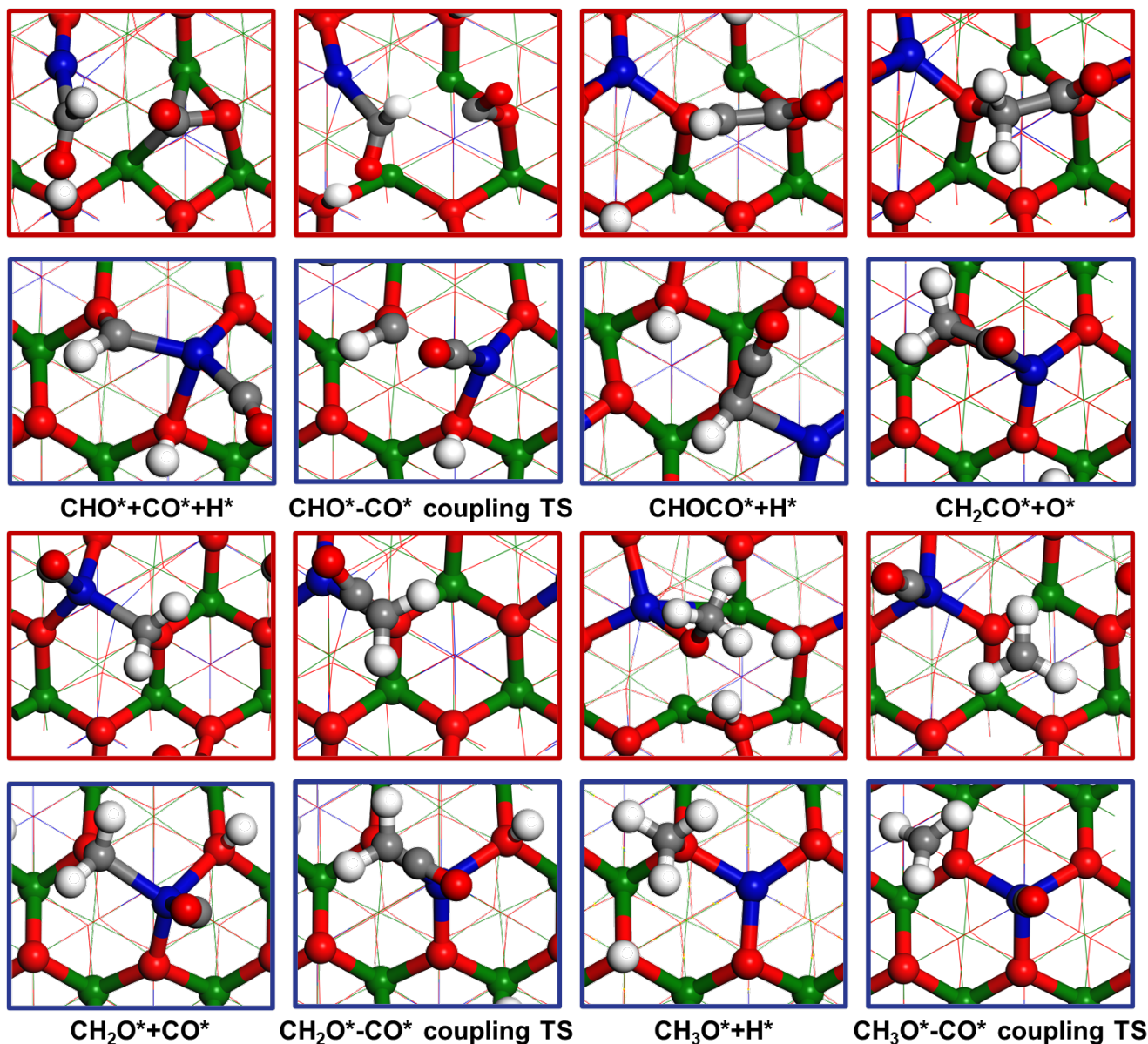


Figure S4 Surface structures of key intermediates and transition states in the C-C coupling pathway on the  $\text{Zn}_3\text{Cr}_3\text{O}_8$  (0001) and  $\text{ZnCr}_2\text{O}_4$  (111) surface (surface-adsorbed species and oxygen-containing adsorbed species are labeled with \*). The frameworks on 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.

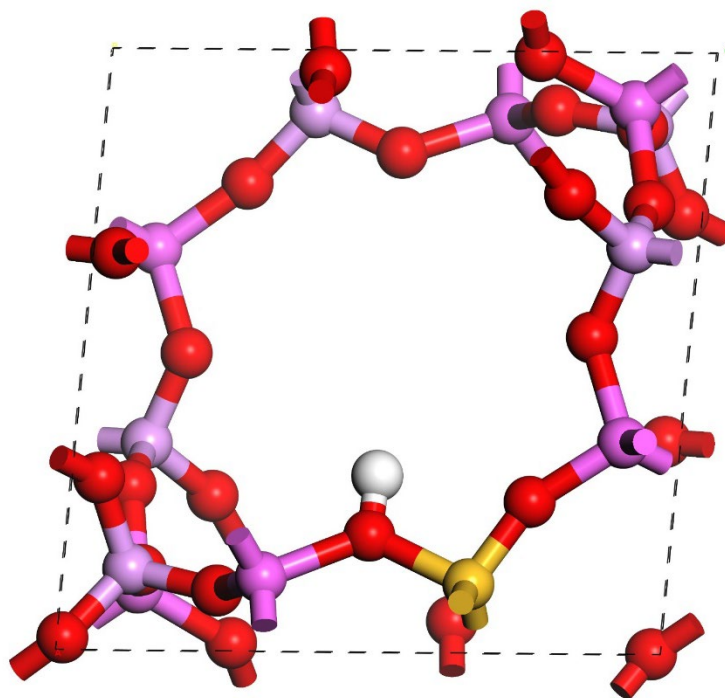


Figure S5 The active site of H site on the SAPO-34 surface.

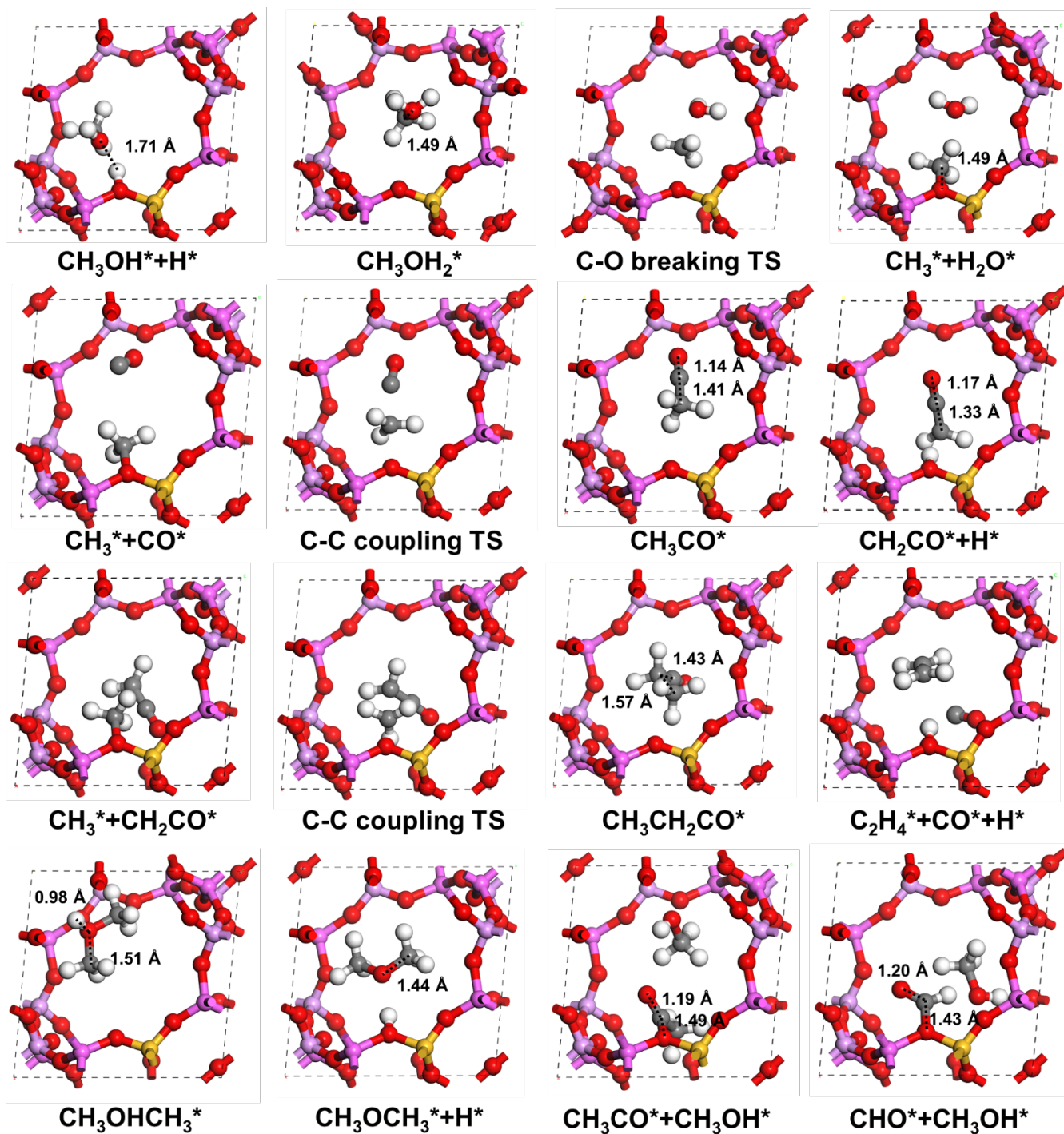


Figure S6 Surface structures of key intermediates and transition states in the C-C coupling pathway on the internal surface of SAPO-34 zeolite (surface-adsorbed species and oxygen-containing adsorbed species are labeled with \*). Al, Si, P, O, C, and H atoms are represented by purple, yellow, pink, red,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

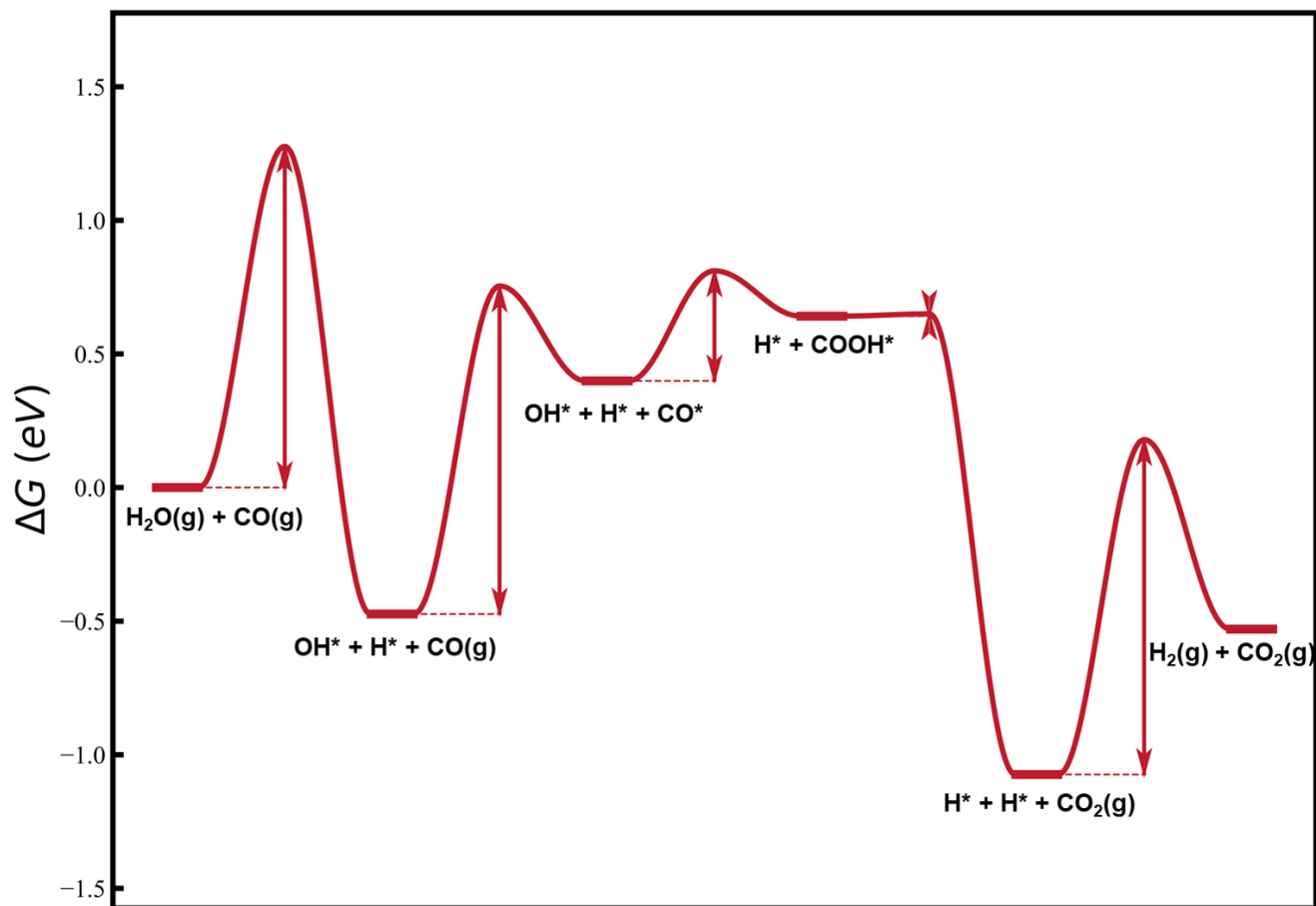


Figure S7 Gibbs free energy reaction profile of the water-gas shift (WGS) pathway catalyzed by  $\text{Zn}_3\text{Cr}_3\text{O}_8$  (0001) surface (Surface adsorbed species are denoted by the symbol \*).

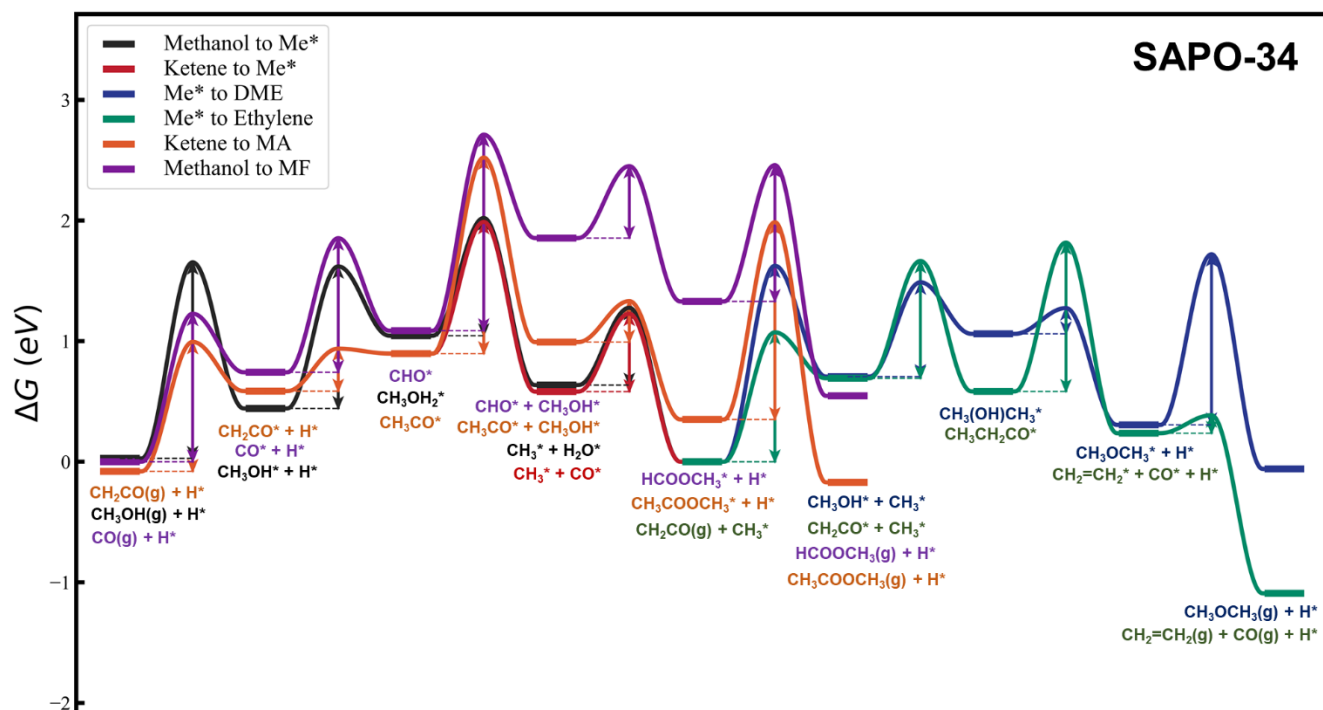


Figure S8 Gibbs free energy reaction profile of methanol and ketene reactions on SAPO-34 catalyst (Surface adsorbed species are denoted by the symbol \*). Distinct colors represent different reaction pathways: methanol to  $\text{CH}_3^*$  (black), ketene to  $\text{CH}_3^*$  (red),  $\text{CH}_3^*$  to dimethyl ether (blue),  $\text{CH}_3^*$  to ethylene (green), ketene to methyl acetate (orange), and methanol to methyl formate (purple).

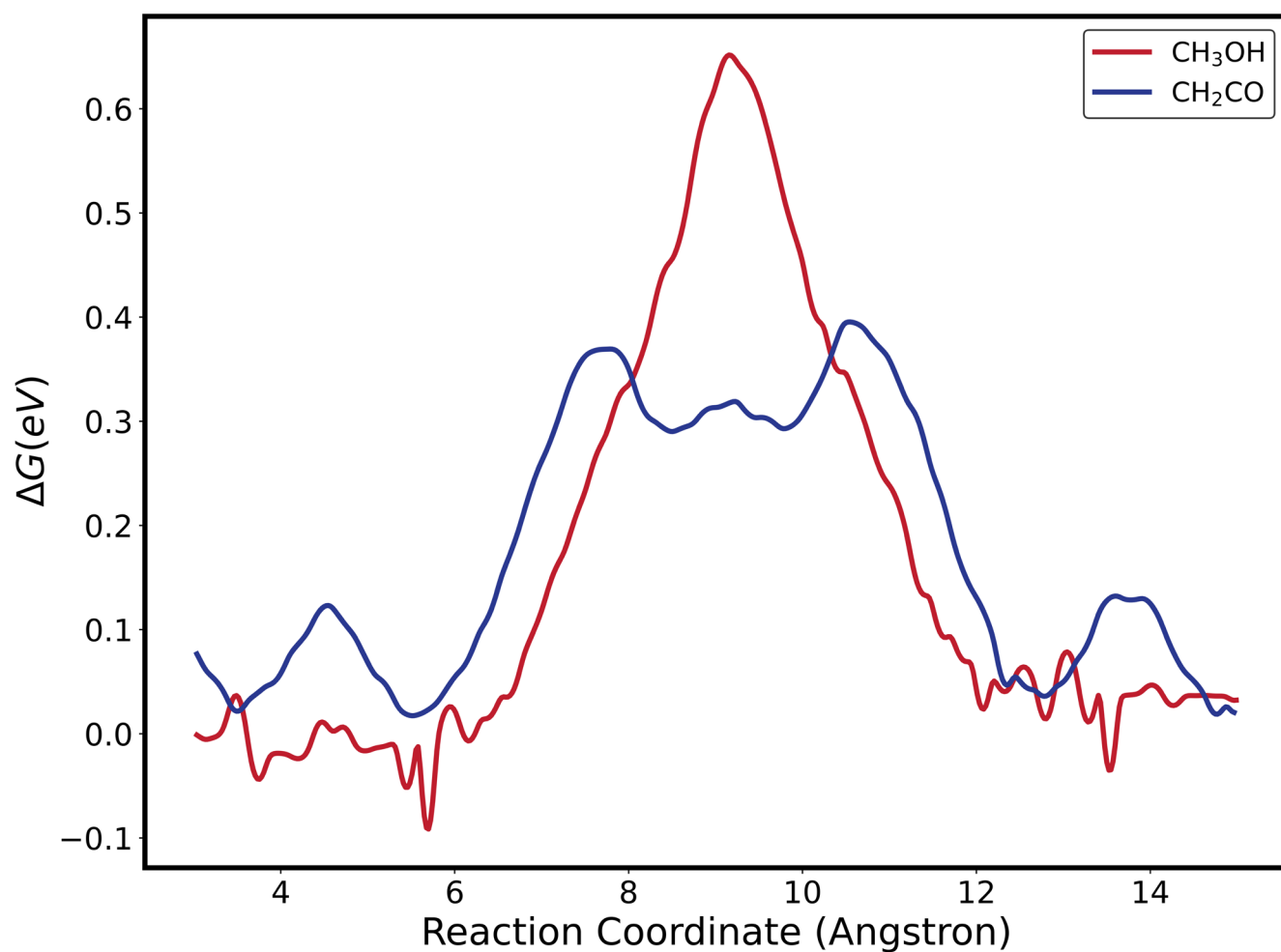


Figure S9 Diffusion free energy barriers of  $\text{CH}_3\text{OH}$  and  $\text{CH}_2\text{CO}$  in the AlPO-34 zeolite utilizing umbrella sampling molecular dynamics method.  $\text{CH}_3\text{OH}$  diffusion within the AlPO-34 is depicted in red line;  $\text{CH}_2\text{CO}$  diffusion in the AlPO-34 are depicted in blue line.



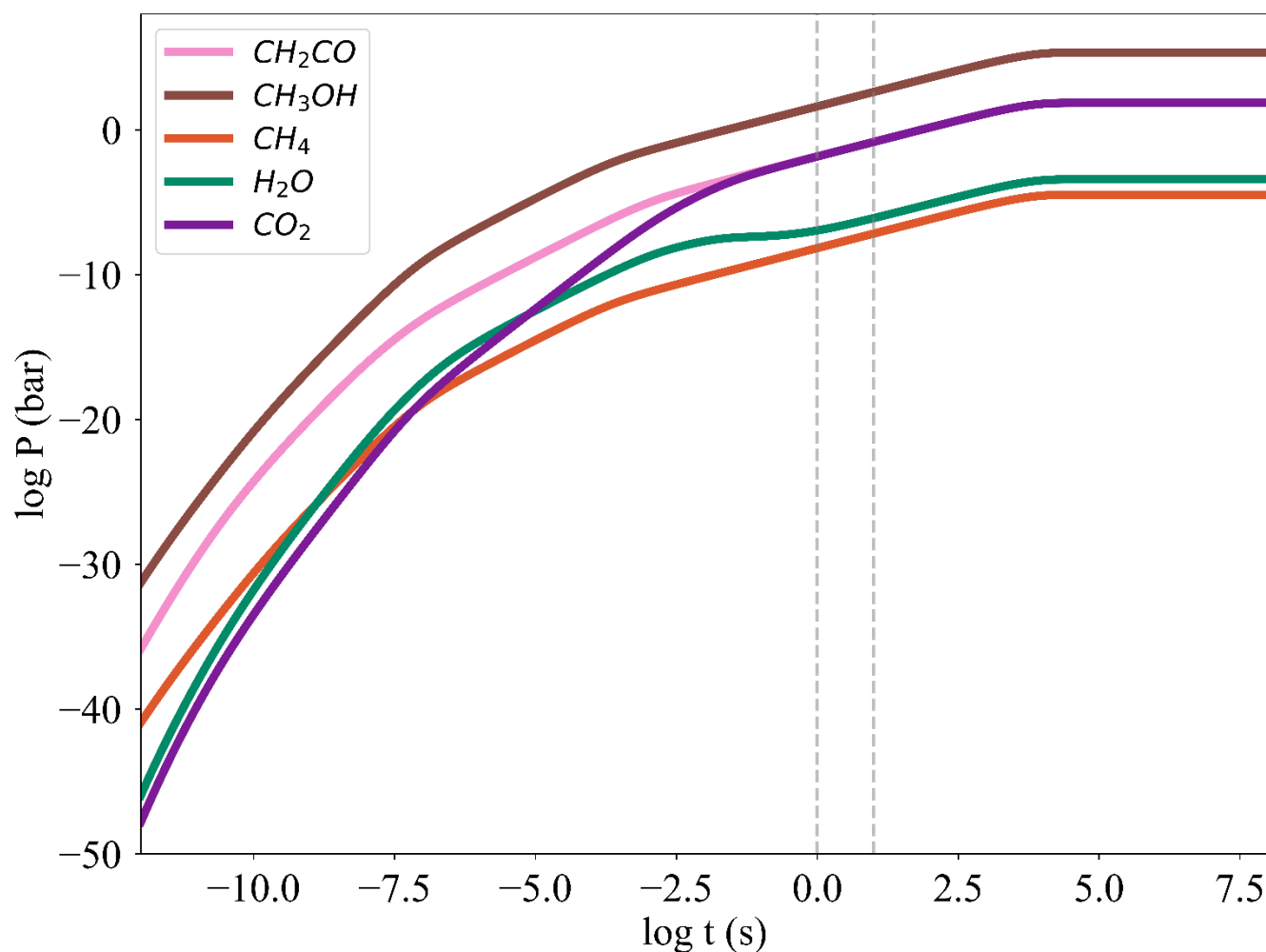


Figure S10 Microkinetic simulation results illustrating the partial pressures of  $CH_2CO$  (pink),  $CH_3OH$  (brown),  $CH_4$  (orange),  $CO_2$  (purple), and  $H_2O$  (green) as a function of time for the  $Zn_3Cr_3O_8$  (0001) surface. Simulations were conducted under typical reaction conditions ( $T = 673$  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.



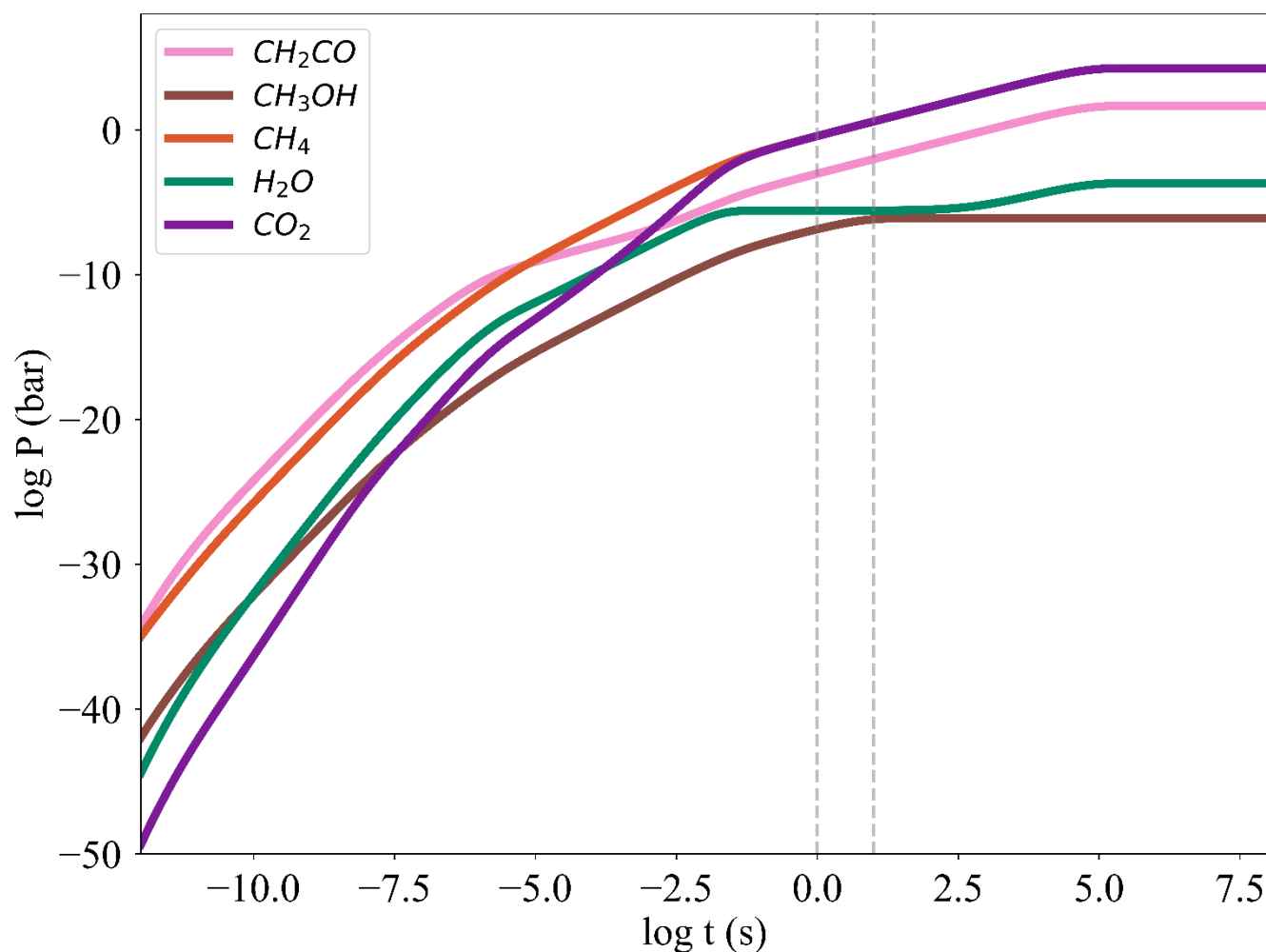


Figure S11 Microkinetic simulation results illustrating the partial pressures of  $CH_2CO$  (pink),  $CH_3OH$  (brown),  $CH_4$  (orange),  $CO_2$  (purple), and  $H_2O$  (green) as a function of time for the  $ZnCr_2O_4$  (111) surface. Simulations were conducted under typical reaction conditions ( $T = 673$  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.

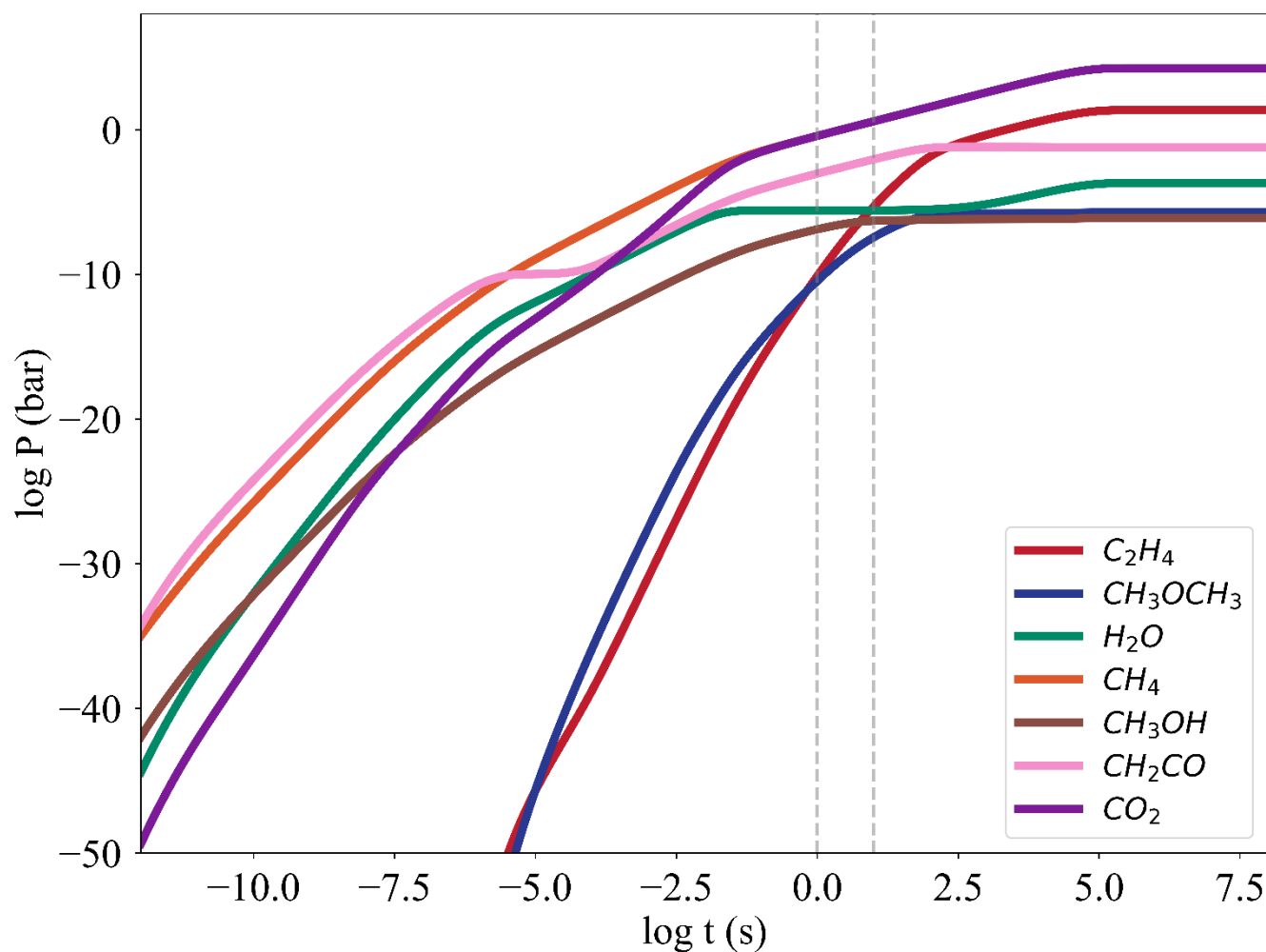


Figure S12 Microkinetic simulation results illustrating the partial pressures of  $C_2H_4$  (red),  $CH_3OCH_3$  (blue),  $H_2O$  (green),  $CH_4$  (orange),  $CH_3OH$  (brown),  $CH_2CO$  (pink), and  $CO_2$  (purple) as a function of time for the  $ZnCr_2O_4|SAPO-34$  catalytic system. Simulations 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.





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



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  $\text{ZnCr}_2\text{O}_4$  (111) | SAPO-34 surface. (#1-#3 indicate three distinct sites on the  $\text{ZnCr}_2\text{O}_4$  (111) surface: the Zn site, O site and  $\text{Cr}_2$  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  $\text{SiO}_4$  tetrahedron and #5 represents the physical adsorption on the 8-MR inner surface).

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

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

| name    | $N_{atom}$ | $E_{G-NN}$ | $E_{DFT}$ | $\Delta E$ (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

➤ Zn<sub>3</sub>Cr<sub>2</sub>O<sub>8</sub> (0001) surface

CH<sub>3</sub>CO\* + 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
```

CH<sub>3</sub>CO\* + 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
```

CH<sub>3</sub>CO\* + 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 | 2.569721107 | 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 |

CH<sub>2</sub>O\*

!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 |

CH<sub>2</sub>O\* + 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

# CH<sub>3</sub>O\* + 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

# CH<sub>3</sub>O\* + 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

```

# **CH<sub>3</sub>CO\* + 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    16.121859007 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

```

# **CH<sub>3</sub>O\***

'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    1.637009730    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
C      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

```

# CH<sub>3</sub>OH\* + 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    |              |             |              |         |          |           |

# CH<sub>3</sub>O\* + 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 | 5.534058000  | 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      | 1.687852314  | 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    |              |             |              |         |          |           |

# CH<sub>3</sub>O\* + 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 2.542335052 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 2.55470035 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
end
end

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

| IDate | Energy       | 15          | -285         | -285.371745 |          |    |        |    |  |
|-------|--------------|-------------|--------------|-------------|----------|----|--------|----|--|
| PBC   | 5.9415       | 5.9415      | 25.2282      | 90.0000     | 120.0000 |    |        |    |  |
| Cr    | 0.142146988  | 3.422872504 | 1.652441846  | CORE        | 1 Cr     | Cr | 0.0000 | 1  |  |
| Cr    | 3.114463007  | 3.242191323 | 1.679979723  | CORE        | 2 Cr     | Cr | 0.0000 | 2  |  |
| Cr    | 4.600052329  | 0.85032375  | 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  | 3.194240000 | 6.617609000  | CORE        | 5 Cr     | Cr | 0.0000 | 5  |  |
| Cr    | 1.642320000  | 2.505680000 | 6.615087000  | CORE        | 6 Cr     | Cr | 0.0000 | 6  |  |
| Cr    | 3.171877254  | 1.667111585 | 11.734823685 | CORE        | 7 Cr     | Cr | 0.0000 | 7  |  |
| Cr    | 0.190201441  | 1.563804000 | 11.578231474 | CORE        | 8 Cr     | Cr | 0.0000 | 8  |  |
| Cr    | -1.296997831 | 4.158048058 | 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  | 0.854356591 | 3.54527273   | CORE        | 11 Zn    | Zn | 0.0000 | 11 |  |
| Zn    | 1.636290462  | 4.27610450  | 4.21013200   | CORE        | 12 Zn    | Zn | 0.0000 | 12 |  |
| Zn    | -1.326089460 | 2.558185046 | 4.779329869  | CORE        | 13 Zn    | Zn | 0.0000 | 13 |  |
| Zn    | -1.309804664 | 2.544370795 | 8.309504848  | CORE        | 14 Zn    | Zn | 0.0000 | 14 |  |
| Zn    | 1.611035118  | 0.881180609 | 9.066485716  | CORE        | 15 Zn    | Zn | 0.0000 | 15 |  |
| Zn    | 2.054979198  | 3.956960294 | 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 | 0.678558314  | CORE        | 20 O     | O  | 0.0000 | 20 |  |
| O     | 1.616981300  | 4.288656453 | 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 | 2.77251126   | CORE        | 23 O     | O  | 0.0000 | 23 |  |
| O     | 1.593797180  | 2.695783865 | 2.768836641  | 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     | 4.611979000  | 0.713714500 | 5.535799000  | CORE        | 28 O     | O  | 0.0000 | 28 |  |
| O     | 1.623490000  | 0.845225000 | 5.530709000  | CORE        | 29 O     | O  | 0.0000 | 29 |  |
| O     | 0.644488000  | 4.271580000 | 6.688042000  | CORE        | 30 O     | O  | 0.0000 | 30 |  |
| O     | 1.288341000  | 1.624328000 | 7.797532000  | CORE        | 31 O     | O  | 0.0000 | 31 |  |
| O     | -1.333926000 | 4.240799000 | 7.786684000  | CORE        | 32 O     | O  | 0.0000 | 32 |  |
| O     | 2.996641700  | 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     | -2.166187935 | 5.122038000 | 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 12.687290177 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



```

!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\* + CO<sub>2</sub>

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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

```

|     |              |             |              |      |    |   |   |        |    |
|-----|--------------|-------------|--------------|------|----|---|---|--------|----|
| 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\* + H<sub>2</sub>\*

!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 7.786683930 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 2.773373759 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 7.786683930 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

# H<sub>2</sub>\*

!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    | 4.612332337  | 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

| PBC=ON |              |             |              |             |         |          |        |    |  |
|--------|--------------|-------------|--------------|-------------|---------|----------|--------|----|--|
| Energy |              | 30          | -261         | -261.574528 |         |          |        |    |  |
| !DATE  |              |             |              |             |         |          |        |    |  |
| PBC    | 5.9415       | 5.9415      | 25.2282      | 90.0000     | 90.0000 | 120.0000 |        |    |  |
| Cr     | 0.158146206  | 3.394132504 | 1.643474879  | CORE        | 1       | Cr Cr    | 0.0000 | 1  |  |
| Cr     | 3.131315770  | 3.394741756 | 1.644115465  | CORE        | 2       | Cr Cr    | 0.0000 | 2  |  |
| Cr     | 4.615739913  | 0.822228709 | 1.670165192  | 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     | 3.17059125   | 1.706411880 | 11.731068460 | CORE        | 7       | Cr Cr    | 0.0000 | 7  |  |
| Cr     | 0.110394125  | 1.597137134 | 11.587681921 | CORE        | 8       | Cr Cr    | 0.0000 | 8  |  |
| Cr     | -1.317950010 | 4.170970362 | 11.636241480 | CORE        | 9       | Cr Cr    | 0.0000 | 9  |  |
| Zn     | 1.646569273  | 0.844459952 | 0.351579114  | CORE        | 10      | Zn Zn    | 0.0000 | 10 |  |
| Zn     | 1.644254343  | 0.815387418 | 3.531836428  | CORE        | 11      | Zn Zn    | 0.0000 | 11 |  |
| Zn     | 1.642277591  | 4.268879257 | 4.169485483  | CORE        | 12      | Zn Zn    | 0.0000 | 12 |  |
| Zn     | -1.329018459 | 2.561091209 | 4.761992464  | CORE        | 13      | Zn Zn    | 0.0000 | 13 |  |
| Zn     | -1.311057523 | 2.548618947 | 8.230465040  | CORE        | 14      | Zn Zn    | 0.0000 | 14 |  |
| Zn     | 1.613113310  | 0.865586916 | 9.066161696  | CORE        | 15      | Zn Zn    | 0.0000 | 15 |  |
| Zn     | 2.053634764  | 3.978394496 | 9.494663871  | CORE        | 16      | Zn Zn    | 0.0000 | 16 |  |
| Zn     | 1.772498001  | 4.169257664 | 12.965540766 | CORE        | 17      | Zn Zn    | 0.0000 | 17 |  |
| O      | 0.062697852  | 1.797193160 | 0.667731467  | CORE        | 18      | O O      | 0.0000 | 18 |  |
| O      | 3.228563482  | 1.799172522 | 0.666680355  | CORE        | 19      | O O      | 0.0000 | 19 |  |
| O      | -1.326013956 | 4.141951240 | 0.679911283  | CORE        | 20      | O O      | 0.0000 | 20 |  |
| O      | 1.645044032  | 4.239226361 | 0.681727686  | CORE        | 21      | O O      | 0.0000 | 21 |  |
| O      | -1.326086677 | 2.548244592 | 2.762062221  | CORE        | 22      | O O      | 0.0000 | 22 |  |
| O      | 0.251954081  | 5.015685502 | 2.780415113  | CORE        | 23      | O O      | 0.0000 | 23 |  |
| O      | 1.644671390  | 2.669992298 | 2.770961404  | CORE        | 24      | O O      | 0.0000 | 24 |  |
| O      | 3.036498614  | 5.014183995 | 2.781704137  | 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      | 1.660141258  | 0.760376880 | 12.709717974 | CORE        | 34      | O O      | 0.0000 | 34 |  |
| O      | -2.617375053 | 5.121585481 | 10.481755197 | CORE        | 35      | O O      | 0.0000 | 35 |  |
| O      | 1.674775818  | 2.422118308 | 10.607139609 | CORE        | 36      | O O      | 0.0000 | 36 |  |
| O      | -1.327391049 | 2.480469675 | 10.575412810 | CORE        | 37      | O O      | 0.0000 | 37 |  |
| O      | 4.626911680  | 0.848153733 | 12.709792925 | CORE        | 38      | O O      | 0.0000 | 38 |  |
| O      | 0.049380001  | 3.221843381 | 12.883137810 | CORE        | 39      | O O      | 0.0000 | 39 |  |
| O      | 3.343478216  | 3.205729976 | 12.962469053 | CORE        | 40      | O O      | 0.0000 | 40 |  |
| H      | -0.570392580 | 2.961078720 | 13.601983470 | CORE        | 41      | H H      | 0.0000 | 41 |  |
| H      | 1.652479241  | 0.739359743 | 13.681837589 | CORE        | 42      | H H      | 0.0000 | 42 |  |
| end    |              |             |              |             |         |          |        |    |  |
| end    |              |             |              |             |         |          |        |    |  |

# OH\* + H\* + CO\*

| !BIOSYM archive 2 |              |             |              |             |         |          |        |    |  |
|-------------------|--------------|-------------|--------------|-------------|---------|----------|--------|----|--|
| PBC=ON            |              |             |              |             |         |          |        |    |  |
| Energy            |              | 31          | -276         | -276.557383 |         |          |        |    |  |
| !DATE             |              |             |              |             |         |          |        |    |  |
| PBC               | 5.9415       | 5.9415      | 25.2282      | 90.0000     | 90.0000 | 120.0000 |        |    |  |
| Cr                | 0.157982893  | 3.396939687 | 1.649038762  | CORE        | 1       | Cr Cr    | 0.0000 | 1  |  |
| Cr                | 3.131603939  | 3.398072014 | 1.650149045  | CORE        | 2       | Cr Cr    | 0.0000 | 2  |  |
| Cr                | 4.616492549  | 0.825776145 | 1.675079451  | 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                | 3.175797702  | 1.753351499 | 11.741695534 | CORE        | 7       | Cr Cr    | 0.0000 | 7  |  |
| Cr                | 0.117658962  | 1.619896436 | 11.575695557 | CORE        | 8       | Cr Cr    | 0.0000 | 8  |  |
| Cr                | -1.316772421 | 4.207499185 | 11.620752392 | CORE        | 9       | Cr Cr    | 0.0000 | 9  |  |
| Zn                | 1.647118148  | 0.847246476 | 0.358110583  | CORE        | 10      | Zn Zn    | 0.0000 | 10 |  |
| Zn                | 1.644362123  | 0.817637761 | 3.542096965  | CORE        | 11      | Zn Zn    | 0.0000 | 11 |  |
| Zn                | 1.642493010  | 4.269725630 | 4.176220843  | CORE        | 12      | Zn Zn    | 0.0000 | 12 |  |
| Zn                | -1.328394794 | 2.561305286 | 4.774220786  | CORE        | 13      | Zn Zn    | 0.0000 | 13 |  |
| Zn                | -1.309862117 | 2.549386100 | 8.269479894  | CORE        | 14      | Zn Zn    | 0.0000 | 14 |  |
| Zn                | 1.616788658  | 0.872651249 | 9.068372285  | CORE        | 15      | Zn Zn    | 0.0000 | 15 |  |
| Zn                | 2.059145186  | 3.988647500 | 9.507454424  | CORE        | 16      | Zn Zn    | 0.0000 | 16 |  |
| Zn                | 1.757503762  | 4.240833360 | 13.327212071 | CORE        | 17      | Zn Zn    | 0.0000 | 17 |  |
| O                 | 0.062268421  | 1.799958140 | 0.672973959  | CORE        | 18      | O O      | 0.0000 | 18 |  |
| O                 | 3.229780069  | 1.801358598 | 0.671204269  | CORE        | 19      | O O      | 0.0000 | 19 |  |
| O                 | -1.325162430 | 4.144050238 | 0.683482161  | CORE        | 20      | O O      | 0.0000 | 20 |  |
| O                 | 1.645181985  | 4.242334226 | 0.686137276  | CORE        | 21      | O O      | 0.0000 | 21 |  |
| O                 | -1.325958383 | 2.551303699 | 2.766630606  | CORE        | 22      | O O      | 0.0000 | 22 |  |
| O                 | 0.252294468  | 5.018926344 | 2.782468750  | CORE        | 23      | O O      | 0.0000 | 23 |  |
| O                 | 1.644750502  | 2.672684584 | 2.773912566  | CORE        | 24      | O O      | 0.0000 | 24 |  |
| O                 | 3.036265822  | 5.017444330 | 2.783651118  | 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                 | 1.669211883  | 0.791912893 | 12.703006831 | CORE        | 34      | O O      | 0.0000 | 34 |  |
| O                 | -2.616740424 | 5.144863674 | 10.467221033 | CORE        | 35      | O O      | 0.0000 | 35 |  |
| O                 | 1.690224793  | 2.405928258 | 10.573291616 | CORE        | 36      | O O      | 0.0000 | 36 |  |
| O                 | -1.324037515 | 2.511055615 | 10.563483310 | CORE        | 37      | O O      | 0.0000 | 37 |  |
| O                 | 4.636523921  | 0.859790388 | 12.687466754 | CORE        | 38      | O O      | 0.0000 | 38 |  |
| O                 | 0.059316951  | 3.258813031 | 12.861392701 | CORE        | 39      | O O      | 0.0000 | 39 |  |
| O                 | 3.336428408  | 3.279238665 | 12.947050581 | CORE        | 40      | O O      | 0.0000 | 40 |  |
| H                 | -0.621896553 | 2.976548104 | 13.518456247 | CORE        | 41      | H H      | 0.0000 | 41 |  |
| H                 | 1.655240478  | 0.735605365 | 13.672674175 | CORE        | 42      | H H      | 0.0000 | 42 |  |
| O                 | 1.916506753  | 3.194911653 | 16.369953947 | CORE        | 43      | O O      | 0.0000 | 43 |  |
| C                 | 1.686397553  | 3.851122341 | 15.453880344 | CORE        | 44      | C C      | 0.0000 | 44 |  |
| end               |              |             |              |             |         |          |        |    |  |
| end               |              |             |              |             |         |          |        |    |  |

# TS CH<sub>3</sub>O\* + CO\* to CH<sub>3</sub>CO\* + O\*

| !BIOSYM archive 2 |              |             |              |             |         |          |        |    |  |
|-------------------|--------------|-------------|--------------|-------------|---------|----------|--------|----|--|
| PBC=ON            |              |             |              |             |         |          |        |    |  |
| Energy            |              | 32          | -281         | -281.865888 |         |          |        |    |  |
| !DATE             |              |             |              |             |         |          |        |    |  |
| PBC               | 5.9415       | 5.9415      | 25.2282      | 90.0000     | 90.0000 | 120.0000 |        |    |  |
| Cr                | 0.181816308  | 3.348393099 | 1.565706826  | CORE        | 1       | Cr Cr    | 0.0000 | 1  |  |
| Cr                | 3.162441050  | 3.345733782 | 1.566885986  | CORE        | 2       | Cr Cr    | 0.0000 | 2  |  |
| Cr                | 4.643815451  | 0.777646200 | 1.596053063  | CORE        | 3       | Cr Cr    | 0.0000 | 3  |  |
| Cr                | -2.789902014 | 5.144116340 | 6.400437892  | CORE        | 4       | Cr Cr    | 0.0000 | 4  |  |
| Cr                | 3.149368407  | 0.011013835 | 6.461186770  | CORE        | 5       | Cr Cr    | 0.0000 | 5  |  |
| Cr                | 1.686305460  | 2.571235353 | 6.548538423  | CORE        | 6       | Cr Cr    | 0.0000 | 6  |  |
| Cr                | 3.176734445  | 1.788713673 | 11.646873597 | CORE        | 7       | Cr Cr    | 0.0000 | 7  |  |
| Cr                | 0.206801521  | 1.704726988 | 11.527399483 | CORE        | 8       | Cr Cr    | 0.0000 | 8  |  |
| Cr                | -1.352516373 | 4.228385063 | 11.668280789 | CORE        | 9       | Cr Cr    | 0.0000 | 9  |  |
| Zn                | 1.676692326  | 0.805122866 | 0.253638786  | CORE        | 10      | Zn Zn    | 0.0000 | 10 |  |
| Zn                | 1.673811025  | 0.773015933 | 3.447112485  | CORE        | 11      | Zn Zn    | 0.0000 | 11 |  |
| Zn                | 1.663419562  | 4.170448056 | 4.047886857  | CORE        | 12      | Zn Zn    | 0.0000 | 12 |  |
| Zn                | -1.273789039 | 2.551962860 | 4.678620611  | CORE        | 13      | Zn Zn    | 0.0000 | 13 |  |
| Zn                | -1.269474807 | 2.597924827 | 8.344137047  | CORE        | 14      | Zn Zn    | 0.0000 | 14 |  |
| Zn                | 1.616755976  | 0.879277432 | 8.976273708  | CORE        | 15      | Zn Zn    | 0.0000 | 15 |  |

|    |              |             |              |      |    |    |    |        |    |
|----|--------------|-------------|--------------|------|----|----|----|--------|----|
| 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 CH<sub>3</sub>O\* + H\* to CH<sub>3</sub>O\*

!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 CH<sub>3</sub>O\* + CO\* to CH<sub>3</sub>CO\* + 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 CH<sub>3</sub>O + H\* + H\* to CH<sub>3</sub>OH\* + 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 CH<sub>3</sub>O\* + H\* + H\* to CH<sub>3</sub> + 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  | 6.559493916 | 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 CH<sub>3</sub>CO\* + O\***

<sup>1</sup>BIOSYM archive 2

PBC=ON

Energy 37 -276 -276.228167

<sup>1</sup>DATE

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 0.028650000 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 CH<sub>3</sub>CO\* + O\***

<sup>1</sup>BIOSYM archive 2

PBC=ON

Energy 38 -284 -284.753011

<sup>1</sup>DATE

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\***

<sup>1</sup>BIOSYM archive 2

PBC=ON

Energy 39 -274 -274.909824

<sup>1</sup>DATE

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 CH<sub>3</sub>O\*

!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

➤ ZnCr<sub>2</sub>O<sub>4</sub> (11) surfaceCH<sub>3</sub>CO\* + O\*

'BIOSYM archive 2

PBC=ON

| Energy |              | 0      | -310        | -310.212153 |              |         |                    |  |
|--------|--------------|--------|-------------|-------------|--------------|---------|--------------------|--|
| IDATE  |              |        |             |             |              |         |                    |  |
| 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     | -2.499933000 |        | 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     | 1.991742191  |        | 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      | 1.17029647   |        | 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    |              |        |             |             |              |         |                    |  |

CH<sub>3</sub>CO\* + 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 |             | 4.262435318  | 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  |        | 3.110570121 |             | 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    |              |        |             |             |              |         |          |           |

CH<sub>3</sub>O\*

'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

# CH<sub>2</sub>O\* + 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

# CH<sub>2</sub>O + 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

CH<sub>3</sub>CO\* + 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

CH<sub>3</sub>O\*

!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

|     |              |              |              |      |    |   |   |        |    |
|-----|--------------|--------------|--------------|------|----|---|---|--------|----|
| 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  | 1.4963711041 | 12.881675536 | CORE | 41 | O | O | 0.0000 | 41 |
| C   | 0.011033190  | 1.2835057719 | 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 |              |              |              |      |    |   |   |        |    |

# CH<sub>3</sub>OH\*

!BIOSYM archive 2

PBC=ON

| 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     | 4.590866226  | 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  | 2.462460967 | 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    |              |             |              |         |         |          |    |        |    |

# CH<sub>3</sub>O\* + CO\*

!BIOSYM archive 2

PBC=ON

| 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 |



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

CH<sub>3</sub>O\* + 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   |              |             |              |             |          |          |    |
| Cr    | 5.9865       | 5.9865      | 25.4420      | 90.0000     | 90.0000  | 120.0000 |    |
| Cr    | 3.498226559  | 1.446606084 | 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  | 0.576298518 | 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 | 2.000575759 | 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   |              |             |              |             |          |          |    |
| Cr    | 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 |

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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      -2.680755464      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  | 4.980259053 | 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   | -2.606808685 | 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 |  |

|     |              |             |              |      |    |   |   |        |    |
|-----|--------------|-------------|--------------|------|----|---|---|--------|----|
| 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 |              |             |              |      |    |   |   |        |    |

TS CH<sub>2</sub>O\* + H\* + CO\* to CH<sub>3</sub>CO\* + OH\*

!BIOSYM archive 2

PBC=ON

| 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      | 0.766883389  | 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    |              |             |              |         |         |          |    |        |    |

TS CH<sub>2</sub>O\* + H\* to CH<sub>3</sub>O\*

!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 | 7.87284394   | 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 CH<sub>2</sub>O\* + CO\* to CH<sub>3</sub>CO\* + O\*

|                  |              |             |              |             |         |          |        |    |  |  |
|------------------|--------------|-------------|--------------|-------------|---------|----------|--------|----|--|--|
| BIOSYM archive 2 |              |             |              |             |         |          |        |    |  |  |
| PBC=ON           |              |             |              |             |         |          |        |    |  |  |
| Energy           |              | 25          | -312         | -312.158094 |         |          |        |    |  |  |
| DATE             |              |             |              |             |         |          |        |    |  |  |
| PBC              | 5.9865       | 5.9865      | 25.4420      | 90.0000     | 90.0000 | 120.0000 |        |    |  |  |
| Cr               | 3.497331169  | 1.446946827 | 1.780427382  | CORE        | 1       | Cr Cr    | 0.0000 | 1  |  |  |
| Cr               | -1.003835780 | 4.019228153 | 1.780242000  | CORE        | 2       | Cr Cr    | 0.0000 | 2  |  |  |
| Cr               | 0.480372508  | 1.447496303 | 1.779000855  | CORE        | 3       | Cr Cr    | 0.0000 | 3  |  |  |
| Cr               | 1.989328124  | 0.576355398 | 4.266043351  | 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  | 2.304373416 | 6.721013140  | CORE        | 7       | Cr Cr    | 0.0000 | 7  |  |  |
| Cr               | 1.986864458  | 4.035209177 | 9.172068059  | CORE        | 8       | Cr Cr    | 0.0000 | 8  |  |  |
| Cr               | 3.487198789  | 3.169692394 | 11.675189714 | CORE        | 9       | Cr Cr    | 0.0000 | 9  |  |  |
| Cr               | 4.963131169  | 0.588018065 | 11.644469101 | CORE        | 10      | Cr Cr    | 0.0000 | 10 |  |  |
| Cr               | 0.474472014  | 3.182206497 | 11.642786855 | CORE        | 11      | Cr Cr    | 0.0000 | 11 |  |  |
| Zn               | 1.991123359  | 4.032319528 | 0.502674858  | CORE        | 12      | Zn Zn    | 0.0000 | 12 |  |  |
| Zn               | 1.988471924  | 4.032761141 | 3.668745994  | CORE        | 13      | Zn Zn    | 0.0000 | 13 |  |  |
| Zn               | -1.003777266 | 2.304482984 | 4.878109697  | CORE        | 14      | Zn Zn    | 0.0000 | 14 |  |  |
| Zn               | -1.006137852 | 2.306080788 | 8.568893165  | CORE        | 15      | Zn Zn    | 0.0000 | 15 |  |  |
| Zn               | 1.989941676  | 0.577374095 | 9.787517222  | CORE        | 16      | Zn Zn    | 0.0000 | 16 |  |  |
| Zn               | 1.934193679  | 0.610303667 | 13.191416930 | CORE        | 17      | Zn Zn    | 0.0000 | 17 |  |  |
| O                | 4.983941979  | 0.691873391 | 0.816750492  | CORE        | 18      | O O      | 0.0000 | 18 |  |  |
| O                | 0.393886578  | 3.110233531 | 0.817420601  | CORE        | 19      | O O      | 0.0000 | 19 |  |  |
| O                | 3.587544613  | 3.110267306 | 0.815457917  | CORE        | 20      | O O      | 0.0000 | 20 |  |  |
| O                | 1.989084033  | 0.576342427 | 0.870973819  | CORE        | 21      | O O      | 0.0000 | 21 |  |  |
| O                | -1.004284088 | 2.304597241 | 2.882168950  | CORE        | 22      | O O      | 0.0000 | 22 |  |  |
| O                | -2.357073917 | 4.981063775 | 2.990803023  | CORE        | 23      | O O      | 0.0000 | 23 |  |  |
| O                | 1.987754805  | 2.137904474 | 2.990876683  | CORE        | 24      | O O      | 0.0000 | 24 |  |  |
| O                | 0.348667950  | 4.979643646 | 2.991181691  | 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                | 0.989912600  | 0.576201004 | 7.778738200  | 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                | -2.648672774 | 4.799894829 | 10.453667706 | CORE        | 34      | O O      | 0.0000 | 34 |  |  |
| O                | 0.632624477  | 4.818007450 | 10.430649250 | CORE        | 35      | O O      | 0.0000 | 35 |  |  |
| O                | 2.001558450  | 2.482986203 | 10.454491580 | CORE        | 36      | O O      | 0.0000 | 36 |  |  |
| O                | -1.016901172 | 2.312960283 | 10.562505659 | CORE        | 37      | O O      | 0.0000 | 37 |  |  |
| O                | 1.983304131  | 4.037442386 | 12.600338590 | CORE        | 38      | O O      | 0.0000 | 38 |  |  |
| O                | 3.511896006  | 1.538344832 | 12.589850533 | CORE        | 39      | O O      | 0.0000 | 39 |  |  |
| O                | -1.073667316 | 3.968234517 | 12.582091525 | CORE        | 40      | O O      | 0.0000 | 40 |  |  |
| O                | 0.348731409  | 1.526480914 | 12.691479513 | CORE        | 41      | O O      | 0.0000 | 41 |  |  |
| O                | 2.193824804  | 0.566369636 | 16.453089746 | CORE        | 42      | O O      | 0.0000 | 42 |  |  |
| C                | -0.492382993 | 2.092440482 | 15.079283395 | CORE        | 43      | C C      | 0.0000 | 43 |  |  |
| C                | 2.095035093  | 0.550471265 | 15.314631618 | CORE        | 44      | C C      | 0.0000 | 44 |  |  |
| H                | -1.220020478 | 2.453535035 | 14.357391378 | CORE        | 45      | H H      | 0.0000 | 45 |  |  |
| H                | 0.319403602  | 2.741634524 | 15.402341207 | CORE        | 46      | H H      | 0.0000 | 46 |  |  |
| H                | -0.635347248 | 1.128797867 | 15.565373781 | CORE        | 47      | H H      | 0.0000 | 47 |  |  |
| end              |              |             |              |             |         |          |        |    |  |  |
| end              |              |             |              |             |         |          |        |    |  |  |

# TS CH<sub>3</sub>O\* + H\* + H\* to CH<sub>3</sub>OH\*

|                  |              |             |              |             |         |          |        |    |  |  |
|------------------|--------------|-------------|--------------|-------------|---------|----------|--------|----|--|--|
| BIOSYM archive 2 |              |             |              |             |         |          |        |    |  |  |
| PBC=ON           |              |             |              |             |         |          |        |    |  |  |
| Energy           |              | 26          | -302         | -302.378758 |         |          |        |    |  |  |
| !DATE            |              |             |              |             |         |          |        |    |  |  |
| PBC              | 5.9865       | 5.9865      | 25.4420      | 90.0000     | 90.0000 | 120.0000 |        |    |  |  |
| Cr               | 3.497224658  | 1.444693197 | 1.758036361  | CORE        | 1       | Cr Cr    | 0.0000 | 1  |  |  |
| Cr               | -1.003136883 | 4.018594333 | 1.758130573  | CORE        | 2       | Cr Cr    | 0.0000 | 2  |  |  |
| Cr               | 0.482371475  | 1.444973173 | 1.757489805  | CORE        | 3       | Cr Cr    | 0.0000 | 3  |  |  |
| Cr               | 1.989883241  | 0.575398840 | 4.238719445  | 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               | 1.999578227  | 4.049769013 | 9.140493797  | CORE        | 8       | Cr Cr    | 0.0000 | 8  |  |  |
| Cr               | 3.389800097  | 3.117520016 | 11.664372795 | CORE        | 9       | Cr Cr    | 0.0000 | 9  |  |  |
| Cr               | 4.842781805  | 0.538425707 | 11.667898067 | CORE        | 10      | Cr Cr    | 0.0000 | 10 |  |  |
| Cr               | 0.442494815  | 3.221162173 | 11.502662403 | CORE        | 11      | Cr Cr    | 0.0000 | 11 |  |  |
| Zn               | 1.990495114  | 4.030640856 | 0.484155630  | CORE        | 12      | Zn Zn    | 0.0000 | 12 |  |  |
| Zn               | 1.990187606  | 4.030867679 | 3.623758967  | CORE        | 13      | Zn Zn    | 0.0000 | 13 |  |  |
| Zn               | -1.002852079 | 2.303996722 | 4.827451484  | CORE        | 14      | Zn Zn    | 0.0000 | 14 |  |  |
| Zn               | -1.010822923 | 2.298553757 | 8.545736333  | CORE        | 15      | Zn Zn    | 0.0000 | 15 |  |  |
| Zn               | 1.914278512  | 0.603195562 | 9.713410341  | CORE        | 16      | Zn Zn    | 0.0000 | 16 |  |  |
| Zn               | 1.964243566  | 0.340432898 | 12.959443947 | CORE        | 17      | Zn Zn    | 0.0000 | 17 |  |  |
| O                | 4.983399404  | 0.688596802 | 0.796751422  | CORE        | 18      | O O      | 0.0000 | 18 |  |  |
| O                | 0.394734951  | 3.109676515 | 0.796784563  | CORE        | 19      | O O      | 0.0000 | 19 |  |  |
| O                | 3.585884848  | 3.109508597 | 0.796588736  | CORE        | 20      | O O      | 0.0000 | 20 |  |  |
| O                | 1.989871851  | 0.574456066 | 0.844892759  | CORE        | 21      | O O      | 0.0000 | 21 |  |  |
| O                | -1.003543797 | 2.302850506 | 2.869676257  | CORE        | 22      | O O      | 0.0000 | 22 |  |  |
| O                | -2.355045605 | 4.979514936 | 2.994787638  | CORE        | 23      | O O      | 0.0000 | 23 |  |  |
| O                | 1.989211657  | 2.135377769 | 2.994567020  | CORE        | 24      | O O      | 0.0000 | 24 |  |  |
| O                | 0.348561749  | 4.978628506 | 2.995239720  | 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 | 7.778784000  | 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                | -2.638797847 | 4.854883421 | 10.563719595 | CORE        | 34      | O O      | 0.0000 | 34 |  |  |
| O                | 0.597201655  | 4.854386077 | 10.394934191 | CORE        | 35      | O O      | 0.0000 | 35 |  |  |
| O                | 1.938391936  | 2.475717439 | 10.414912523 | CORE        | 36      | O O      | 0.0000 | 36 |  |  |
| O                | -1.052814583 | 2.262585646 | 10.598895809 | CORE        | 37      | O O      | 0.0000 | 37 |  |  |
| O                | 1.875757071  | 4.000579719 | 12.606167602 | CORE        | 38      | O O      | 0.0000 | 38 |  |  |
| O                | 3.395070876  | 1.439093305 | 12.683728249 | CORE        | 39      | O O      | 0.0000 | 39 |  |  |
| O                | -1.031409938 | 3.656345576 | 12.869389981 | CORE        | 40      | O O      | 0.0000 | 40 |  |  |
| O                | 0.041994300  | 1.437013428 | 13.403778846 | CORE        | 41      | O O      | 0.0000 | 41 |  |  |
| C                | -0.311867532 | 0.935238716 | 14.736891109 | CORE        | 42      | C C      | 0.0000 | 42 |  |  |
| H                | 4.632715992  | 1.208748353 | 14.942544058 | CORE        | 43      | H H      | 0.0000 | 43 |  |  |
| H                | 0.361806985  | 1.394229941 | 15.475017875 | CORE        | 44      | H H      | 0.0000 | 44 |  |  |
| H                | 2.775808875  | 5.027354095 | 14.723104708 | CORE        | 45      | H H      | 0.0000 | 45 |  |  |
| H                | -0.417781400 | 2.450077884 | 13.360347832 | CORE        | 46      | H H      | 0.0000 | 46 |  |  |
| end              |              |             |              |             |         |          |        |    |  |  |



|    |              |             |              |      |    |    |    |        |    |
|----|--------------|-------------|--------------|------|----|----|----|--------|----|
| 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 CH<sub>3</sub>O\*

| !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 |             | 0.4455567751 | 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 |             | 13.729986470 | 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

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    | 1.990849492  | 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

```

# 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

```

➤ SAPO-34 surface

TS CH<sub>3</sub>CH<sub>2</sub>CO\* to HS + C<sub>2</sub>H<sub>4</sub>\* + 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  | 7.916562030  | 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  | 3.322869667 | CORE    | 44 H H   | 0.0000 44 |
| H      | 5.501235699  | 2.131502550  | 4.352108383 | CORE    | 45 H H   | 0.0000 45 |
| end    |              |              |             |         |          |           |
| end    |              |              |             |         |          |           |

TS CH<sub>3</sub>CH<sub>2</sub>CO\* to HS + CH<sub>2</sub>CH<sub>2</sub>CO\*

!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 CH<sub>3</sub>CO\* to HS CH<sub>3</sub>CO\*

!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 CH<sub>3</sub>OH<sub>2</sub><sup>+</sup> to CH<sub>3</sub>S H<sub>2</sub>O<sup>+</sup>

!BIOSYM archive 2

PBC=ON

|       | Energy       |              | 3           | -266    | -266.609484 |         |    |        |    |
|-------|--------------|--------------|-------------|---------|-------------|---------|----|--------|----|
| !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     | 5.325444183  | 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     | 8.325920004  | 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  | 2.032548146  | 2.158907374 | 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 CH<sub>3</sub>OHCH<sub>3</sub><sup>+</sup> to HS + CH<sub>3</sub>OCH<sub>3</sub><sup>+</sup>

!BIOSYM archive 2

PBC=ON

|       | Energy       |             | 4           | -284    | -284.051827 |         |    |        |    |
|-------|--------------|-------------|-------------|---------|-------------|---------|----|--------|----|
| !DATE |              |             |             |         |             |         |    |        |    |
| PBC   | 9.3040       | 9.3040      | 9.3040      | 94.5972 | 94.5972     | 94.5972 |    |        |    |
| Al    | 2.353654000  | 8.064435000 | 0.968225600 | CORE    | 2           | 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 |

|     |              |              |             |      |    |   |   |        |    |
|-----|--------------|--------------|-------------|------|----|---|---|--------|----|
| O   | 8.497935420  | 1.897910157  | 6.367064923 | CORE | 27 | O | O | 0.0000 | 27 |
| O   | 1.477534337  | -0.429024571 | 7.160445863 | CORE | 28 | O | O | 0.0000 | 28 |
| O   | 6.028704980  | 0.931262663  | 6.828420880 | CORE | 29 | O | O | 0.0000 | 29 |
| O   | -0.442205062 | 6.330792888  | 6.983841948 | CORE | 30 | O | O | 0.0000 | 30 |
| O   | 0.406373162  | 4.129762851  | 7.734078636 | CORE | 31 | O | O | 0.0000 | 31 |
| O   | 3.389613289  | 0.990824629  | 7.876234943 | CORE | 32 | O | O | 0.0000 | 32 |
| O   | 1.084107369  | 1.601405998  | 8.600344588 | CORE | 33 | O | O | 0.0000 | 33 |
| O   | 4.404911471  | 8.212330606  | 8.785956058 | CORE | 34 | O | O | 0.0000 | 34 |
| O   | -1.175066144 | 5.450429060  | 9.188606247 | CORE | 35 | O | O | 0.0000 | 35 |
| P   | 7.503717539  | 3.152599578  | 0.929944949 | CORE | 36 | P | P | 0.0000 | 36 |
| O   | 3.504152202  | 2.604176607  | 3.535358153 | CORE | 37 | O | O | 0.0000 | 37 |
| H   | 4.256058887  | 2.007178939  | 3.343763944 | CORE | 38 | H | H | 0.0000 | 38 |
| C   | 3.355436776  | 2.774422622  | 5.037446699 | CORE | 39 | C | C | 0.0000 | 39 |
| H   | 3.090104460  | 3.815356443  | 5.201929139 | CORE | 40 | H | H | 0.0000 | 40 |
| H   | 4.308161256  | 2.504295400  | 5.486812128 | CORE | 41 | H | H | 0.0000 | 41 |
| H   | 2.550377314  | 2.100174116  | 5.315536096 | CORE | 42 | H | H | 0.0000 | 42 |
| H   | 3.502961057  | 3.482268762  | 1.653004870 | CORE | 43 | H | H | 0.0000 | 43 |
| C   | 3.573205159  | 3.841235843  | 2.677141709 | CORE | 44 | C | C | 0.0000 | 44 |
| H   | 2.699957418  | 4.425223384  | 2.958680053 | CORE | 45 | H | H | 0.0000 | 45 |
| H   | 4.510806369  | 4.356788344  | 2.880562594 | CORE | 46 | H | H | 0.0000 | 46 |
| end |              |              |             |      |    |   |   |        |    |
| end |              |              |             |      |    |   |   |        |    |

# TS CH<sub>3</sub>CO\* + CH<sub>3</sub>CO\* to CH<sub>3</sub>CH<sub>2</sub>CO\* + CO\*

|                   |              |              |             |             |         |         |    |        |    |
|-------------------|--------------|--------------|-------------|-------------|---------|---------|----|--------|----|
| !BIOSYM archive 2 |              |              |             |             |         |         |    |        |    |
| PBC=ON            |              |              |             |             |         |         |    |        |    |
| Energy            |              | 5            | -298        | -298.100616 |         |         |    |        |    |
| !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                 | 5.551685456  | 8.114417566  | 1.168362740 | CORE        | 2       | P       | P  | 0.0000 | 2  |
| Si                | 7.508373244  | 0.584046263  | 6.118771126 | CORE        | 3       | Si      | Si | 0.0000 | 3  |
| Al                | 7.878580278  | 0.561678384  | 3.145866643 | CORE        | 4       | Al      | Al | 0.0000 | 4  |
| P                 | 0.166950081  | 7.786312821  | 3.215834118 | CORE        | 5       | P       | P  | 0.0000 | 5  |
| Al                | 7.732602976  | 6.020753331  | 1.253268462 | CORE        | 6       | Al      | Al | 0.0000 | 6  |
| Al                | -0.144609463 | 7.843116323  | 6.229247578 | CORE        | 7       | Al      | Al | 0.0000 | 7  |
| Al                | 0.001184260  | 2.389859090  | 8.185509900 | CORE        | 8       | Al      | Al | 0.0000 | 8  |
| P                 | 2.233917219  | 0.321999970  | 8.310075170 | CORE        | 9       | P       | P  | 0.0000 | 9  |
| P                 | 0.014047708  | 5.439018588  | 8.262247696 | CORE        | 10      | P       | P  | 0.0000 | 10 |
| Al                | 5.462181233  | 0.411750118  | 8.324229409 | CORE        | 11      | Al      | Al | 0.0000 | 11 |
| O                 | 1.195599517  | 5.988170292  | 9.066156517 | CORE        | 12      | O       | O  | 0.0000 | 12 |
| O                 | 6.073822041  | 1.853948575  | 9.165220449 | CORE        | 13      | O       | O  | 0.0000 | 13 |
| O                 | -0.052290603 | 3.188586322  | 0.508873668 | CORE        | 14      | O       | O  | 0.0000 | 14 |
| O                 | 2.554528945  | 0.326340835  | 0.320953141 | CORE        | 15      | O       | O  | 0.0000 | 15 |
| O                 | 6.195255280  | 6.752339146  | 0.876177795 | CORE        | 16      | O       | O  | 0.0000 | 16 |
| O                 | 4.043612688  | 7.933972378  | 1.245148052 | CORE        | 17      | O       | O  | 0.0000 | 17 |
| O                 | 7.388169103  | 4.351349932  | 1.670193430 | CORE        | 18      | O       | O  | 0.0000 | 18 |
| O                 | 7.844334436  | 1.952714079  | 2.102763806 | CORE        | 19      | O       | O  | 0.0000 | 19 |
| O                 | 1.480249069  | 7.797095102  | 2.440637148 | CORE        | 20      | O       | O  | 0.0000 | 20 |
| O                 | 6.038529433  | 8.612202109  | 2.532296532 | CORE        | 21      | O       | O  | 0.0000 | 21 |
| O                 | 8.531805356  | 6.690084998  | 2.666749393 | CORE        | 22      | O       | O  | 0.0000 | 22 |
| O                 | 0.227285620  | -0.111399805 | 3.111884861 | CORE        | 23      | O       | O  | 0.0000 | 23 |
| O                 | 7.366108009  | 1.221259770  | 4.632115388 | CORE        | 24      | O       | O  | 0.0000 | 24 |
| O                 | 0.526703651  | 7.430887495  | 4.654477844 | CORE        | 25      | O       | O  | 0.0000 | 25 |
| O                 | 7.588818097  | 8.466244061  | 6.033711805 | CORE        | 26      | O       | O  | 0.0000 | 26 |
| O                 | 8.364238199  | 1.666334712  | 6.979328037 | CORE        | 27      | O       | O  | 0.0000 | 27 |
| O                 | 1.794042279  | -0.413275700 | 7.036631719 | CORE        | 28      | O       | O  | 0.0000 | 28 |
| O                 | 6.044153884  | 0.336989021  | 6.733707631 | CORE        | 29      | O       | O  | 0.0000 | 29 |
| O                 | -0.255873920 | 6.291726434  | 7.031506323 | CORE        | 30      | O       | O  | 0.0000 | 30 |
| O                 | 0.378708461  | 4.048240231  | 7.754908350 | CORE        | 31      | O       | O  | 0.0000 | 31 |
| O                 | 3.73320187   | 0.501936140  | 8.316246850 | CORE        | 32      | O       | O  | 0.0000 | 32 |
| O                 | 1.598414396  | 1.705960184  | 8.376718744 | CORE        | 33      | O       | O  | 0.0000 | 33 |
| O                 | 5.938702545  | 9.094833279  | 0.059599521 | CORE        | 34      | O       | O  | 0.0000 | 34 |
| O                 | 8.045708038  | 5.390129851  | 9.118076747 | CORE        | 35      | O       | O  | 0.0000 | 35 |
| P                 | 7.814865486  | 3.014653188  | 1.028814120 | CORE        | 36      | P       | P  | 0.0000 | 36 |
| O                 | 5.827248180  | 4.186676538  | 4.687106786 | CORE        | 37      | O       | O  | 0.0000 | 37 |
| C                 | 6.955727408  | 4.062822907  | 4.625443125 | CORE        | 38      | C       | C  | 0.0000 | 38 |
| H                 | -0.197906284 | 4.698801368  | 5.316748700 | CORE        | 39      | H       | H  | 0.0000 | 39 |
| C                 | -0.334587187 | 3.880205053  | 4.630039560 | CORE        | 40      | C       | C  | 0.0000 | 40 |
| H                 | -0.281711249 | 4.068642144  | 3.572471004 | CORE        | 41      | H       | H  | 0.0000 | 41 |
| H                 | -0.472038739 | 2.880490413  | 5.002879122 | CORE        | 42      | H       | H  | 0.0000 | 42 |
| H                 | 1.903762787  | 2.809439063  | 3.657258185 | CORE        | 43      | H       | H  | 0.0000 | 43 |
| C                 | 2.523061160  | 4.429559079  | 4.787480643 | CORE        | 44      | C       | C  | 0.0000 | 44 |
| O                 | 3.033569036  | 5.460552721  | 4.927368319 | CORE        | 45      | O       | O  | 0.0000 | 45 |
| C                 | 1.850465858  | 3.280167528  | 4.634902644 | CORE        | 46      | C       | C  | 0.0000 | 46 |
| H                 | 1.850025601  | 2.628266158  | 5.503577411 | CORE        | 47      | H       | H  | 0.0000 | 47 |
| end               |              |              |             |             |         |         |    |        |    |
| end               |              |              |             |             |         |         |    |        |    |

# TS CH<sub>3</sub>CO\* + CH<sub>3</sub>OH\* to HS + CH<sub>3</sub>COOCH<sub>3</sub>\*

|                   |              |              |             |         |         |         |    |        |    |
|-------------------|--------------|--------------|-------------|---------|---------|---------|----|--------|----|
| !BIOSYM archive 2 |              |              |             |         |         |         |    |        |    |
| PBC=ON            |              |              |             |         |         |         |    |        |    |
| Energy            | 6            | -298         | -298.959262 |         |         |         |    |        |    |
| !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                 | 5.454475685  | 8.066330320  | 1.051553924 | CORE    | 2       | P       | P  | 0.0000 | 2  |
| Si                | 7.538059165  | 0.757833791  | 6.008244676 | CORE    | 3       | Si      | Si | 0.0000 | 3  |
| Al                | 7.909389861  | 0.659946026  | 3.012506071 | CORE    | 4       | Al      | Al | 0.0000 | 4  |
| P                 | 0.102997530  | 7.774989100  | 3.244593309 | CORE    | 5       | P       | P  | 0.0000 | 5  |
| Al                | 7.741156759  | 6.009570808  | 1.304202494 | CORE    | 6       | Al      | Al | 0.0000 | 6  |
| Al                | -0.311816731 | 7.845230543  | 6.202189820 | CORE    | 7       | Al      | Al | 0.0000 | 7  |
| Al                | 0.006077769  | 2.497611629  | 7.915855985 | CORE    | 8       | Al      | Al | 0.0000 | 8  |
| P                 | 2.188758384  | 0.374826736  | 8.288655448 | CORE    | 9       | P       | P  | 0.0000 | 9  |
| P                 | -0.038251746 | 5.531391496  | 8.222238038 | CORE    | 10      | P       | P  | 0.0000 | 10 |
| Al                | 5.318945156  | 0.424033310  | 8.325214943 | CORE    | 11      | Al      | Al | 0.0000 | 11 |
| O                 | 1.167246872  | 6.223425627  | 8.870603404 | CORE    | 12      | O       | O  | 0.0000 | 12 |
| O                 | 6.499622971  | 2.420831293  | 0.308056936 | CORE    | 13      | O       | O  | 0.0000 | 13 |
| O                 | 8.118907615  | 2.397657783  | 9.188385539 | CORE    | 14      | O       | O  | 0.0000 | 14 |
| O                 | 2.936242418  | 0.446136615  | 0.404735435 | CORE    | 15      | O       | O  | 0.0000 | 15 |
| O                 | 6.234423301  | 6.768022167  | 0.842651957 | CORE    | 16      | O       | O  | 0.0000 | 16 |
| O                 | 4.006810978  | 7.723689894  | 1.408904065 | CORE    | 17      | O       | O  | 0.0000 | 17 |
| O                 | 7.398117596  | 4.334596751  | 1.625644523 | CORE    | 18      | O       | O  | 0.0000 | 18 |
| O                 | 8.282304288  | 2.054490228  | 2.047239620 | CORE    | 19      | O       | O  | 0.0000 | 19 |
| O                 | 1.355191912  | 7.778018050  | 2.367842709 | CORE    | 20      | O       | O  | 0.0000 | 20 |
| O                 | 6.053119456  | 8.851439711  | 2.220291121 | CORE    | 21      | O       | O  | 0.0000 | 21 |
| O                 | 8.418137879  | 6.695154392  | 2.770936568 | CORE    | 22      | O       | O  | 0.0000 | 22 |
| O                 | 0.175507563  | -0.114204770 | 3.173268502 | CORE    | 23      | O       | O  | 0.0000 | 23 |
| O                 | 7.068392339  | 1.270343963  | 4.467980261 | CORE    | 24      | O       | O  | 0.0000 | 24 |
| O                 | 0.525244085  | 7.477640590  | 4.685240766 | CORE    | 25      | O       | O  | 0.0000 | 25 |
| O                 | 7.467819861  | 8.577241824  | 5.842162550 | CORE    | 26      | O       | O  | 0.0000 | 26 |
| O                 | -0.681098682 | 1.844064283  | 6.491527084 | CORE    | 27      | O       | O  | 0.0000 | 27 |
| O                 | 1.516665957  | -0.460935457 | 7.198841458 | CORE    | 28      | O       | O  | 0.0000 | 28 |
| O                 | 6.197651385  | 0.717405506  | 6.888660411 | CORE    | 29      | O       | O  | 0.0000 | 29 |
| O                 | -0.578776457 | 6.335811112  | 7.041318737 | CORE    | 30      | O       | O  | 0.0000 | 30 |
| O                 | 0.424375283  | 4.176510631  | 7.708468674 | CORE    | 31      | O       | O  | 0.0000 | 31 |
| O                 | 3.637992997  | 0.655649760  | 7.859132380 | CORE    | 32      | O       | O  | 0.0000 | 32 |
| O                 | 1.467123566  | 1.702838878  | 8.471156416 | CORE    | 33      | O       | O  | 0.0000 | 33 |
| O                 | 4.773585369  | 8.080836062  | 8.993893583 | CORE    | 34      | O       | O  | 0.0000 | 34 |
| O                 | -0.417665472 | 6.203279369  | 0.013115357 | CORE    | 35      | O       | O  | 0.0000 | 35 |
| P                 | 7.759121635  | 2.997881112  | 0.967465394 | CORE    | 36      | P       | P  | 0.0000 | 36 |
| O                 | 5.491614928  | 2.671757754  | 3.070535693 | CORE    | 37      | O       | O  | 0.0000 | 37 |
| C                 | 5.887131921  | 2.736977522  | 4.164234304 | CORE    | 38      | C       | C  | 0.0000 | 38 |

|     |             |              |             |      |    |   |   |        |    |
|-----|-------------|--------------|-------------|------|----|---|---|--------|----|
| 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 + CH<sub>3</sub>OH\* to HS + HCOOCH<sub>3</sub>\*

!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 + CH<sub>3</sub>CH<sub>2</sub>CO\* to HS + C<sub>2</sub>H<sub>5</sub>\* + 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

|                   |              |              |             |             |         |         |    |        |    |
|-------------------|--------------|--------------|-------------|-------------|---------|---------|----|--------|----|
| !BIOSYM archive 2 |              |              |             |             |         |         |    |        |    |
| PBC=ON            |              |              |             |             |         |         |    |        |    |
| Energy            |              | 9            | -250        | -250.955914 |         |         |    |        |    |
| !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                 | 5.430825946  | 8.220947388  | 0.830152469 | CORE        | 2       | P       | P  | 0.0000 | 2  |
| Si                | 7.457744673  | 0.757091285  | 5.917170412 | CORE        | 3       | Si      | Si | 0.0000 | 3  |
| Al                | 7.957662956  | 0.775364975  | 2.826181230 | CORE        | 4       | Al      | Al | 0.0000 | 4  |
| P                 | 0.063748046  | 7.861335491  | 3.159693258 | CORE        | 5       | P       | P  | 0.0000 | 5  |
| Al                | 7.676586576  | 6.124689281  | 1.188127823 | CORE        | 6       | Al      | Al | 0.0000 | 6  |
| Al                | -0.371368889 | 7.876180599  | 6.224818855 | CORE        | 7       | Al      | Al | 0.0000 | 7  |
| Al                | -0.146427222 | 2.552392391  | 7.886640449 | CORE        | 8       | Al      | Al | 0.0000 | 8  |
| P                 | 2.053529266  | 0.409319532  | 8.315552606 | CORE        | 9       | P       | P  | 0.0000 | 9  |
| P                 | 0.006966070  | 5.535364925  | 8.197102354 | CORE        | 10      | P       | P  | 0.0000 | 10 |
| Al                | 5.134137728  | 0.562217214  | 8.168297097 | CORE        | 11      | Al      | Al | 0.0000 | 11 |
| O                 | 1.212729736  | 6.205280535  | 8.869072828 | CORE        | 12      | O       | O  | 0.0000 | 12 |
| O                 | 6.447349670  | 2.446313983  | 0.188265543 | CORE        | 13      | O       | O  | 0.0000 | 13 |
| O                 | 7.977602187  | 2.608473509  | 9.153822930 | CORE        | 14      | O       | O  | 0.0000 | 14 |
| O                 | 2.868572654  | 0.434920625  | 0.400262001 | CORE        | 15      | O       | O  | 0.0000 | 15 |
| O                 | 6.262334580  | 6.965715588  | 0.595137057 | CORE        | 16      | O       | O  | 0.0000 | 16 |
| O                 | 4.043941493  | 7.830315008  | 1.355886854 | CORE        | 17      | O       | O  | 0.0000 | 17 |
| O                 | 7.119691741  | 4.489047364  | 1.477010372 | CORE        | 18      | O       | O  | 0.0000 | 18 |
| O                 | 8.159014683  | 2.307625856  | 2.043216323 | CORE        | 19      | O       | O  | 0.0000 | 19 |
| O                 | 1.381158125  | 7.752646523  | 2.385106521 | CORE        | 20      | O       | O  | 0.0000 | 20 |
| O                 | 6.098833429  | 9.093455845  | 1.888490766 | CORE        | 21      | O       | O  | 0.0000 | 21 |
| O                 | 8.348690368  | 6.816577950  | 2.662668617 | CORE        | 22      | O       | O  | 0.0000 | 22 |
| O                 | 0.221908098  | 0.001343819  | 2.958998278 | CORE        | 23      | O       | O  | 0.0000 | 23 |
| O                 | 7.151746038  | 1.045134622  | 4.339864054 | CORE        | 24      | O       | O  | 0.0000 | 24 |
| O                 | 0.359924560  | 7.627959468  | 4.636937426 | CORE        | 25      | O       | O  | 0.0000 | 25 |
| O                 | 7.353289272  | 8.580798967  | 6.146732924 | CORE        | 26      | O       | O  | 0.0000 | 26 |
| O                 | 8.375406417  | 1.926647143  | 6.497038062 | CORE        | 27      | O       | O  | 0.0000 | 27 |
| O                 | 1.513573157  | -0.452687988 | 7.175638258 | CORE        | 28      | O       | O  | 0.0000 | 28 |
| O                 | 5.872727355  | 0.796964706  | 6.548840127 | CORE        | 29      | O       | O  | 0.0000 | 29 |
| O                 | -0.493320873 | 6.324544350  | 6.995255129 | CORE        | 30      | O       | O  | 0.0000 | 30 |
| O                 | 0.459406414  | 4.169645255  | 7.693362628 | CORE        | 31      | O       | O  | 0.0000 | 31 |
| O                 | 3.450980149  | 0.905305480  | 7.928232864 | CORE        | 32      | O       | O  | 0.0000 | 32 |
| O                 | 1.168473699  | 1.621283717  | 8.544784809 | CORE        | 33      | O       | O  | 0.0000 | 33 |
| O                 | 4.574334574  | 8.180633744  | 8.736416208 | CORE        | 34      | O       | O  | 0.0000 | 34 |
| O                 | -1.132226964 | 5.434330856  | 9.215282676 | CORE        | 35      | O       | O  | 0.0000 | 35 |
| P                 | 7.609410292  | 3.156133719  | 0.901162437 | CORE        | 36      | P       | P  | 0.0000 | 36 |
| O                 | 3.554727377  | 0.833810545  | 5.136656907 | CORE        | 37      | O       | O  | 0.0000 | 37 |
| C                 | 4.673687752  | 1.058961437  | 5.027358631 | CORE        | 38      | C       | C  | 0.0000 | 38 |
| H                 | 5.610410574  | 1.274952256  | 4.415944570 | CORE        | 39      | H       | H  | 0.0000 | 39 |
| end               |              |              |             |             |         |         |    |        |    |
| end               |              |              |             |             |         |         |    |        |    |

TS HS + CH<sub>3</sub>OH\* to CH<sub>3</sub>OH<sub>2</sub>\*

|                   |              |              |             |             |         |         |    |        |    |
|-------------------|--------------|--------------|-------------|-------------|---------|---------|----|--------|----|
| !BIOSYM archive 2 |              |              |             |             |         |         |    |        |    |
| PBC=ON            |              |              |             |             |         |         |    |        |    |
| Energy            |              | 10           | -266        | -266.935228 |         |         |    |        |    |
| !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                 | 5.410871824  | 8.255273821  | 0.837797182 | CORE        | 2       | P       | P  | 0.0000 | 2  |
| Si                | 7.409662397  | 0.810748356  | 5.879124157 | CORE        | 3       | Si      | Si | 0.0000 | 3  |
| Al                | 7.954157347  | 0.790802043  | 2.883735408 | CORE        | 4       | Al      | Al | 0.0000 | 4  |
| P                 | 0.054739260  | 7.880622560  | 3.166051843 | CORE        | 5       | P       | P  | 0.0000 | 5  |
| Al                | 7.652158622  | 6.158827319  | 1.172780678 | CORE        | 6       | Al      | Al | 0.0000 | 6  |
| Al                | -0.398862414 | 7.908710904  | 6.204075351 | CORE        | 7       | Al      | Al | 0.0000 | 7  |
| Al                | -0.198598862 | 2.519705615  | 7.800320725 | CORE        | 8       | Al      | Al | 0.0000 | 8  |
| P                 | 2.040336637  | 0.429818112  | 8.293040104 | CORE        | 9       | P       | P  | 0.0000 | 9  |
| P                 | -0.000657205 | 5.534810028  | 8.202066060 | CORE        | 10      | P       | P  | 0.0000 | 10 |
| Al                | 5.134671721  | 0.612720269  | 8.170680248 | CORE        | 11      | Al      | Al | 0.0000 | 11 |
| O                 | 1.219495294  | 6.161483115  | 8.904167350 | CORE        | 12      | O       | O  | 0.0000 | 12 |
| O                 | 6.296964345  | 2.428520400  | 0.378161741 | CORE        | 13      | O       | O  | 0.0000 | 13 |
| O                 | 7.824569877  | 2.513350250  | 9.008247176 | CORE        | 14      | O       | O  | 0.0000 | 14 |
| O                 | 2.877532483  | 0.442182385  | 0.384914346 | CORE        | 15      | O       | O  | 0.0000 | 15 |
| O                 | 6.204473697  | 6.966888312  | 0.601201858 | CORE        | 16      | O       | O  | 0.0000 | 16 |
| O                 | 4.035866703  | 7.886299592  | 1.441054997 | CORE        | 17      | O       | O  | 0.0000 | 17 |
| O                 | 7.150889827  | 4.498995738  | 1.472534898 | CORE        | 18      | O       | O  | 0.0000 | 18 |
| O                 | 8.191588025  | 2.320290742  | 2.033339303 | CORE        | 19      | O       | O  | 0.0000 | 19 |
| O                 | 1.371043268  | 7.775271168  | 2.380996175 | CORE        | 20      | O       | O  | 0.0000 | 20 |
| O                 | 6.897898094  | -0.147595227 | 1.844002095 | CORE        | 21      | O       | O  | 0.0000 | 21 |
| O                 | 8.326197237  | 6.861176854  | 2.641569344 | CORE        | 22      | O       | O  | 0.0000 | 22 |
| O                 | 0.238909805  | 0.035678967  | 2.995571596 | CORE        | 23      | O       | O  | 0.0000 | 23 |
| O                 | 7.025620976  | 1.065310250  | 4.304820197 | CORE        | 24      | O       | O  | 0.0000 | 24 |
| O                 | 0.367183998  | 7.599895279  | 4.629855192 | CORE        | 25      | O       | O  | 0.0000 | 25 |
| O                 | 7.355076470  | 8.615219196  | 6.037029284 | CORE        | 26      | O       | O  | 0.0000 | 26 |
| O                 | 8.515133466  | 1.930165069  | 6.313848236 | CORE        | 27      | O       | O  | 0.0000 | 27 |
| O                 | 1.518720472  | -0.435148933 | 7.151540789 | CORE        | 28      | O       | O  | 0.0000 | 28 |
| O                 | 6.064144776  | 0.917734619  | 6.780373178 | CORE        | 29      | O       | O  | 0.0000 | 29 |
| O                 | -0.465200817 | 6.358273459  | 7.012549173 | CORE        | 30      | O       | O  | 0.0000 | 30 |
| O                 | 0.416608356  | 4.154745722  | 7.712624773 | CORE        | 31      | O       | O  | 0.0000 | 31 |
| O                 | 3.426858492  | 0.965261105  | 7.922028614 | CORE        | 32      | O       | O  | 0.0000 | 32 |
| O                 | 1.110231596  | 1.612040673  | 8.563846471 | CORE        | 33      | O       | O  | 0.0000 | 33 |
| O                 | 4.477266664  | 8.200404024  | 8.754516199 | CORE        | 34      | O       | O  | 0.0000 | 34 |
| O                 | -1.152901872 | 5.445421250  | 9.209764242 | CORE        | 35      | O       | O  | 0.0000 | 35 |
| P                 | 7.574420447  | 3.135120088  | 0.889791638 | CORE        | 36      | P       | P  | 0.0000 | 36 |
| H                 | 5.561943752  | 2.339022518  | 2.769464692 | CORE        | 37      | H       | H  | 0.0000 | 37 |
| O                 | 4.691635712  | 2.370317264  | 3.219954226 | CORE        | 38      | O       | O  | 0.0000 | 38 |
| H                 | 4.388728350  | 1.451699141  | 3.363534221 | CORE        | 39      | H       | H  | 0.0000 | 39 |
| C                 | 3.693450827  | 3.322485569  | 2.603812127 | CORE        | 40      | C       | C  | 0.0000 | 40 |
| H                 | 2.872993031  | 3.347033527  | 3.315455360 | CORE        | 41      | H       | H  | 0.0000 | 41 |
| H                 | 3.403482506  | 2.956950735  | 1.623547183 | CORE        | 42      | H       | H  | 0.0000 | 42 |
| H                 | 4.229865083  | 4.267085736  | 2.564633198 | CORE        | 43      | H       | H  | 0.0000 | 43 |
| end               |              |              |             |             |         |         |    |        |    |
| end               |              |              |             |             |         |         |    |        |    |

TS CH<sub>3</sub>S + CH<sub>3</sub>CO\* to CH<sub>3</sub>CH<sub>2</sub>CO\*

|                   |              |        |             |             |         |         |    |    |           |
|-------------------|--------------|--------|-------------|-------------|---------|---------|----|----|-----------|
| !BIOSYM archive 2 |              |        |             |             |         |         |    |    |           |
| PBC=ON            |              |        |             |             |         |         |    |    |           |
| Energy            |              | 11     | -284        | -284.582310 |         |         |    |    |           |
| !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                 | 5.354752371  |        | 8.167154654 | 0.948011120 | CORE    | 2       | P  | P  | 0.0000 2  |
| Si                | 7.407718771  |        | 0.760078749 | 5.990015318 | CORE    | 3       | Si | Si | 0.0000 3  |
| Al                | 7.805576388  |        | 0.763118945 | 2.973177635 | CORE    | 4       | Al | Al | 0.0000 4  |
| P                 | 0.006919179  |        | 7.880814019 | 3.188500401 | CORE    | 5       | P  | P  | 0.0000 5  |
| Al                | 7.652368071  |        | 6.116044248 | 1.217626276 | CORE    | 6       | Al | Al | 0.0000 6  |
| Al                | -0.385210152 |        | 7.876516308 | 6.184390655 | CORE    | 7       | Al | Al | 0.0000 7  |
| Al                | -0.200837664 |        | 2.497914349 | 7.905655869 | CORE    | 8       | Al | Al | 0.0000 8  |
| P                 | 2.058752121  |        | 0.416780112 | 8.280560158 | CORE    | 9       | P  | P  | 0.0000 9  |
| P                 | -0.044174134 |        | 5.527897559 | 8.209044118 | CORE    | 10      | P  | P  | 0.0000 10 |
| Al                | 5.100854566  |        | 0.551705382 | 8.273190591 | CORE    | 11      | Al | Al | 0.0000 11 |
| O                 | 1.169068246  |        | 6.178137521 | 8.891888137 | CORE    | 12      | O  | O  | 0.0000 12 |
| O                 | 6.272547990  |        | 2.433926962 | 0.389187079 | CORE    | 13      | O  | O  | 0.0000 13 |
| O                 | 7.849775670  |        | 2.457350692 | 9.132767122 | CORE    | 14      | O  | O  | 0.0000 14 |
| O                 | 2.957527101  |        | 0.427921052 | 0.354441186 | CORE    | 15      | O  | O  | 0.0000 15 |
| O                 | 6.211423831  |        | 6.935029117 | 0.659800211 | CORE    | 16      | O  | O  | 0.0000 16 |
| O                 | 3.984736365  |        | 7.695696929 | 1.474678196 | CORE    | 17      | O  | O  | 0.0000 17 |
| O                 | 7.148658934  |        | 4.470427346 | 1.543249136 | CORE    | 18      | O  | O  | 0.0000 18 |



|     |              |              |             |      |    |   |   |        |    |
|-----|--------------|--------------|-------------|------|----|---|---|--------|----|
| 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 | 6.531383666  | 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 CH<sub>3</sub>S + CO\* to CH<sub>3</sub>CO\*

!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 CH<sub>3</sub>S + CH<sub>3</sub>OH\* to CH<sub>3</sub>OHCH<sub>3</sub>\*

!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  | 2.313380192  | 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 |             |             |             |      |    |   |   |        |    |
| end |             |             |             |      |    |   |   |        |    |

# CH<sub>3</sub>CH<sub>2</sub>CO\* + 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 |
| end |              |              |             |         |         |         |    |        |    |
| end |              |              |             |         |         |         |    |        |    |

# CH<sub>3</sub>CH<sub>2</sub>CO\*

!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 |              |              |             |         |         |         |    |        |    |

CH<sub>3</sub>CO\*

'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    |              |        |              |             |             |         |                    |  |

CH<sub>3</sub>OH\*

'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  |             | 7.105203898 | 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    |              |        |              |             |             |         |          |           |

CH<sub>3</sub>OHCH<sub>3</sub>\*

'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 | 0.4219221202 | 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

**CH<sub>3</sub>COS + CH<sub>3</sub>CO\***

!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

**CH<sub>3</sub>COS + CH<sub>3</sub>OH\***

!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 |

|     |              |              |             |      |    |   |   |        |    |
|-----|--------------|--------------|-------------|------|----|---|---|--------|----|
| O   | 7.409379994  | 8.596534923  | 5.782032812 | CORE | 26 | O | O | 0.0000 | 26 |
| O   | -0.686805963 | 1.831909978  | 6.542786794 | CORE | 27 | O | O | 0.0000 | 27 |
| O   | 1.358092495  | -0.395248701 | 7.262465579 | CORE | 28 | O | O | 0.0000 | 28 |
| O   | 6.151082278  | 0.773551979  | 6.868956136 | CORE | 29 | O | O | 0.0000 | 29 |
| O   | -0.598999120 | 6.361255526  | 7.023936033 | CORE | 30 | O | O | 0.0000 | 30 |
| O   | 0.387583149  | 4.198868288  | 7.714234318 | CORE | 31 | O | O | 0.0000 | 31 |
| O   | 3.507814521  | 0.730782442  | 7.805665757 | CORE | 32 | O | O | 0.0000 | 32 |
| O   | 1.362137416  | 1.719827006  | 6.608466405 | CORE | 33 | O | O | 0.0000 | 33 |
| O   | 4.680927548  | 8.236208590  | 9.019605410 | CORE | 34 | O | O | 0.0000 | 34 |
| O   | -0.426697189 | 6.246607170  | 0.016525420 | CORE | 35 | O | O | 0.0000 | 35 |
| P   | 7.609323874  | 3.092643523  | 0.943136118 | CORE | 36 | P | P | 0.0000 | 36 |
| O   | 5.174049874  | 2.250715408  | 3.583247241 | CORE | 37 | O | O | 0.0000 | 37 |
| O   | 6.117828564  | 2.460097923  | 4.283864672 | CORE | 38 | C | C | 0.0000 | 38 |
| H   | 5.923112167  | 4.531913726  | 4.592447540 | CORE | 39 | H | H | 0.0000 | 39 |
| C   | 6.515505111  | 3.712065907  | 4.994447892 | CORE | 40 | C | C | 0.0000 | 40 |
| H   | 7.585009893  | 3.901821251  | 4.887213476 | CORE | 41 | H | H | 0.0000 | 41 |
| H   | 6.299900817  | 3.606429795  | 6.062181539 | CORE | 42 | H | H | 0.0000 | 42 |
| H   | 3.265236491  | 4.800681324  | 4.110296452 | CORE | 43 | H | H | 0.0000 | 43 |
| H   | 3.222013136  | 4.025677573  | 5.726404949 | CORE | 44 | H | H | 0.0000 | 44 |
| C   | 2.609496095  | 4.412971204  | 4.900393486 | CORE | 45 | C | C | 0.0000 | 45 |
| H   | 1.992737890  | 5.229773969  | 5.272835828 | CORE | 46 | H | H | 0.0000 | 46 |
| O   | 1.711028974  | 3.412817700  | 4.395319742 | CORE | 47 | O | O | 0.0000 | 47 |
| H   | 2.240774691  | 2.729320090  | 3.961924535 | CORE | 48 | H | H | 0.0000 | 48 |
| end |              |              |             |      |    |   |   |        |    |
| end |              |              |             |      |    |   |   |        |    |

# CHOS + CH<sub>3</sub>OH\*

!BIOSYM archive 2

PBC=ON

|       | Energy       | 21           | -281        | -281.759423 |         |         |    |        |    |
|-------|--------------|--------------|-------------|-------------|---------|---------|----|--------|----|
| !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     | 5.379532102  | 8.033257373  | 0.979472841 | CORE        | 2       | P       | P  | 0.0000 | 2  |
| Si    | 7.530628747  | 0.625769905  | 6.099564115 | CORE        | 3       | Si      | Si | 0.0000 | 3  |
| Al    | 7.879884799  | 6.829020176  | 2.922808818 | CORE        | 4       | Al      | Al | 0.0000 | 4  |
| P     | 0.057320111  | 7.810449531  | 3.199772280 | CORE        | 5       | P       | P  | 0.0000 | 5  |
| Al    | 7.665932370  | 6.049168390  | 1.233080049 | CORE        | 6       | Al      | Al | 0.0000 | 6  |
| Al    | -0.254575095 | 7.777018481  | 6.155082895 | CORE        | 7       | Al      | Al | 0.0000 | 7  |
| Al    | -0.125037367 | 2.461876866  | 7.912496533 | CORE        | 8       | Al      | Al | 0.0000 | 8  |
| P     | 2.148566298  | 0.369158813  | 8.226794027 | CORE        | 9       | P       | P  | 0.0000 | 9  |
| P     | -0.032434892 | 5.492189357  | 8.227264125 | CORE        | 10      | P       | P  | 0.0000 | 10 |
| Al    | 5.184560459  | 0.452030335  | 8.313511021 | CORE        | 11      | Al      | Al | 0.0000 | 11 |
| O     | 1.172793950  | 6.149303232  | 8.913348348 | CORE        | 12      | O       | O  | 0.0000 | 12 |
| O     | 6.385058455  | 2.405264436  | 0.334288245 | CORE        | 13      | O       | O  | 0.0000 | 13 |
| O     | 8.006618101  | 2.339563944  | 9.206903693 | CORE        | 14      | O       | O  | 0.0000 | 14 |
| O     | 2.966049107  | 0.406763813  | 0.318968582 | CORE        | 15      | O       | O  | 0.0000 | 15 |
| O     | 6.150841343  | 6.746691637  | 0.665684687 | CORE        | 16      | O       | O  | 0.0000 | 16 |
| O     | 3.981508549  | 7.688452500  | 1.501118041 | CORE        | 17      | O       | O  | 0.0000 | 17 |
| O     | 7.270738377  | 4.387103319  | 1.567451906 | CORE        | 18      | O       | O  | 0.0000 | 18 |
| O     | 8.116020682  | 2.145281888  | 2.145663742 | CORE        | 19      | O       | O  | 0.0000 | 19 |
| O     | 1.288242109  | 7.851254987  | 2.312012818 | CORE        | 20      | O       | O  | 0.0000 | 20 |
| O     | 6.145387372  | 8.780543537  | 2.075111997 | CORE        | 21      | O       | O  | 0.0000 | 21 |
| O     | 8.341002883  | 6.78602717   | 2.673718609 | CORE        | 22      | O       | O  | 0.0000 | 22 |
| O     | 0.146353878  | -0.059418406 | 3.225495951 | CORE        | 23      | O       | O  | 0.0000 | 23 |
| O     | 6.910769449  | 1.028556111  | 4.470408083 | CORE        | 24      | O       | O  | 0.0000 | 24 |
| O     | 0.505107156  | 7.422722353  | 4.606203365 | CORE        | 25      | O       | O  | 0.0000 | 25 |
| O     | 7.507414847  | 8.503491671  | 5.852737728 | CORE        | 26      | O       | O  | 0.0000 | 26 |
| O     | 8.523220290  | 1.827957609  | 6.444807040 | CORE        | 27      | O       | O  | 0.0000 | 27 |
| O     | 1.561793464  | -0.499792693 | 7.114252627 | CORE        | 28      | O       | O  | 0.0000 | 28 |
| O     | 6.197796007  | 0.551768283  | 6.943323052 | CORE        | 29      | O       | O  | 0.0000 | 29 |
| O     | -0.489018829 | 6.288486614  | 7.013809961 | CORE        | 30      | O       | O  | 0.0000 | 30 |
| O     | 0.392226773  | 4.111407628  | 7.747220783 | CORE        | 31      | O       | O  | 0.0000 | 31 |
| O     | 3.553336274  | 0.805346235  | 7.802150338 | CORE        | 32      | O       | O  | 0.0000 | 32 |
| O     | 1.295524728  | 1.606131984  | 8.455898972 | CORE        | 33      | O       | O  | 0.0000 | 33 |
| O     | 4.525756038  | 8.078722364  | 8.953135877 | CORE        | 34      | O       | O  | 0.0000 | 34 |
| O     | -1.207159573 | 5.402022267  | 9.205564084 | CORE        | 35      | O       | O  | 0.0000 | 35 |
| P     | 7.627584143  | 3.021021195  | 0.985070759 | CORE        | 36      | P       | P  | 0.0000 | 36 |
| O     | 5.119699986  | 1.685547317  | 3.220523512 | CORE        | 37      | O       | O  | 0.0000 | 37 |
| C     | 5.599915807  | 1.580089574  | 4.310541920 | CORE        | 38      | C       | C  | 0.0000 | 38 |
| H     | 5.176351086  | 1.860606387  | 5.275744239 | CORE        | 39      | H       | H  | 0.0000 | 39 |
| H     | 4.896317094  | 4.132375114  | 7.508856687 | CORE        | 40      | H       | H  | 0.0000 | 40 |
| O     | 4.941885659  | 3.897662213  | 6.571601109 | CORE        | 41      | O       | O  | 0.0000 | 41 |
| C     | 3.649694410  | 4.165390423  | 5.988601455 | CORE        | 42      | C       | C  | 0.0000 | 42 |
| H     | 2.902113527  | 3.444403092  | 6.334466418 | CORE        | 43      | H       | H  | 0.0000 | 43 |
| H     | 3.305335705  | 5.178705962  | 6.220514014 | CORE        | 44      | H       | H  | 0.0000 | 44 |
| H     | 3.766194186  | 4.068623055  | 4.907056776 | CORE        | 45      | H       | H  | 0.0000 | 45 |
| end   |              |              |             |             |         |         |    |        |    |
| end   |              |              |             |             |         |         |    |        |    |

# CHOS

!BIOSYM archive 2

PBC=ON

|       | Energy       | 22           | -251        | -251.830447 |         |         |    |        |    |
|-------|--------------|--------------|-------------|-------------|---------|---------|----|--------|----|
| !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     | 5.372046141  | 8.113535725  | 0.998211558 | CORE        | 2       | P       | P  | 0.0000 | 2  |
| Si    | 7.487994351  | 0.674650528  | 6.128824869 | CORE        | 3       | Si      | Si | 0.0000 | 3  |
| Al    | 7.880255228  | 0.711212702  | 2.928852644 | CORE        | 4       | Al      | Al | 0.0000 | 4  |
| P     | 0.043558620  | 7.872272588  | 3.211397460 | CORE        | 5       | P       | P  | 0.0000 | 5  |
| Al    | 7.667260666  | 6.109639268  | 1.242023314 | CORE        | 6       | Al      | Al | 0.0000 | 6  |
| O     | -0.284232456 | 7.828709595  | 6.185129458 | CORE        | 7       | Al      | Al | 0.0000 | 7  |
| Al    | -0.149373824 | 2.495007526  | 7.928651446 | CORE        | 8       | Al      | Al | 0.0000 | 8  |
| P     | 2.118315852  | 0.407339736  | 8.265881323 | CORE        | 9       | P       | P  | 0.0000 | 9  |
| P     | -0.023857964 | 5.515268194  | 8.235236126 | CORE        | 10      | P       | P  | 0.0000 | 10 |
| Al    | 5.139409489  | 0.536785811  | 8.353740869 | CORE        | 11      | Al      | Al | 0.0000 | 11 |
| O     | 1.189461813  | 6.163318607  | 8.912602105 | CORE        | 12      | O       | O  | 0.0000 | 12 |
| O     | 6.341972857  | 2.458733805  | 0.399122878 | CORE        | 13      | O       | O  | 0.0000 | 13 |
| O     | 7.930461263  | 2.408488965  | 9.173331289 | CORE        | 14      | O       | O  | 0.0000 | 14 |
| O     | 2.983802532  | 0.416280089  | 0.335189617 | CORE        | 15      | O       | O  | 0.0000 | 15 |
| O     | 6.189408168  | 6.864170885  | 0.673440276 | CORE        | 16      | O       | O  | 0.0000 | 16 |
| O     | 3.984057515  | 7.721929796  | 1.516983503 | CORE        | 17      | O       | O  | 0.0000 | 17 |
| O     | 7.264738023  | 4.453453668  | 1.598566547 | CORE        | 18      | O       | O  | 0.0000 | 18 |
| O     | 8.148557724  | 2.216002591  | 2.142859763 | CORE        | 19      | O       | O  | 0.0000 | 19 |
| O     | 1.277327922  | 7.889721625  | 2.322369722 | CORE        | 20      | O       | O  | 0.0000 | 20 |
| O     | 6.094398932  | 8.889119832  | 2.105766959 | CORE        | 21      | O       | O  | 0.0000 | 21 |
| O     | 8.318072139  | 6.855591673  | 2.692150038 | CORE        | 22      | O       | O  | 0.0000 | 22 |
| O     | 0.139443794  | 0.007438045  | 3.228530629 | CORE        | 23      | O       | O  | 0.0000 | 23 |
| O     | 6.880249145  | 1.060844718  | 4.481941285 | CORE        | 24      | O       | O  | 0.0000 | 24 |
| O     | 0.472081699  | 7.500643533  | 4.627920950 | CORE        | 25      | O       | O  | 0.0000 | 25 |
| O     | 7.458889340  | 8.541817323  | 5.917905050 | CORE        | 26      | O       | O  | 0.0000 | 26 |
| O     | 8.495740744  | 1.870619270  | 6.453166312 | CORE        | 27      | O       | O  | 0.0000 | 27 |
| O     | 1.544002109  | -0.451842630 | 7.138025804 | CORE        | 28      | O       | O  | 0.0000 | 28 |
| O     | 6.143725838  | 0.661465916  | 6.967336983 | CORE        | 29      | O       | O  | 0.0000 | 29 |
| O     | -0.489879160 | 6.326487746  | 7.033560298 | CORE        | 30      | O       | O  | 0.0000 | 30 |
| O     | 0.393482434  | 4.134883398  | 7.749448049 | CORE        | 31      | O       | O  | 0.0000 | 31 |
| O     | 3.506694329  | 0.902279409  | 7.837896745 | CORE        | 32      | O       | O  | 0.0000 | 32 |
| O     | 1.217753460  | 1.601773403  | 8.539496121 | CORE        | 33      | O       | O  | 0.0000 | 33 |
| O     | 4.494910320  | 8.162219671  | 8.974785498 | CORE        | 34      | O       | O  | 0.0000 | 34 |
| O     | -1.183296029 | 5.424614859  | 9.230983168 | CORE        | 35      | O       | O  | 0.0000 | 35 |
| P     | 7.601089353  | 3.088657463  | 1.002603741 | CORE        | 36      | P       | P  | 0.0000 | 36 |
| O     | 5.149824718  | 1.855523322  | 3.212583553 | CORE        | 37      | O       | O  | 0.0000 | 37 |



|    |              |              |             |      |    |    |    |        |    |
|----|--------------|--------------|-------------|------|----|----|----|--------|----|
| 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 + CH<sub>3</sub>COOCH<sub>3</sub>\*

|                  |              |              |             |             |         |         |    |        |    |
|------------------|--------------|--------------|-------------|-------------|---------|---------|----|--------|----|
| 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 |
| H                | 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  
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  | 0.71837008  | 6.085563605 | CORE        | 3       | Si      | Si | 0.0000 | 3  |
| Al               | 7.893261079  | 0.779001987 | 2.880889341 | 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 |

|     |              |              |                  |    |   |   |        |    |
|-----|--------------|--------------|------------------|----|---|---|--------|----|
| O   | 8.071820770  | 2.327568742  | 2.143914567 CORE | 19 | O | O | 0.0000 | 19 |
| O   | 1.288297172  | 7.861835216  | 2.340633337 CORE | 20 | O | O | 0.0000 | 20 |
| O   | 6.035401568  | 9.077474006  | 2.001166710 CORE | 21 | O | O | 0.0000 | 21 |
| O   | 8.301776359  | 6.853430534  | 2.697490829 CORE | 22 | O | O | 0.0000 | 22 |
| O   | 0.132774719  | 0.025238161  | 3.130746339 CORE | 23 | O | O | 0.0000 | 23 |
| O   | 6.981048451  | 1.085446796  | 4.435651044 CORE | 24 | O | O | 0.0000 | 24 |
| O   | 0.406648399  | 7.574447215  | 4.640342771 CORE | 25 | O | O | 0.0000 | 25 |
| O   | 7.373712431  | 8.556059146  | 5.973414792 CORE | 26 | O | O | 0.0000 | 26 |
| O   | 8.519136167  | 1.874766482  | 6.441370114 CORE | 27 | O | O | 0.0000 | 27 |
| O   | 1.464194483  | -0.409776948 | 7.156381057 CORE | 28 | O | O | 0.0000 | 28 |
| O   | 6.066447663  | 0.834263749  | 6.854822484 CORE | 29 | O | O | 0.0000 | 29 |
| O   | -0.491666446 | 6.346638311  | 7.041455559 CORE | 30 | O | O | 0.0000 | 30 |
| O   | 0.370691383  | 4.145852961  | 7.741958844 CORE | 31 | O | O | 0.0000 | 31 |
| O   | 3.433813306  | 0.936905516  | 7.825477212 CORE | 32 | O | O | 0.0000 | 32 |
| O   | 1.165295909  | 1.618288672  | 8.600933332 CORE | 33 | O | O | 0.0000 | 33 |
| O   | 4.466298822  | 8.214032972  | 8.860685236 CORE | 34 | O | O | 0.0000 | 34 |
| O   | -0.413156753 | 6.254069543  | 0.015719904 CORE | 35 | O | O | 0.0000 | 35 |
| P   | 7.523886011  | 3.137859548  | 0.955394083 CORE | 36 | P | P | 0.0000 | 36 |
| O   | 5.748604080  | 4.205386714  | 4.445451686 CORE | 37 | O | O | 0.0000 | 37 |
| C   | 6.094076197  | 4.659221009  | 5.436915827 CORE | 38 | C | C | 0.0000 | 38 |
| H   | 6.104520244  | 1.492552811  | 4.374097394 CORE | 39 | H | H | 0.0000 | 39 |
| end |              |              |                  |    |   |   |        |    |
| end |              |              |                  |    |   |   |        |    |

# HS + CH<sub>3</sub>OCH<sub>3</sub>\*

!BIOSYM archive 2

PBC=ON

|       | Energy       |              | 28               | -284    | -284.953247 |         |        |    |  |
|-------|--------------|--------------|------------------|---------|-------------|---------|--------|----|--|
| !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     | 5.376037328  | 8.165349299  | 0.932423709 CORE | 2       | P           | P       | 0.0000 | 2  |  |
| Si    | 7.451976326  | 0.780142273  | 6.042039441 CORE | 3       | Si          | Si      | 0.0000 | 3  |  |
| Al    | 7.872173957  | 0.751273047  | 2.885584819 CORE | 4       | Al          | Al      | 0.0000 | 4  |  |
| P     | 0.041435866  | 7.870634126  | 3.213293113 CORE | 5       | P           | P       | 0.0000 | 5  |  |
| Al    | 7.676175281  | 6.109029596  | 1.260771160 CORE | 6       | Al          | Al      | 0.0000 | 6  |  |
| Al    | -0.374309243 | 7.891391800  | 6.199717690 CORE | 7       | Al          | Al      | 0.0000 | 7  |  |
| Al    | -0.144006999 | 2.546226989  | 7.899704199 CORE | 8       | Al          | Al      | 0.0000 | 8  |  |
| P     | 2.059014509  | 0.429863066  | 8.320255655 CORE | 9       | P           | P       | 0.0000 | 9  |  |
| P     | -0.048745040 | 5.558627883  | 8.221756610 CORE | 10      | P           | P       | 0.0000 | 10 |  |
| Al    | 5.128130662  | 0.545088493  | 8.256418381 CORE | 11      | Al          | Al      | 0.0000 | 11 |  |
| O     | 1.179880690  | 6.211970773  | 8.870163893 CORE | 12      | O           | O       | 0.0000 | 12 |  |
| O     | 6.336498980  | 2.416202274  | 0.362090141 CORE | 13      | O           | O       | 0.0000 | 13 |  |
| O     | 7.893067929  | 2.477024873  | 9.106166347 CORE | 14      | O           | O       | 0.0000 | 14 |  |
| O     | 2.916724856  | 0.449007287  | 0.401403914 CORE | 15      | O           | O       | 0.0000 | 15 |  |
| O     | 6.258143941  | 6.947808010  | 0.677598739 CORE | 16      | O           | O       | 0.0000 | 16 |  |
| O     | 3.999259495  | 7.703025906  | 1.429128471 CORE | 17      | O           | O       | 0.0000 | 17 |  |
| O     | 7.181727783  | 4.455290919  | 1.536480307 CORE | 18      | O           | O       | 0.0000 | 18 |  |
| O     | 8.171810593  | 2.250425942  | 2.074925143 CORE | 19      | O           | O       | 0.0000 | 19 |  |
| O     | 1.293489763  | 7.850103167  | 2.342249530 CORE | 20      | O           | O       | 0.0000 | 20 |  |
| O     | 6.002155379  | 9.028299203  | 2.034574998 CORE | 21      | O           | O       | 0.0000 | 21 |  |
| O     | 8.338293804  | 6.805091430  | 2.735966485 CORE | 22      | O           | O       | 0.0000 | 22 |  |
| O     | 0.113829154  | -0.009895392 | 3.128078706 CORE | 23      | O           | O       | 0.0000 | 23 |  |
| O     | 6.964859829  | 1.187471115  | 4.411225038 CORE | 24      | O           | O       | 0.0000 | 24 |  |
| O     | 0.446950986  | 7.594270100  | 4.659730708 CORE | 25      | O           | O       | 0.0000 | 25 |  |
| O     | 7.387494228  | 8.614207476  | 5.874180952 CORE | 26      | O           | O       | 0.0000 | 26 |  |
| O     | 8.527968446  | 1.902206247  | 6.432316538 CORE | 27      | O           | O       | 0.0000 | 27 |  |
| O     | 1.412669326  | -0.411651663 | 7.221859124 CORE | 28      | O           | O       | 0.0000 | 28 |  |
| O     | 6.086011879  | 0.813975130  | 6.860185311 CORE | 29      | O           | O       | 0.0000 | 29 |  |
| O     | -0.589274662 | 6.386251358  | 7.059300908 CORE | 30      | O           | O       | 0.0000 | 30 |  |
| O     | 0.374806488  | 4.195170337  | 7.687114020 CORE | 31      | O           | O       | 0.0000 | 31 |  |
| O     | 3.455875773  | 0.855237262  | 7.856029223 CORE | 32      | O           | O       | 0.0000 | 32 |  |
| O     | 1.224073660  | 1.681923036  | 8.581351889 CORE | 33      | O           | O       | 0.0000 | 33 |  |
| O     | 4.492737398  | 8.159346149  | 8.871849419 CORE | 34      | O           | O       | 0.0000 | 34 |  |
| O     | -0.404206594 | 6.227923627  | 0.036620563 CORE | 35      | O           | O       | 0.0000 | 35 |  |
| P     | 7.582010409  | 3.102001462  | 0.940287696 CORE | 36      | P           | P       | 0.0000 | 36 |  |
| O     | 4.205358565  | 2.774366732  | 3.884295980 CORE | 37      | O           | O       | 0.0000 | 37 |  |
| H     | 6.124860058  | 1.684763421  | 4.320278827 CORE | 38      | H           | H       | 0.0000 | 38 |  |
| C     | 3.307919950  | 2.888083385  | 4.999833063 CORE | 39      | C           | C       | 0.0000 | 39 |  |
| H     | 3.283642672  | 3.918284327  | 5.382095280 CORE | 40      | H           | H       | 0.0000 | 40 |  |
| H     | 3.664053318  | 2.214495490  | 5.774269684 CORE | 41      | H           | H       | 0.0000 | 41 |  |
| H     | 2.286756345  | 2.599170971  | 4.706131125 CORE | 42      | H           | H       | 0.0000 | 42 |  |
| H     | 4.424030842  | 3.407202317  | 1.944348596 CORE | 43      | H           | H       | 0.0000 | 43 |  |
| C     | 3.780676720  | 3.613935678  | 2.796475154 CORE | 44      | C           | C       | 0.0000 | 44 |  |
| H     | 2.738173653  | 3.391459553  | 2.529961984 CORE | 45      | H           | H       | 0.0000 | 45 |  |
| H     | 3.863187949  | 4.676488231  | 3.068654559 CORE | 46      | H           | H       | 0.0000 | 46 |  |
| end   |              |              |                  |         |             |         |        |    |  |
| end   |              |              |                  |         |             |         |        |    |  |

# HS + HCOOCH<sub>3</sub>\*

!BIOSYM archive 2

PBC=ON

| !DATE | Energy       |              | 29     | -282             | -282.389197 |         |    |    |        |    |
|-------|--------------|--------------|--------|------------------|-------------|---------|----|----|--------|----|
| PBC   | 9.3040       | 9.3040       | 9.3040 | 94.5972          | 94.5972     | 94.5972 |    |    |        |    |
| Al    | 2.353654000  | 8.064435000  |        | 0.968225600 CORE | 2           | 1       | Al | Al | 0.0000 | 1  |
| P     | 5.465941599  | 8.128791917  |        | 0.845334657 CORE | 2           | 2       | P  | P  | 0.0000 | 2  |
| Si    | 7.506119685  | 0.761548050  |        | 5.886195269 CORE | 3           | 3       | Si | Si | 0.0000 | 3  |
| Al    | 7.961978213  | 0.689886740  |        | 2.885486665 CORE | 4           | 4       | Al | Al | 0.0000 | 4  |
| P     | 0.083337070  | 7.808206820  |        | 3.168808630 CORE | 5           | 5       | P  | P  | 0.0000 | 5  |
| Al    | 7.675300521  | 6.041202061  |        | 1.190309048 CORE | 6           | 6       | Al | Al | 0.0000 | 6  |
| Al    | -0.299052885 | 7.863640914  |        | 6.226367060 CORE | 7           | 7       | Al | Al | 0.0000 | 7  |
| Al    | -0.138953530 | 2.532257400  |        | 7.845965415 CORE | 8           | 8       | Al | Al | 0.0000 | 8  |
| P     | 2.128222626  | 0.365671906  |        | 8.206002663 CORE | 9           | 9       | P  | P  | 0.0000 | 9  |
| P     | 0.007738643  | 5.493149448  |        | 8.222648823 CORE | 10          | 10      | P  | P  | 0.0000 | 10 |
| Al    | 5.210865897  | 0.463316667  |        | 8.286550875 CORE | 11          | 11      | Al | Al | 0.0000 | 11 |
| O     | 1.209402758  | 6.098233207  |        | 8.959128793 CORE | 12          | 12      | O  | O  | 0.0000 | 12 |
| O     | 6.591184520  | 2.344685680  |        | 0.245482781 CORE | 13          | 13      | O  | O  | 0.0000 | 13 |
| O     | 8.880275573  | 3.304318122  |        | 0.008134581 CORE | 14          | 14      | O  | O  | 0.0000 | 14 |
| O     | 2.789148565  | 0.372672603  |        | 0.275533484 CORE | 15          | 15      | O  | O  | 0.0000 | 15 |
| O     | 6.186112569  | 6.798756011  |        | 0.647999504 CORE | 16          | 16      | O  | O  | 0.0000 | 16 |
| O     | 4.048112327  | 7.891033916  |        | 1.379343890 CORE | 17          | 17      | O  | O  | 0.0000 | 17 |
| O     | 7.210622407  | 4.392156986  |        | 1.519616694 CORE | 18          | 18      | O  | O  | 0.0000 | 18 |
| O     | 8.252147490  | 2.227786705  |        | 2.136068738 CORE | 19          | 19      | O  | O  | 0.0000 | 19 |
| O     | 1.417253709  | 7.761519216  |        | 2.414601142 CORE | 20          | 20      | O  | O  | 0.0000 | 20 |
| O     | 6.226352716  | 8.982119613  |        | 1.843606831 CORE | 21          | 21      | O  | O  | 0.0000 | 21 |
| O     | 8.381568927  | 6.789605528  |        | 2.605995209 CORE | 22          | 22      | O  | O  | 0.0000 | 22 |
| O     | 0.247384591  | -0.045976057 |        | 3.054408549 CORE | 23          | 23      | O  | O  | 0.0000 | 23 |
| O     | 7.090193338  | 0.881077799  |        | 4.351564004 CORE | 24          | 24      | O  | O  | 0.0000 | 24 |
| O     | 0.338041390  | 7.471480721  |        | 4.633599916 CORE | 25          | 25      | O  | O  | 0.0000 | 25 |
| O     | 7.463553650  | 8.653115717  |        | 6.286514475 CORE | 26          | 26      | O  | O  | 0.0000 | 26 |
| O     | 8.295806560  | 2.031423888  |        | 6.449369973 CORE | 27          | 27      | O  | O  | 0.0000 | 27 |
| O     | 1.736651393  | -0.489879140 |        | 6.996925737 CORE | 28          | 28      | O  | O  | 0.0000 | 28 |
| O     | 5.925556274  | 0.772086338  |        | 6.643829017 CORE | 29          | 29      | O  | O  | 0.0000 | 29 |
| O     | -0.466633690 | 6.365841626  |        | 7.074154633 CORE | 30          | 30      | O  | O  | 0.0000 | 30 |
| O     | 0.455178741  | 4.155441958  |        | 7.643555987 CORE | 31          | 31      | O  | O  | 0.0000 | 31 |
| O     | 3.562138515  | 0.861889375  |        | 7.980130987 CORE | 32          | 32      | O  | O  | 0.0000 | 32 |
| O     | 1.240295011  | 1.585693238  |        | 8.309348476 CORE | 33          | 33      | O  | O  | 0.0000 | 33 |
| O     | 4.662369614  | 8.056403666  |        | 8.723635667 CORE | 34          | 34      | O  | O  | 0.0000 | 34 |
| O     | -1.169782803 | 5.331679099  |        | 9.184725552 CORE | 35          | 35      | O  | O  | 0.0000 | 35 |
| P     | 7.739306545  | 3.063258229  |        | 0.974217137 CORE | 36          | 36      | P  | P  | 0.0000 | 36 |
| O     | 3.444030917  | 2.249805767  |        | 2.823852077 CORE | 37          | 37      | O  | O  | 0.0000 | 37 |
| C     | 3.897746969  | 1.595434087  |        | 3.730353997 CORE | 38          | 38      | C  | C  | 0.0000 | 38 |



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 + CH<sub>3</sub>OH\*

!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 | 5.555185062  | 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   | -1.172721962 | 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

#### CH<sub>3</sub>S + CH<sub>3</sub>CO\*

!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 |

|     |              |              |             |      |    |    |    |        |    |
|-----|--------------|--------------|-------------|------|----|----|----|--------|----|
| P   | 2.098994908  | 0.359773202  | 8.236098888 | CORE | 9  | P  | P  | 0.0000 | 9  |
| P   | -0.036837061 | 5.488669788  | 8.229884433 | CORE | 10 | P  | P  | 0.0000 | 10 |
| Al  | 5.160458558  | 0.442868238  | 8.227648061 | CORE | 11 | Al | Al | 0.0000 | 11 |
| O   | 1.171207535  | 6.163801493  | 8.897192865 | CORE | 12 | O  | O  | 0.0000 | 12 |
| O   | 6.367534550  | 2.297462005  | 0.347684281 | CORE | 13 | O  | O  | 0.0000 | 13 |
| O   | 7.913141430  | 2.366582944  | 9.066465399 | CORE | 14 | O  | O  | 0.0000 | 14 |
| O   | 2.924642420  | 0.418333722  | 0.348127812 | CORE | 15 | O  | O  | 0.0000 | 15 |
| O   | 6.187716155  | 6.796135715  | 0.668935484 | CORE | 16 | O  | O  | 0.0000 | 16 |
| O   | 4.001346457  | 7.726551618  | 1.468489993 | CORE | 17 | O  | O  | 0.0000 | 17 |
| O   | 7.210511873  | 4.344063131  | 1.511766994 | CORE | 18 | O  | O  | 0.0000 | 18 |
| O   | 8.215133103  | 2.148957379  | 2.050561706 | CORE | 19 | O  | O  | 0.0000 | 19 |
| O   | 1.319736746  | 7.714857692  | 2.335594386 | CORE | 20 | O  | O  | 0.0000 | 20 |
| O   | 6.118957860  | 8.913222378  | 1.968102164 | CORE | 21 | O  | O  | 0.0000 | 21 |
| O   | 8.329704977  | 6.724508543  | 2.680848888 | CORE | 22 | O  | O  | 0.0000 | 22 |
| O   | 0.176480423  | -0.111731512 | 3.150277568 | CORE | 23 | O  | O  | 0.0000 | 23 |
| O   | 6.963440763  | 1.047319062  | 4.357730849 | CORE | 24 | O  | O  | 0.0000 | 24 |
| O   | 0.463530013  | 7.405884903  | 4.628566270 | CORE | 25 | O  | O  | 0.0000 | 25 |
| O   | 7.460279068  | 8.533824458  | 5.827931724 | CORE | 26 | O  | O  | 0.0000 | 26 |
| O   | 8.500655471  | 1.857080844  | 6.359990920 | CORE | 27 | O  | O  | 0.0000 | 27 |
| O   | 1.529075554  | -0.534423443 | 7.135500587 | CORE | 28 | O  | O  | 0.0000 | 28 |
| O   | 6.134925511  | 0.647185011  | 6.837498735 | CORE | 29 | O  | O  | 0.0000 | 29 |
| O   | -0.564320475 | 6.304444805  | 7.055137841 | CORE | 30 | O  | O  | 0.0000 | 30 |
| O   | 0.406691001  | 4.126043713  | 7.706840597 | CORE | 31 | O  | O  | 0.0000 | 31 |
| O   | 3.500729012  | 0.809677111  | 7.816556968 | CORE | 32 | O  | O  | 0.0000 | 32 |
| O   | 1.218189249  | 1.581605919  | 8.444702173 | CORE | 33 | O  | O  | 0.0000 | 33 |
| O   | 4.503587905  | 8.049369320  | 8.839050370 | CORE | 34 | O  | O  | 0.0000 | 34 |
| O   | -0.419592141 | 6.146963173  | 0.012616168 | CORE | 35 | O  | O  | 0.0000 | 35 |
| P   | 7.615229275  | 2.992632834  | 0.912163184 | CORE | 36 | P  | P  | 0.0000 | 36 |
| O   | 5.833961206  | 4.953999184  | 6.136880482 | CORE | 37 | O  | O  | 0.0000 | 37 |
| C   | 4.938985023  | 5.411769000  | 5.523904964 | CORE | 38 | C  | C  | 0.0000 | 38 |
| H   | 4.904738175  | 1.296835437  | 4.639853273 | CORE | 39 | H  | H  | 0.0000 | 39 |
| C   | 3.930140818  | 5.897618424  | 4.837139672 | CORE | 40 | C  | C  | 0.0000 | 40 |
| H   | 4.093056478  | 6.369231981  | 3.876611131 | CORE | 41 | H  | H  | 0.0000 | 41 |
| H   | 2.926679138  | 5.806561333  | 5.232099641 | CORE | 42 | H  | H  | 0.0000 | 42 |
| C   | 5.717065284  | 1.824264007  | 4.144354006 | CORE | 43 | C  | C  | 0.0000 | 43 |
| H   | 5.536281490  | 1.878191748  | 3.072717056 | CORE | 44 | H  | H  | 0.0000 | 44 |
| H   | 5.851669271  | 2.820717301  | 4.559550478 | CORE | 45 | H  | H  | 0.0000 | 45 |
| end |              |              |             |      |    |    |    |        |    |
| end |              |              |             |      |    |    |    |        |    |

# CH<sub>3</sub>S + CO\*

!BIOSYM archive 2

PBC=ON

|       | Energy       |              | 33          | -268    | -268.710733 |         |    |        |    |
|-------|--------------|--------------|-------------|---------|-------------|---------|----|--------|----|
| !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     | 5.430011157  | 8.140398889  | 0.933672871 | CORE    | 2           | P       | P  | 0.0000 | 2  |
| Si    | 7.523783996  | 0.741963026  | 6.002387289 | CORE    | 3           | Si      | Si | 0.0000 | 3  |
| Al    | 7.984651624  | 0.691448249  | 2.881287421 | CORE    | 4           | Al      | Al | 0.0000 | 4  |
| P     | 0.094863314  | 7.800213985  | 3.218280234 | CORE    | 5           | P       | P  | 0.0000 | 5  |
| Al    | 7.699959781  | 6.069967134  | 1.248075074 | CORE    | 6           | Al      | Al | 0.0000 | 6  |
| Al    | -0.299884378 | 7.852707205  | 6.186537495 | CORE    | 7           | Al      | Al | 0.0000 | 7  |
| Al    | -0.091449844 | 2.515542163  | 7.847197702 | CORE    | 8           | Al      | Al | 0.0000 | 8  |
| P     | 2.130195820  | 0.408445046  | 8.273931358 | CORE    | 9           | P       | P  | 0.0000 | 9  |
| P     | -0.020341959 | 5.534513070  | 8.217644608 | CORE    | 10          | P       | P  | 0.0000 | 10 |
| Al    | 5.214215958  | 0.505038264  | 8.252265580 | CORE    | 11          | Al      | Al | 0.0000 | 11 |
| O     | 1.206399713  | 6.181586583  | 8.878055684 | CORE    | 12          | O       | O  | 0.0000 | 12 |
| O     | 4.068220432  | 2.373326639  | 0.363419774 | CORE    | 13          | O       | O  | 0.0000 | 13 |
| O     | 7.966642237  | 2.404588879  | 9.076896875 | CORE    | 14          | O       | O  | 0.0000 | 14 |
| O     | 2.923154642  | 0.432107557  | 0.363569781 | CORE    | 15          | O       | O  | 0.0000 | 15 |
| O     | 6.233009918  | 6.859143888  | 0.712863871 | CORE    | 16          | O       | O  | 0.0000 | 16 |
| O     | 4.022628448  | 7.788588736  | 1.427508399 | CORE    | 17          | O       | O  | 0.0000 | 17 |
| O     | 7.282541196  | 4.399068518  | 1.529845111 | CORE    | 18          | O       | O  | 0.0000 | 18 |
| O     | 8.261100162  | 2.192571362  | 2.060727553 | CORE    | 19          | O       | O  | 0.0000 | 19 |
| O     | 1.349528389  | 7.760747018  | 2.352904502 | CORE    | 20          | O       | O  | 0.0000 | 20 |
| O     | 6.113851090  | 8.972905516  | 2.025016417 | CORE    | 21          | O       | O  | 0.0000 | 21 |
| O     | 8.352784064  | 6.787783414  | 2.716033816 | CORE    | 22          | O       | O  | 0.0000 | 22 |
| O     | 0.227514706  | -0.050488363 | 3.152155271 | CORE    | 23          | O       | O  | 0.0000 | 23 |
| O     | 7.009761333  | 1.113013380  | 4.373846298 | CORE    | 24          | O       | O  | 0.0000 | 24 |
| O     | 0.490454881  | 7.476827530  | 4.653060769 | CORE    | 25          | O       | O  | 0.0000 | 25 |
| O     | 7.474558758  | 8.585980164  | 5.841402465 | CORE    | 26          | O       | O  | 0.0000 | 26 |
| O     | 8.580131567  | 1.893137840  | 6.367718480 | CORE    | 27          | O       | O  | 0.0000 | 27 |
| O     | 1.528865346  | -0.440798694 | 7.153502726 | CORE    | 28          | O       | O  | 0.0000 | 28 |
| O     | 6.185204297  | 0.757014007  | 6.863898999 | CORE    | 29          | O       | O  | 0.0000 | 29 |
| O     | -0.559541851 | 6.373283939  | 7.065034459 | CORE    | 30          | O       | O  | 0.0000 | 30 |
| O     | 0.394441824  | 4.177165863  | 7.665975579 | CORE    | 31          | O       | O  | 0.0000 | 31 |
| O     | 3.543245022  | 0.827113685  | 7.856732529 | CORE    | 32          | O       | O  | 0.0000 | 32 |
| O     | 1.289597180  | 1.660320558  | 8.501196153 | CORE    | 33          | O       | O  | 0.0000 | 33 |
| O     | 4.621613509  | 8.120883494  | 8.859548697 | CORE    | 34          | O       | O  | 0.0000 | 34 |
| O     | -0.386297510 | 6.205674700  | 0.022365245 | CORE    | 35          | O       | O  | 0.0000 | 35 |
| P     | 7.667686936  | 3.044505814  | 0.925593252 | CORE    | 36          | P       | P  | 0.0000 | 36 |
| O     | 1.816170264  | 4.459565545  | 4.253987376 | CORE    | 37          | O       | O  | 0.0000 | 37 |
| O     | 2.237498695  | 5.580889889  | 3.657885534 | CORE    | 38          | C       | C  | 0.0000 | 38 |
| H     | 5.193088187  | 1.372730817  | 3.371130430 | CORE    | 39          | H       | H  | 0.0000 | 39 |
| C     | 5.783115900  | 1.904723762  | 4.117438798 | CORE    | 40          | C       | C  | 0.0000 | 40 |
| H     | 6.078938332  | 2.887841623  | 3.753749793 | CORE    | 41          | H       | H  | 0.0000 | 41 |
| H     | 5.232528170  | 1.978278876  | 5.049679464 | CORE    | 42          | H       | H  | 0.0000 | 42 |
| end   |              |              |             |         |             |         |    |        |    |
| end   |              |              |             |         |             |         |    |        |    |

# CH<sub>3</sub>S + H<sub>2</sub>O\*

!BIOSYM archive 2

PBC=ON

|       | Energy       |              | 34          | -267    | -267.790724 |         |    |        |    |
|-------|--------------|--------------|-------------|---------|-------------|---------|----|--------|----|
| !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     | 5.408977079  | 8.093181216  | 1.049249871 | CORE    | 2           | P       | P  | 0.0000 | 2  |
| Si    | 7.545663029  | 0.698692035  | 6.085007446 | CORE    | 3           | Si      | Si | 0.0000 | 3  |
| Al    | 7.913995470  | 0.643578786  | 2.994237175 | CORE    | 4           | Al      | Al | 0.0000 | 4  |
| P     | 0.108424277  | 7.793686723  | 3.255685214 | CORE    | 5           | P       | P  | 0.0000 | 5  |
| Al    | 7.716439103  | 6.038972920  | 1.330983793 | CORE    | 6           | Al      | Al | 0.0000 | 6  |
| Al    | -0.303760779 | 7.829241171  | 6.209264080 | CORE    | 7           | Al      | Al | 0.0000 | 7  |
| Al    | -0.061673722 | 2.489497070  | 7.943999631 | CORE    | 8           | Al      | Al | 0.0000 | 8  |
| P     | 2.146233461  | 0.392220168  | 8.308446359 | CORE    | 9           | P       | P  | 0.0000 | 9  |
| P     | -0.059883685 | 5.531348821  | 8.246572158 | CORE    | 10          | P       | P  | 0.0000 | 10 |
| Al    | 5.223227683  | 0.473511210  | 8.328027628 | CORE    | 11          | Al      | Al | 0.0000 | 11 |
| O     | 1.162232851  | 6.215133939  | 8.874297085 | CORE    | 12          | O       | O  | 0.0000 | 12 |
| O     | 6.400264261  | 2.413219293  | 0.386453827 | CORE    | 13          | O       | O  | 0.0000 | 13 |
| O     | 8.019226128  | 2.369236128  | 9.196444204 | CORE    | 14          | O       | O  | 0.0000 | 14 |
| O     | 2.958937974  | 0.445367509  | 0.416050007 | CORE    | 15          | O       | O  | 0.0000 | 15 |
| O     | 6.251282989  | 6.840636976  | 0.824159963 | CORE    | 16          | O       | O  | 0.0000 | 16 |
| O     | 3.989780280  | 7.675760754  | 1.440760314 | CORE    | 17          | O       | O  | 0.0000 | 17 |
| O     | 7.325579426  | 4.367934490  | 1.630447420 | CORE    | 18          | O       | O  | 0.0000 | 18 |
| O     | 8.198814664  | 2.108419485  | 2.119555705 | CORE    | 19          | O       | O  | 0.0000 | 19 |
| O     | 1.343544756  | 7.782427861  | 2.362507369 | CORE    | 20          | O       | O  | 0.0000 | 20 |
| O     | 5.999686782  | 8.904262968  | 2.212035489 | CORE    | 21          | O       | O  | 0.0000 | 21 |
| O     | 8.400982554  | 6.728153787  | 2.795118297 | CORE    | 22          | O       | O  | 0.0000 | 22 |
| O     | 0.181346500  | -0.089577611 | 3.182892358 | CORE    | 23          | O       | O  | 0.0000 | 23 |
| O     | 7.019318441  | 1.166793729  | 4.495626880 | CORE    | 24          | O       | O  | 0.0000 | 24 |
| O     | 0.547092953  | 7.494711451  | 4.691306891 | CORE    | 25          | O       | O  | 0.0000 | 25 |
| O     | 7.476918763  | 8.547846989  | 5.814781807 | CORE    | 26          | O       | O  | 0.0000 | 26 |

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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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# CH<sub>3</sub>S + CH<sub>3</sub>OH\*

!BIOSYM archive 2

PBC=ON

```

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

```

# CH<sub>3</sub>S

!BIOSYM archive 2

PBC=ON

```

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 2.786942414 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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