Supplementary material

Interaction of electronically excited CO($a^3\Pi_r$) molecules with H, H_2, and H_2O: Potential energy surfaces and reaction kinetics

Alexey V. Pelevkin, Boris I. Loukhovitski, and Alexander S. Sharipov

Central Institute of Aviation Motors, Moscow, Russia

E-mail: aleksandr.sharipov@phystech.edu, assharipov@ciam.ru

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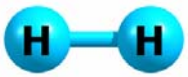
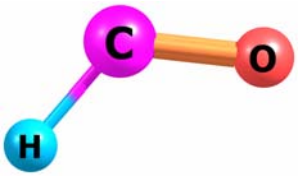
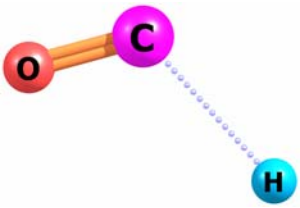
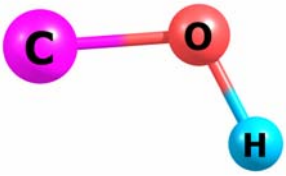
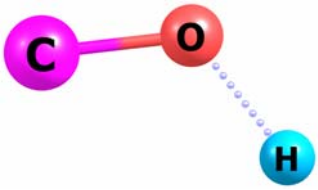
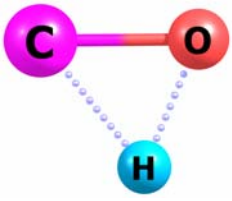
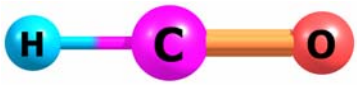
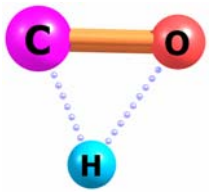
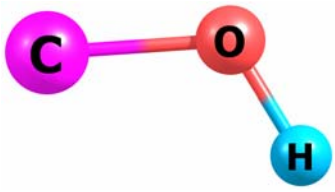
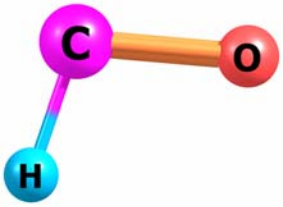
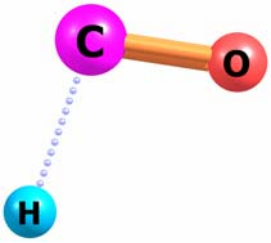
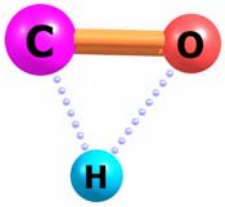
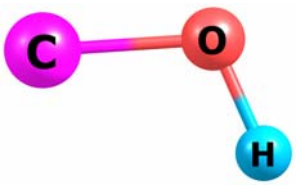
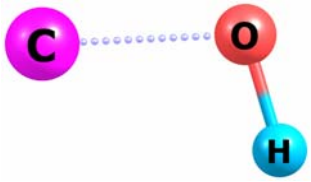
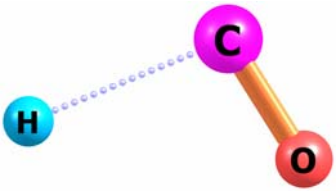
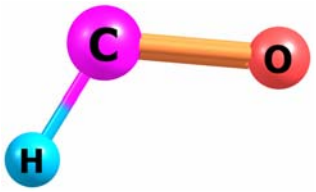
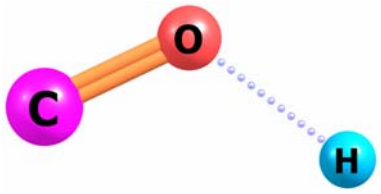
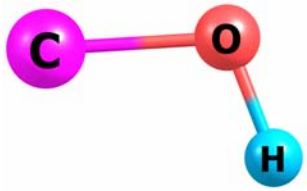
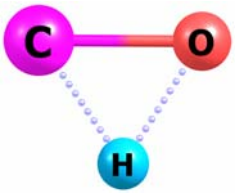
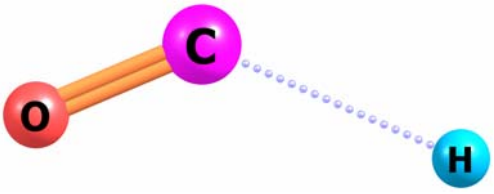
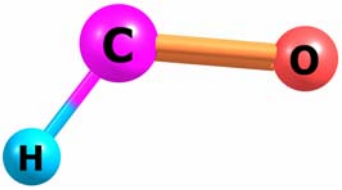
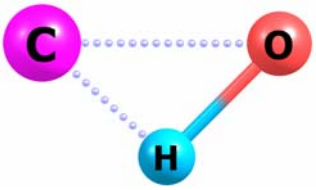
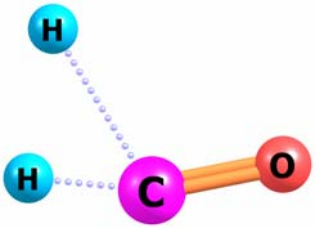
Preamble

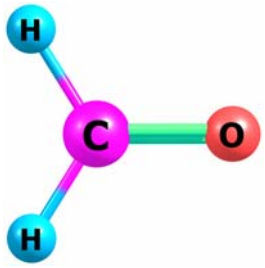
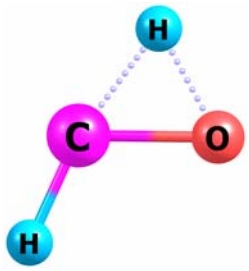
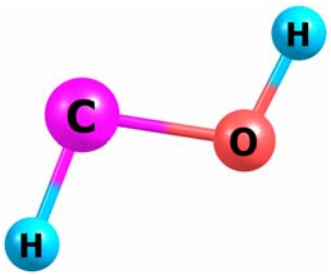
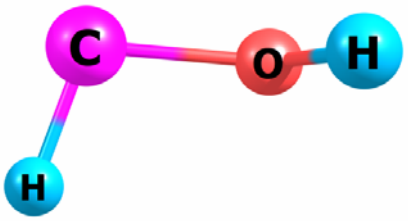
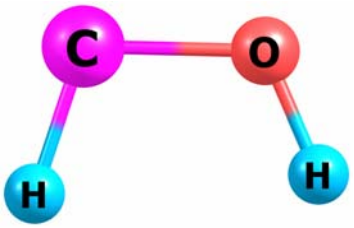
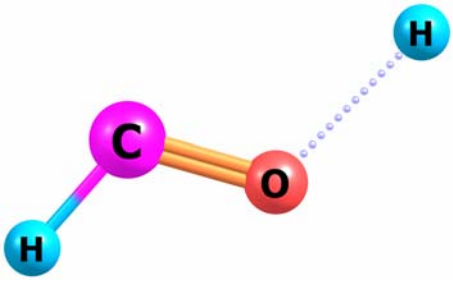
The structures, frequencies of normal vibrations, and rotational constants for reactants, products, and transitions states, obtained in the present work, are presented in **Table S1**. The corresponding structures are also given in the Cartesian GAMESS-like input format in **Table S2**.

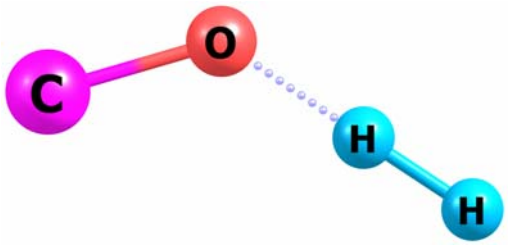
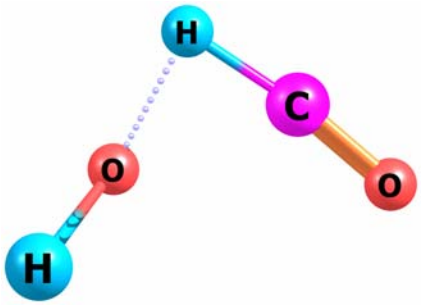
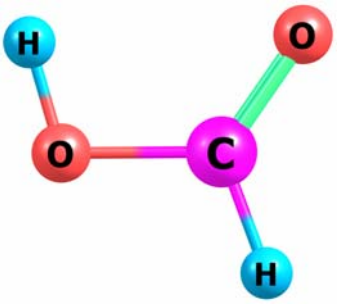
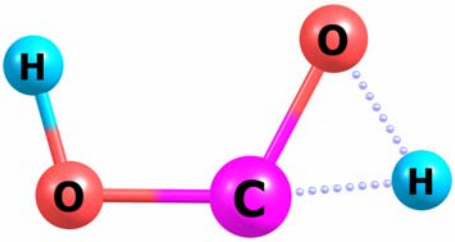
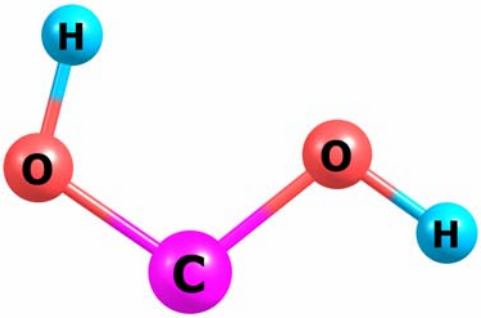
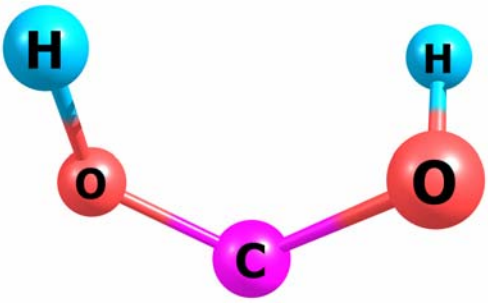
Table S1. Structure and properties of reactants, products, and transitions states.

Structure	Rotational constants A_0, B_0, C_0, K	Vibrational frequencies ω_1,..,ω_n, cm^{-1}	Image
CO($X^1\Sigma$)	2.756	2151.56	
CO($a^3\Pi_r$)	2.403	1724.15	
OH($X^2\Sigma$)	26.829	3739.76	
H_2	86.811	4361.11	
H_2O	13.552, 21.124, 37.803	1623.84, 3787.50, 3876.21	
$^2IM_0$ (CHO)	2.008, 2.132, 34.347	1105.29, 1863.46, 2670.84	
$^2TS_0$ (CHO)	1.755, 2.065, 11.684	765.34*i*, 363.05, 2097.21	
$^2IM_1$ (CHO)	1.887, 2.001, 33.144	1137.58, 1381.87, 3344.62	
$^2TS_1$ (CHO)	2.005, 2.174, 25.821	2486.87*i*, 975.92, 1792.76	
$^2TS_2$ (CHO)	1.958, 2.139, 23.198	2124.30*i*, 1411.00, 2429.65	

$^{2}IM_{2}$ (CHO)	1.912	832.58, 832.62, 1809.73, 3432.65	
$^{2}TS_{3}$ (CHO)	1.993, 2.217, 19.710	1523.41*i*, 1498.49, 2437.12	
$^{2}IM_{3}$ (CHO)	1.797, 1.890, 36.851	724.30, 1299.18, 3750.39	
$^{2}IM_{5}$ (CHO)	1.589, 1.707, 22.999	1072.67, 1382.19, 2729.95	
$^{2}TS_{4}$ (CHO)	1.799, 2.107, 12.313	1343.82*i*, 903.37, 2065.83	
$^{2}TS_{5}$ (CHO)	1.996, 2.221, 19.759	1416.44*i*, 1591.41, 3171.99	
$^{2}IM_{6}$ (CHO)	1.768, 1.874, 31.181	1105.95, 1410.23, 3312.54	
$^{2}TS_{6}$ (CHO)	1.211, 1.264, 28.911	1455.48*i*, 939.11, 3598.44	
$^{4}TS_{0}$ (CHO)	1.636, 2.040, 8.254	1675.87*i*, 429.34, 1460.49	

$^4IM_0$ (CHO)	1.534, 1.617, 29.842	953.78, 1237.89, 3095.86	
$^4TS_1$ (CHO)	1.748, 1.970, 15.530	1521.75*i*, 663.79, 1544.92	
$^4IM_1$ (CHO)	1.678, 1.774, 31.096	1100.88, 1275.60, 3695.98	
$^4TS_2$ (CHO)	1.704, 1.840, 23.150	1923.87*i*, 1158.34, 2391.88	
$^4TS_3$ (CHO)	1.215, 1.321, 15.127	722.67*i*, 151.62, 1187.68	
$^4IM_2$ (CHO)	1.468, 1.535, 33.866	1049.19, 1135.10, 3103.54	
$^4TS_4$ (CHO)	1.027, 1.061, 32.340	1289.99*i*, 515.62, 1986.19	
$^1TS_0$ (CH_2O)	1.502, 1.712, 12.275	1821.61*i*, 807.75, 840.32, 1311.36, 1817.68, 3145.66	

CH_2O	1.631, 1.851, 13.701	1163.20, 1248.99, 1524.48, 1738.46, 2893.81, 3002.26	
$^1TS_1$ (CH_2O)	1.579, 1.811, 12.370	2089.88*i*, 800.37, 1280.11, 1374.31, 2582.33, 2872.89	
trans-HCOH	1.546, 1.741, 13.776	1092.62, 1196.57, 1296.65, 1483.17, 2826.92, 3690.95	
$^1TS_2$ (CH_2O)	1.524, 1.559, 14.272	1493.11*i*, 749.16, 1184.70, 1376.86, 2894.76, 3799.26	
cis-HCOH	1.539, 1.739, 13.340	996.89, 1203.24, 1315.93, 1447.48, 2738.95, 3565.87	
$^1TS_3$ (CH_2O)	1.520, 1.766, 10.925	1039.71*i*, 678.31, 746.52, 1081.83, 1724.70, 3120.72	
$^3TS_0$ (CH_2O)	0.927	428.86*i*, 68.96, 165.61, 263.99, 304.12, 1736.01, 3882.99	

$^{3}TS_1$ (CH_2O)	1.239, 1.390, 11.388	2848.21*i*, 227.67, 741.38, 822.83, 1355.21, 1684.88	
$^{1}TS_0$ (CH_2O_2)	0.366, 0.397, 3.798	1591.95*i*, 277.72, 344.38, 674.69, 764.42, 992.16, 1884.77, 2658.52, 3719.47	
HCOOH	0.499, 0.576, 3.736	631.86, 713.58, 1077.55, 1138.58, 1318.11, 1443.23, 1792.68, 3125.15, 3722.55	
$^{1}TS_1$ (CH_2O_2)	0.499, 0.574, 3.844	1956.33*i*, 405.88, 608.19, 676.26, 1140.08, 1263.70, 1457.79, 2517.81, 3493.51	
trans-$C(OH)_2$	0.509, 0.597, 3.479	632.61, 663.01, 773.54, 1079.69, 1154.10, 1311.53, 1392.37, 3495.16, 3730.74	
$^{1}TS_2$ (CH_2O_2)	0.510, 0.587, 3.132	668.04i, 624.40, 810.21, 955.48, 1027.05, 1205.08, 1270.06, 3375.95, 3738.68	

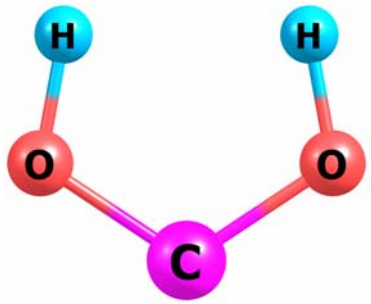
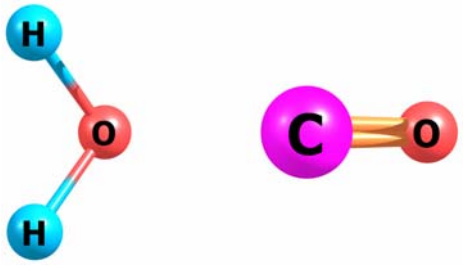
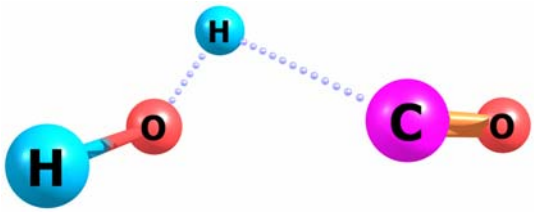
cis-$C(OH)_2$	0.506, 0.597, 3.298	478.59, 677.47, 728.17, 1084.92, 1190.18, 1289.86, 1372.24, 3292.85, 3374.57	
$^3IM_0$ (CH_2O_2)	0.323, 0.335, 4.803	170.73, 183.51, 459.85, 585.96, 600.15, 1595.71, 1690.01, 3715.81, 3816.99	
$^3TS_0$ (CH_2O_2)	0.282, 0.288, 7.565	780.56*i*, 136.06, 350.31, 451.92, 707.85, 1502.61, 1755.03, 2466.44, 3715.02	

Table S2. Structures of critical points in Cartesian coordinates (in Å).

```
$DATA
 CO(X1)
C1
CARBON      6.0      0.000000000          0.000000000          0.000000000
OXYGEN      8.0      1.132607334          0.000000000          0.000000000
 $END

$DATA
 CO(a3)
C1
CARBON      6.0      0.000000000          0.000000000          0.000000000
OXYGEN      8.0      1.213039669          0.000000000          0.000000000
 $END

$DATA
 OH(X2)
C1
OXYGEN      8.0      0.000000000          0.000000000          0.000000000
HYDROGEN    1.0      0.975767563          0.000000000          0.000000000
 $END

$DATA
 H2
C1
OXYGEN      8.0      0.000000000          0.000000000          0.000000000
HYDROGEN    1.0      0.975767563          0.000000000          0.000000000
 $END

$DATA
 H2O
C1
HYDROGEN    1.0      0.000000000          0.000000000          0.963300311
OXYGEN      8.0      0.000000000          0.000000000          0.000000000
HYDROGEN    1.0      0.938011115          0.000000000         -0.219246887
 $END

$DATA
 2IM0_CHO
C1
HYDROGEN    1.0      1.354524709         -0.749812350          0.000000000
CARBON      6.0      0.622136327          0.102250736          0.000000000
OXYGEN      8.0     -0.552098123         -0.029467449          0.000000000
$END

$DATA
 2TS0_CHO
C1
HYDROGEN    1.0      1.824984267         -1.182726340          0.000000000
CARBON      6.0      0.561509888          0.213657614          0.000000000
OXYGEN      8.0     -0.536257061         -0.085771674          0.000000000
$END
```

```
$DATA
 2IM1_CHO
C1
HYDROGEN    1.0     -0.966211143        -0.802741830         0.000000000
CARBON      6.0      0.763079223        -0.024043856         0.000000000
OXYGEN      8.0     -0.511611440         0.068618677         0.000000000
$END

$DATA
 2TS1_CHO
C1
HYDROGEN    1.0      1.218421500        -0.880042887         0.000000000
CARBON      6.0     -0.719954196        -0.047161160         0.000000000
OXYGEN      8.0      0.463365827         0.090832843         0.000000000
$END

$DATA
 2TS2_CHO
C1
HYDROGEN    1.0     -0.105784409        -1.000114023         0.000000000
CARBON      6.0      0.738032528         0.028841168         0.000000000
OXYGEN      8.0     -0.547035161         0.041378532         0.000000000
$END

$DATA
 2IM2_CHO
C1
HYDROGEN    1.0      0.000000000         0.000000000         1.686101868
CARBON      6.0      0.000000000         0.000000000         0.619283801
OXYGEN      8.0      0.000000000         0.000000000        -0.570850429
$END

$DATA
 2TS3_CHO
C1
HYDROGEN    1.0     -0.230443997         1.082797877         0.000000000
CARBON      6.0     -0.711297207        -0.056219253         0.000000000
OXYGEN      8.0      0.548162741        -0.026048270         0.000000000
$END

$DATA
 2IM3_CHO
C1
HYDROGEN    1.0     -1.027491810        -0.759031822         0.000000000
CARBON      6.0      0.784176472        -0.024563696         0.000000000
OXYGEN      8.0     -0.523578172         0.066254552         0.000000000
$END

$DATA
 2IM5_CHO
C1
HYDROGEN    1.0      1.108314917        -0.958470401         0.000000000
CARBON      6.0      0.744474464         0.101831573         0.000000000
OXYGEN      8.0     -0.628367465        -0.016005619         0.000000000
$END
```

```
$DATA
 2TS4_CHO
C1
HYDROGEN    1.0     -1.158841708         1.287006484         0.000000000
CARBON      6.0     -0.651877525        -0.153229399         0.000000000
OXYGEN      8.0      0.562081308         0.033865491         0.000000000
$END

$DATA
 2TS5_CHO
C1
HYDROGEN    1.0      0.242823499        -1.081127780         0.000000000
CARBON      6.0      0.710096229         0.057076210         0.000000000
OXYGEN      8.0     -0.548041742         0.025300116         0.000000000
$END

$DATA
 2IM6_CHO
C1
HYDROGEN    1.0     -0.927497523         0.832571928         0.000000000
CARBON      6.0      0.790472586         0.020732991         0.000000000
OXYGEN      8.0     -0.534602311        -0.068014305         0.000000000
$END

$DATA
 2TS6_CHO
C1
HYDROGEN    1.0     -0.940200441        -0.874488859         0.000000000
CARBON      6.0      0.966279244        -0.012353462         0.000000000
OXYGEN      8.0     -0.665698864         0.064368807         0.000000000
$END

$DATA
 4TS0_CHO
C1
HYDROGEN    1.0     -1.340203598         1.539397259         0.000000000
CARBON      6.0     -0.642027568        -0.204000565         0.000000000
OXYGEN      8.0      0.566118941         0.056053065         0.000000000
$END

$DATA
 4IM0_CHO
C1
HYDROGEN    1.0      1.318424652        -0.827075449         0.000000000
CARBON      6.0      0.744725930         0.098203581         0.000000000
OXYGEN      8.0     -0.641794951        -0.021562838         0.000000000
$END

$DATA
 4TS1_CHO
C1
HYDROGEN    1.0      1.388721987         1.118409769         0.000000000
CARBON      6.0     -0.749977824         0.070041867         0.000000000
OXYGEN      8.0      0.475160232        -0.123018118         0.000000000
$END
```

```
$DATA
 4IM1_CHO
C1
HYDROGEN    1.0     -0.903625147         0.836864098         0.000000000
CARBON      6.0      0.813648446         0.018000142         0.000000000
OXYGEN      8.0     -0.553493914        -0.066234462         0.000000000
$END

$DATA
 4TS2_CHO
C1
HYDROGEN    1.0     -0.072569544         1.001455075         0.000000000
CARBON      6.0     -0.789249170        -0.040615179         0.000000000
OXYGEN      8.0      0.596697790        -0.032629712         0.000000000
$END

$DATA
 4TS3_CHO
C1
HYDROGEN    1.0     -2.438440738         1.007864364         0.000000000
CARBON      6.0     -0.672581912        -0.196961928         0.000000000
OXYGEN      8.0      0.658240933         0.084263821         0.000000000
$END

$DATA
 4IM2_CHO
C1
HYDROGEN    1.0      1.417911913        -0.771122052         0.000000000
CARBON      6.0      0.756487432         0.095070491         0.000000000
OXYGEN      8.0     -0.656887489        -0.022737847         0.000000000
$END

$DATA
 4TS4_CHO
C1
HYDROGEN    1.0     -0.081040859         0.847341910         0.000000000
CARBON      6.0     -1.039873264        -0.033778207         0.000000000
OXYGEN      8.0      0.785259446        -0.028048541         0.000000000
$END

$DATA
 1TS0_CH2O
C1
HYDROGEN    1.0      1.419371246        -1.245146999         0.000000000
HYDROGEN    1.0      1.635188452         0.064829476         0.000000000
CARBON      6.0      0.548217999         0.173073515         0.000000000
OXYGEN      8.0     -0.603759422        -0.055475690         0.000000000
$END

$DATA
 CH2O
C1
HYDROGEN    1.0      1.189591489         0.938833748         0.000000000
HYDROGEN    1.0      1.184459600        -0.935381996         0.000000000
CARBON      6.0      0.606311954        -0.000762522         0.000000000
OXYGEN      8.0     -0.604465514         0.000354582         0.000000000
$END
```

```
$DATA
 1TS1_CH2O
C1
HYDROGEN    1.0      0.143782029         1.009950444         0.000000000
HYDROGEN    1.0     -1.260711876        -0.887882567         0.000000000
CARBON      6.0     -0.706831340         0.076518530         0.000000000
OXYGEN      8.0      0.600668956        -0.065098548         0.000000000
$END

$DATA
 trans-HCOH
C1
HYDROGEN    1.0      0.999409610        -0.781180059         0.000000000
HYDROGEN    1.0     -1.140079398         0.919279959         0.000000000
CARBON      6.0     -0.738339413        -0.123060066         0.000000000
OXYGEN      8.0      0.562794257         0.083622869         0.000000000
$END

$DATA
 1TS2_CH2O
C1
HYDROGEN    1.0      1.711825659        -0.864526451         1.596844710
HYDROGEN    1.0      0.000000000         0.000000000         0.000000000
CARBON      6.0      0.000000000         0.000000000         1.113185296
OXYGEN      8.0      1.306044602         0.000000000         1.468241792
$END

$DATA
 cis-HCOH
C1
HYDROGEN    1.0      0.952145306         0.842861537         0.000000000
HYDROGEN    1.0     -1.096609841         0.983032908         0.000000000
CARBON      6.0     -0.744731824        -0.083966992         0.000000000
OXYGEN      8.0      0.567829195        -0.052052694         0.000000000
$END

$DATA
 1TS3_CH2O
C1
HYDROGEN    1.0     -1.618305362         1.009801580         0.000000000
HYDROGEN    1.0      1.405583631        -0.666554811         0.000000000
CARBON      6.0      0.665740824         0.175307921         0.000000000
OXYGEN      8.0     -0.486061104        -0.153150454         0.000000000
$END

$DATA
 3TS0_CH2O
C1
HYDROGEN    1.0      0.000000000         0.000000000         3.084797375
HYDROGEN    1.0      0.000000000         0.000000000         2.322904749
CARBON      6.0      0.000000000         0.000000000         0.497685697
OXYGEN      8.0      0.000000000         0.000000000        -0.714117538
$END
```

```
$DATA
 3TS1_CH2O
C1
HYDROGEN    1.0     -1.399052822         0.471960759         0.000000000
HYDROGEN    1.0     -2.166581183         0.976616382         0.000000000
CARBON      6.0      0.827783710         0.151075932         0.000000000
OXYGEN      8.0     -0.396367934        -0.204616558         0.000000000
$END

$DATA
 1TS0_CH2O2
C1
HYDROGEN    1.0      0.124148750        -0.892880427        -0.365441127
OXYGEN      8.0      0.000000000         0.000000000         0.000000000
HYDROGEN    1.0      0.000000000         0.000000000         1.439213433
CARBON      6.0      1.142353115         0.000000000         1.477391363
OXYGEN      8.0      2.268620283        -0.235958244         1.356351384
$END

$DATA
 HCOOH
C1
HYDROGEN    1.0      1.006630620         1.084465177         0.000000000
OXYGEN      8.0      1.138557399         0.122010877         0.000000000
HYDROGEN    1.0     -0.032790752        -1.501074291         0.000000000
CARBON      6.0     -0.099535291        -0.413964285         0.000000000
OXYGEN      8.0     -1.125242955         0.214811306         0.000000000
$END

$DATA
 1TS1_CH2O2
C1
HYDROGEN    1.0     -0.939719964         1.077991370         0.000000000
OXYGEN      8.0     -1.136644926         0.113852721         0.000000000
HYDROGEN    1.0      1.196550733        -0.961035843         0.000000000
CARBON      6.0      0.030593610        -0.498146408         0.000000000
OXYGEN      8.0      1.097509740         0.252506714         0.000000000
$END

$DATA
 trans-C(OH)2
C1
HYDROGEN    1.0     -0.853837093         1.103299942         0.000000000
OXYGEN      8.0     -1.095529274         0.151743796         0.000000000
HYDROGEN    1.0      1.825972982        -0.317010491         0.000000000
CARBON      6.0     -0.009830423        -0.598001532         0.000000000
OXYGEN      8.0      1.041651023         0.247356681         0.000000000
$END

$DATA
 1TS2_CH2O2
C1
HYDROGEN    1.0      0.931793939         0.029314384        -0.313431770
OXYGEN      8.0      0.000000000         0.000000000         0.000000000
HYDROGEN    1.0      1.640575883        -0.915544466         1.711450934
CARBON      6.0      0.000000000         0.000000000         1.307696659
OXYGEN      8.0      1.320478892         0.000000000         1.744375710
$END
```

```
$DATA
 cis-C(OH)2
C1
HYDROGEN    1.0      0.926542831         0.000000000         1.121254623
OXYGEN      8.0      1.102431686         0.000000000         0.148836106
HYDROGEN    1.0     -0.926542831         0.000000000         1.121254623
CARBON      6.0      0.000000000         0.000000000        -0.585108093
OXYGEN      8.0     -1.102431686         0.000000000         0.148836106
$END

$DATA
 3IM0_CH2O2
C1
HYDROGEN    1.0     -0.575312292        -0.775396534        -0.092398408
OXYGEN      8.0      0.000000000         0.000000000         0.000000000
HYDROGEN    1.0     -0.580416538         0.771563958        -0.092397085
CARBON      6.0      0.000000000         0.000000000         1.901312681
OXYGEN      8.0      0.958086821         0.000000000         2.653705301
$END

$DATA
 3TS0_CH2O2
C1
HYDROGEN    1.0     -1.495386774        -0.469963083         0.069901799
OXYGEN      8.0     -0.602985045        -0.833245512        -0.097669468
HYDROGEN    1.0      0.000000000         0.000000000         0.000000000
CARBON      6.0      0.000000000         0.000000000         1.667728239
OXYGEN      8.0      0.853607647         0.000000000         2.520814443
$END
```