

**Supporting Information**

**for**

**Singlet ( $^1\Delta_g$ ) O<sub>2</sub> initiated gas phase oxidation as  
a potential tropospheric decay channel for ketene**

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In the MESMER program, kinetic calculations are carried out through construction of stochastic energy grained master equation by describing the time dependent rovibrational population density  $[p_m(E)]$  for a particular isomeric species (m) on the PES having total rovibrational energy E. For one dimensional master equation, E is the independent variable. The energy grained master equation keeping E as continuous variable can be expressed by the following differential equation:

$$\begin{aligned} \frac{dp_m(E)}{dt} = & \omega \int_{E_{0m}}^{\infty} P(E|E') p_m(E') dE' - \omega p_m(E) \\ & + \sum_{n \neq m}^M k_{mn}(E) p_n(E) - \sum_{n \neq m}^M k_{nm}(E) p_n(E) - k_{Sm}(E) p_m(E) \\ & + K_{Rm}^{eq} k_{Rm}(E) \frac{\rho_m(E) e^{-\beta E}}{Q_m(\beta)} n_A p_B - k_{Rm}(E) p_m(E) \end{aligned} \quad (1)$$

There are seven terms on right hand side of the above equation. Among them, positive terms correspond to the population flux into the energy grain associated with the chemical species m  $[mE]$  and negative terms correspond to the population flux out of  $[mE]$ . The first term on the right hand side of the above equation represents the population increase in  $[mE]$  through collisional energy transfer.  $\omega$  represents the Lennard-Jones collision frequency and  $P(E|E)$  represents the probability of collision with bath gas (considering  $N_2$  for our investigation). The second term in the above equation corresponds to the population loss from  $[mE]$  due to collision. The reversible population gain for  $p_m(E)$  at a constant energy E through the reaction that transfers population from isomer n to isomer m is described by the third term whereas the fourth term represents the population loss for  $p_m(E)$  at a constant energy E through the reaction that transfers the population from isomer m to isomer n. The  $k_{mn}(E)$  and  $k_{nm}(E)$  terms represent the microcanonical rate coefficient for population transfer from isomer n to isomer m and isomer m to isomer n, respectively. The fifth term corresponds to the irreversible population loss from  $[mE]$  through the reactions that transfer population from isomer m to products S having microcanonical rate coefficient  $k_{Sm}(E)$ . The sixth and seventh terms represent the so called "bimolecular" source term and apply only to those isomers which are populated via bimolecular association reactions. It is based on the assumption that

two bimolecular reactants say A and B are maintained in a Boltzmann distribution and the reactant A is in sufficient large amount compare to reactant B making this condition follow pseudo-first order kinetics. Also, under this condition, the sixth and seventh terms describe the population gain by [mE] due to bimolecular association of reactants A and B (altogether denoted as R) and the population from [mE] via redissociation to the reactants. Here, the  $k_{Rm}(E)$  is the rate coefficient at which [mE] redissociates to give the bimolecular reactants, R, and  $K_{Rm}^{eq}$  represents the equilibrium constant between isomer m and the reactants. The rovibrational partition function for isomer m ( $Q_m(\beta)$ ) is given by  $Q_m(\beta) = \int dE \rho_m(E) e^{-\beta E}$ . In the sixth term,  $n_A$  corresponds to the number density of reactant A and  $p_B$  represents the population in reactant B. The phenomenological rate coefficients are calculated from the eigenvalues and eigenvectors of the system using Bartis-Widom method. Inverse Laplace transform (ILT) method has used to obtain microcanonical rate coefficients from an existing Arrhenius form. Generally, the required Arrhenius parameters for the ILT method in MESMER are usually obtained from experimental data through the fitting process. But there exist no experimental studies on the kinetics of the reaction of Ketene and  $^1\text{O}_2$ . So, we have calculated the rate coefficient of the bimolecular barrierless association step using KTOOLS from Multiwell at different temperatures. Molecular geometry optimization and normal mode vibrational frequency calculations of reactant and trial transition state along the unimolecular dissociation reaction path have been carried out at M06-2X/aug-cc-pVTZ level of theory. Further, the energetics of the unimolecular dissociation reaction path have been extrapolated up to reported all the corrected energy limits using a two point fitting method. By fitting these rate coefficient values, we have calculated the Arrhenius bimolecular association parameter for the studied reaction. Under the high pressure condition, the equilibrium constant for  $(A + B \xrightleftharpoons[k_b]{k_a} C)$  can be expressed as:

$$K = \frac{k'_a}{k_d} = \frac{\chi_C}{\chi_B} \quad (2)$$

where forward rate coefficient  $k'_a = k_a A$ .  $\chi_C$  and  $\chi_B$  are the equilibrium fraction of C

and B, respectively. The canonical high pressure rate coefficient may be expressed as:

$$k_d(\beta) = K_e(\beta)k_a(\beta) \quad (3)$$

In case of  $k_a(\beta)$  having a modified Arrhenius expression, the equation becomes:

$$\frac{W(E)}{h} = k(E)\rho(E) = A_0\beta_0^n L^{-1}[K_e(\beta)\frac{Q(\beta)}{\beta^n}e^{-\beta E_a}] \quad (4)$$

The final result obtained is:

$$k(E)\rho(E) = \frac{A_0\beta_0^n}{\Gamma(n+1.5)}\left(\frac{2\pi\mu}{h^2}\right)^{\frac{3}{2}}\left(\frac{g_A g_B}{g_C}\right) \int_0^E d\tau \rho_R(E-\tau)(\tau - E_a - \Delta H_0^0)^{n+0.5} u(\tau - E_a - \Delta H_0^0) \quad (5)$$

where  $\rho_R E$  is the convolved density of states for the associating pair,  $\Delta H_0^0$  is the enthalpy of reaction,  $\mu$  is the reduced mass of the system and  $g_X$  is the spin degeneracy of species X.

Table S1: T1-diagnostic values of all the studied species calculated at CCSD(T)/aug-cc-pVTZ//CCSD(T)-F12/cc-pVDZ-F12 level

Species	T1-Diagnostic
H <sub>2</sub> C <sub>2</sub> O	0.016516
<sup>1</sup> O <sub>2</sub>	0.015602
RC	0.017854
TS	0.045512
PC	0.017264
CH <sub>2</sub> O	0.015650
CO <sub>2</sub>	0.017947

Table S2: Concentrations of <sup>1</sup>O<sub>2</sub> (molecules cm<sup>-3</sup>) at different altitudes in troposphere

Altitude (km)	T (K)	P (atm)	<sup>1</sup> O <sub>2</sub>
0	298	1	$1.7 \times 10^8$
5	259	0.535	$1.0 \times 10^8$
10	230	0.266	$5.8 \times 10^7$
15	213	0.120	$2.8 \times 10^7$

Table S3: Absolute electronic energies, ZPE corrections and thermal corrections to Gibbs Free energies at 298K of all the studied species calculated at CCSD(T)/CBS//CCSD(T)-F12/cc-pVDZ-F12 level (All values are in Hartrees)

Species	CCSD(T)-F12/ cc-pVDZ-F12	CCSD(T)/ CBS	ZPE Correction	Thermal Correction to Gibbs Free Energy
H <sub>2</sub> C <sub>2</sub> O	-152.394060	-152.431767	0.031426	0.007801
<sup>1</sup> O <sub>2</sub>	-150.118161	-150.155250	0.003420	-0.015530
RC	-302.612299	-302.689841	0.043314	0.016324
TS	-302.576611	-302.652545	0.039176	0.011930
PC	-302.739704	-302.815794	0.039574	0.008785
CH <sub>2</sub> O	-188.373463	-188.420100	0.026667	0.005007
CO <sub>2</sub>	-114.361450	-114.390795	0.010070	-0.010588

Table S4: Contribution of core electron and full triple excitations along with perturbative quartic excitations of all the studied species calculated at all-electron CCSD(T)/aug-cc-pCVTZ and CCSDT(Q)/cc-pVDZ levels of theory respectively (All values are in Hartrees)

Species	E <sub>CORE</sub>	E <sub>T(Q)</sub>
H <sub>2</sub> C <sub>2</sub> O	-0.159284	-0.002303
<sup>1</sup> O <sub>2</sub>	-0.114012	-0.012856
RC	-0.273036	-0.004161
TS	-0.272515	-0.008297
PC	-0.273785	-0.003773
CH <sub>2</sub> O + CO <sub>2</sub>	-0.273841	-0.003842

Table S5: Absolute electronic energies and ZPE corrections at 298K of all the studied species calculated at M06-2X/aug-cc-pVTZ level of theory (All values are in Hartrees)

Species	E <sub>M06-2X/AUG-CC-PVTZ</sub>	ZPE Correction
H <sub>2</sub> C <sub>2</sub> O	-152.598693	0.031916
<sup>1</sup> O <sub>2</sub>	-150.265705	0.003986
TS <sup>1</sup>	-302.862518	0.039604
RC	-302.973247	0.044287
TS <sup>2</sup>	-302.907606	0.040058
PC	-303.098737	0.040525

Table S6: Optimized geometries of all the species in Cartesian Coordinates and normal mode frequencies calculated at CCSD(T)-F12/cc-pVDZ-F12 level

Species	Cartesian Coordinates(Å)	Frequencies( $\text{cm}^{-1}$ )
CH <sub>2</sub> CO	C 0.000218 -1.213823 -0.000000	
	H -0.941969 -1.736735 0.000000	438.64 511.61 584.74
	H 0.9425914 -1.736399 0.000000	993.20 1153.78 1415.68
	C -0.000015 0.102624 -0.000000	2195.26 3196.02 3305.43
	O -0.000227 1.265446 0.000000	
<sup>1</sup> O <sub>2</sub>	O 0.000000 0.000000 0.609918	
	O 0.000000 0.000000 -0.609918	1501.35
RC	C -0.600348 0.973487 0.000235	
	H -0.727823 1.567643 -0.903489	221.94 484.45 506.35
	H -0.727715 1.567192 0.904272	736.63 819.74 917.58
	C 0.602414 0.062691 -0.000086	1020.89 1024.71 1146.46
	O 1.785085 0.108656 -0.000051	1153.96 1309.59 1487.84
	O -0.191863 -1.064871 -0.000152	1941.44 3085.68 3155.69
	O -1.425043 -0.212257 -0.000006	
TS	C -0.743828 -0.867698 0.000309	
	H -0.808884 -1.465843 0.912245	742.40i 195.12 450.77
	H -0.805574 -1.475273 -0.905318	539.34 591.33 729.55
	C 0.537645 -0.019178 -0.000835	934.62 962.34 1040.82
	O 1.686872 -0.408044 -0.012201	1200.81 1285.45 1491.24
	O 0.264812 1.236559 0.011329	1633.05 3015.12 3126.98
	O -1.630666 0.206762 -0.005549	
PC	C -2.133239 0.169285 0.000000	
	H -1.776872 1.211567 0.000112	41.58 85.71 106.49
	H -3.223531 0.011126 0.000025	149.79 159.13 662.65
	C 1.316957 0.167193 -0.000009	678.73 1195.10 1275.73
	O 1.789886 -0.892738 0.000073	1352.07 1534.26 1772.59
	O 0.875573 1.245089 0.000003	2392.32 2942.87 3022.18
	O -1.361682 -0.760871 -0.000139	
CH <sub>2</sub> O	C -0.531570 0.000033 0.000008	
	O 0.675038 -0.000072 -0.000003	1186.47 1271.50 1536.92
	H -1.111283 0.937962 0.000013	1778.81 2930.21 3001.76
	H -1.111436 -0.937801 0.000013	
CO <sub>2</sub>	C 1.263257 0.164127 0.000018	
	O 1.728233 -0.901455 0.000017	675.48 1352.36 2392.29
	O 0.798281 1.229709 0.000019	

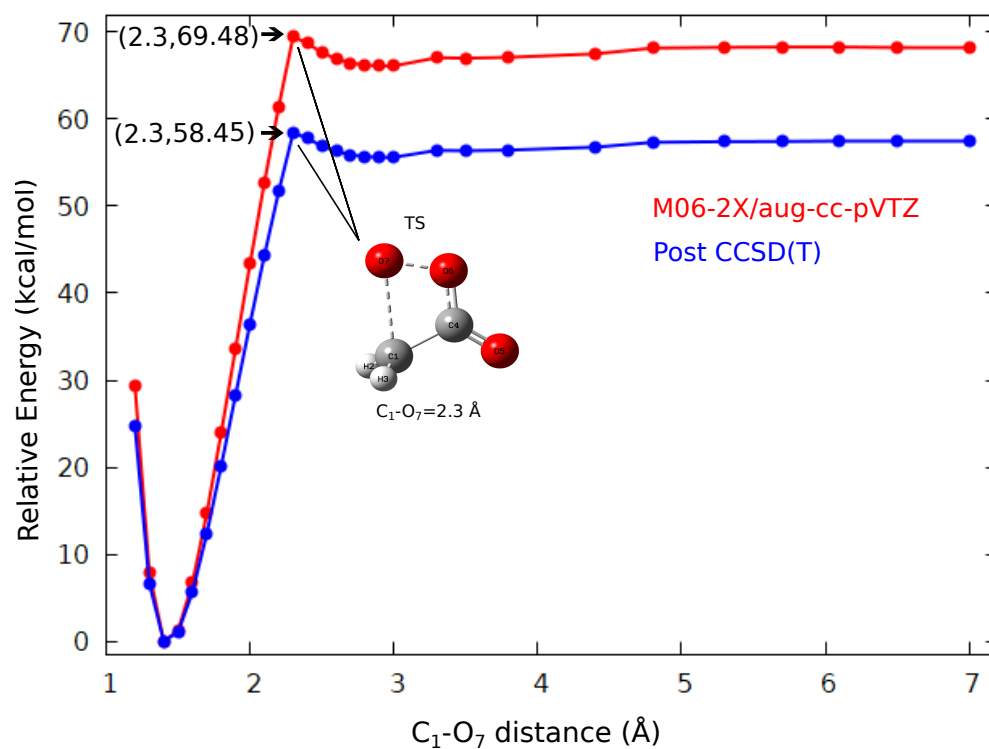


Figure S1: Relaxed potential energy scan profile for the bimolecular addition step at M06-2X/aug-cc-pVTZ level and the projected scan profile considering energy values after Post-CCSD(T) corrections



Listing 1: KTOOLS input file for  $\text{H}_2\text{C}_2\text{O} + {}^1\text{O}_2$

```

1 C2H2O-O2
2 KCAL MCC ! Ekey, Sskey
3 nosavefiles ! Whatdo
4 40000 10. ! Emax Egrain
5 500 1 ! Jmax Jgrain
6 301 902 40000. ! 1D double array parameters: Imax1, Isize, Emax2
7 15 ! Nt number of temperatures
8 200. 210. 220. 230. 240. 250. 260. 270. 280. 290. 298. 300. 310. 320. 330.
9 1 32 2 ! no. of reactants, no. of of trial transition states, no.
    of products
10
11 reac rc -57.45 1.4
12 C2H2O3
13 a) (blank comment line)
14 b) (blank comment line)
15 c) (blank comment line)
16 1 1 1
17 0.0 1
18 17 'HAR' AMUA
19 1 vib 233.9246 0.0 1
20 2 vib 496.6897 0.0 1
21 3 vib 507.0428 0.0 1
22 4 vib 766.1007 0.0 1
23 5 vib 944.4380 0.0 1
24 6 vib 994.7600 0.0 1
25 7 vib 1020.6032 0.0 1
26 8 vib 1061.0997 0.0 1
27 9 vib 1154.6336 0.0 1
28 10 vib 1178.2013 0.0 1
29 11 vib 1317.7260 0.0 1
30 12 vib 1483.5546 0.0 1
31 13 vib 2001.3337 0.0 1
32 14 vib 3107.3201 0.0 1
33 15 vib 3172.4158 0.0 1
34 16 kro 36.1475 1.0 1 ! K-rotor
35 17 jro 109.3677 1.0 2 ! 2D adiabatic rotor
36
37 ctst rc-150 -56.42 1.5 0.0
38 C2H2O3
39 a) (blank comment line)
40 b) (blank comment line)
41 c) (blank comment line)
42 1 1 1

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43	0.0		1			
44	17	'HAR'	AMUA			
45	1	vib	257.3995	0.0	1	
46	2	vib	506.1280	0.0	1	
47	3	vib	516.8213	0.0	1	
48	4	vib	756.6622	0.0	1	
49	5	vib	860.5564	0.0	1	
50	6	vib	979.3644	0.0	1	
51	7	vib	997.2725	0.0	1	
52	8	vib	1013.0451	0.0	1	
53	9	vib	1117.5384	0.0	1	
54	10	vib	1185.6223	0.0	1	
55	11	vib	1299.2602	0.0	1	
56	12	vib	1466.7381	0.0	1	
57	13	vib	1993.1187	0.0	1	
58	14	vib	3124.7119	0.0	1	
59	15	vib	3202.5328	0.0	1	
60	16	kro	36.9869	1.0	1	! K-rotor
61	17	jro	109.9797	1.0	2	! 2D adiabatic rotor
62						
63	ctst	rc-160	-51.82	1.6	0.0	
64	C2H2O3					
65	a)	(blank comment line)				
66	b)	(blank comment line)				
67	c)	(blank comment line)				
68	1	1	1			
69	0.0		1			
70	17	'HAR'	AMUA			
71	1	vib	268.3791	0.0	1	
72	2	vib	513.6877	0.0	1	
73	3	vib	525.4037	0.0	1	
74	4	vib	629.0777	0.0	1	
75	5	vib	757.5638	0.0	1	
76	6	vib	960.8159	0.0	1	
77	7	vib	979.7570	0.0	1	
78	8	vib	1001.3211	0.0	1	
79	9	vib	1073.1534	0.0	1	
80	10	vib	1185.8990	0.0	1	
81	11	vib	1276.0358	0.0	1	
82	12	vib	1450.2517	0.0	1	
83	13	vib	1979.8535	0.0	1	
84	14	vib	3145.6311	0.0	1	
85	15	vib	3237.4320	0.0	1	
86	16	kro	38.3121	1.0	1	! K-rotor

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87 17 jro 111.0083 1.0 2 ! 2D adiabatic rotor
88
89 ctst rc-170 -45.09 1.7 0.0
90 C2H2O3
91 a) (blank comment line)
92 b) (blank comment line)
93 c) (blank comment line)
94 1 1 1
95 0.0 1
96 17 'HAR' AMUA
97 1 vib 265.3281 0.0 1
98 2 vib 439.0093 0.0 1
99 3 vib 517.4886 0.0 1
100 4 vib 531.3683 0.0 1
101 5 vib 738.2343 0.0 1
102 6 vib 922.7754 0.0 1
103 7 vib 950.1680 0.0 1
104 8 vib 1001.4307 0.0 1
105 9 vib 1050.7836 0.0 1
106 10 vib 1162.4843 0.0 1
107 11 vib 1270.9386 0.0 1
108 12 vib 1441.0780 0.0 1
109 13 vib 1966.0878 0.0 1
110 14 vib 3158.5782 0.0 1
111 15 vib 3260.7902 0.0 1
112 16 kro 39.6936 1.0 1 ! K-rotor
113 17 jro 112.0764 1.0 2 ! 2D adiabatic rotor
114
115 ctst rc-180 -37.31 1.8 0.0
116 C2H2O3
117 a) (blank comment line)
118 b) (blank comment line)
119 c) (blank comment line)
120 1 1 1
121 0.0 1
122 17 'HAR' AMUA
123 1 vib 254.8934 0.0 1
124 2 vib 261.8494 0.0 1
125 3 vib 516.2014 0.0 1
126 4 vib 536.8489 0.0 1
127 5 vib 719.6186 0.0 1
128 6 vib 855.2021 0.0 1
129 7 vib 939.8046 0.0 1
130 8 vib 1000.3981 0.0 1

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131	9	vib	1040.0081	0.0	1	
132	10	vib	1128.0332	0.0	1	
133	11	vib	1276.3843	0.0	1	
134	12	vib	1436.4178	0.0	1	
135	13	vib	1951.8550	0.0	1	
136	14	vib	3166.2232	0.0	1	
137	15	vib	3276.2410	0.0	1	
138	16	kro	41.1034	1.0	1	! K-rotor
139	17	jro	113.1958	1.0	2	! 2D adiabatic rotor
140						
141	ctst	rc-190	-29.14	1.9	0.0	
142	C2H2O3					
143	a) (blank comment line)					
144	b) (blank comment line)					
145	c) (blank comment line)					
146	1	1	1			
147	0.0		1			
148	16	'HAR'	AMUA			
149	1	vib	241.6475	0.0	1	
150	2	vib	511.8684	0.0	1	
151	3	vib	542.2182	0.0	1	
152	4	vib	700.8664	0.0	1	
153	5	vib	786.8424	0.0	1	
154	6	vib	927.5503	0.0	1	
155	7	vib	996.8544	0.0	1	
156	8	vib	1033.8431	0.0	1	
157	9	vib	1094.4125	0.0	1	
158	10	vib	1282.2545	0.0	1	
159	11	vib	1433.7900	0.0	1	
160	12	vib	1937.0968	0.0	1	
161	13	vib	3170.3743	0.0	1	
162	14	vib	3287.2007	0.0	1	
163	15	kro	42.5522	1.0	1	! K-rotor
164	16	jro	114.3471	1.0	2	! 2D adiabatic rotor
165						
166	ctst	rc-200	-20.99	2.0	0.0	
167	C2H2O3					
168	a) (blank comment line)					
169	b) (blank comment line)					
170	c) (blank comment line)					
171	1	1	1			
172	0.0		1			
173	16	'HAR'	AMUA			
174	1	vib	226.9239	0.0	1	

175	2	vib	504.2141	0.0	1	
176	3	vib	543.9503	0.0	1	
177	4	vib	683.8212	0.0	1	
178	5	vib	721.6322	0.0	1	
179	6	vib	917.6551	0.0	1	
180	7	vib	995.3888	0.0	1	
181	8	vib	1029.8394	0.0	1	
182	9	vib	1069.9976	0.0	1	
183	10	vib	1290.4826	0.0	1	
184	11	vib	1433.7586	0.0	1	
185	12	vib	1921.9115	0.0	1	
186	13	vib	3171.3910	0.0	1	
187	14	vib	3292.7333	0.0	1	
188	15	kro	43.8642	1.0	1	! K-rotor
189	16	jro	115.5559	1.0	2	! 2D adiabatic rotor
190						
191	ctst	rc-210	-13.13	2.1	0.0	
192	C2H2O3					
193	a)	(blank comment line)				
194	b)	(blank comment line)				
195	c)	(blank comment line)				
196	1	1	1			
197	0.0		1			
198	16	'HAR'	AMUA			
199	1	vib	212.2406	0.0	1	
200	2	vib	494.0442	0.0	1	
201	3	vib	540.3273	0.0	1	
202	4	vib	659.9595	0.0	1	
203	5	vib	668.6052	0.0	1	
204	6	vib	906.2850	0.0	1	
205	7	vib	989.4404	0.0	1	
206	8	vib	1025.3138	0.0	1	
207	9	vib	1052.1726	0.0	1	
208	10	vib	1298.4768	0.0	1	
209	11	vib	1433.9797	0.0	1	
210	12	vib	1905.6419	0.0	1	
211	13	vib	3170.2834	0.0	1	
212	14	vib	3295.4117	0.0	1	
213	15	kro	45.1369	1.0	1	! K-rotor
214	16	jro	116.7984	1.0	2	! 2D adiabatic rotor
215						
216	ctst	rc-220	-5.75	2.2	0.0	
217	C2H2O3					
218	a)	(blank comment line)				

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219 b) (blank comment line)
220 c) (blank comment line)
221 1 1 1
222 0.0 1
223 16 'HAR' AMUA
224 1 vib 194.9812 0.0 1
225 2 vib 480.6069 0.0 1
226 3 vib 524.3945 0.0 1
227 4 vib 608.2459 0.0 1
228 5 vib 655.3152 0.0 1
229 6 vib 898.8233 0.0 1
230 7 vib 984.5046 0.0 1
231 8 vib 1021.7438 0.0 1
232 9 vib 1039.7991 0.0 1
233 10 vib 1307.7032 0.0 1
234 11 vib 1436.0448 0.0 1
235 12 vib 1884.5254 0.0 1
236 13 vib 3169.4995 0.0 1
237 14 vib 3296.8632 0.0 1
238 15 kro 46.0334 1.0 1 ! K-rotor
239 16 jro 118.1831 1.0 2 ! 2D adiabatic rotor
240
241 ctst rc-230 0.99 2.3 0.0
242 C2H2O3
243 a) (blank comment line)
244 b) (blank comment line)
245 c) (blank comment line)
246 1 1 1
247 0.0 1
248 16 'HAR' AMUA
249 1 vib 181.8405 0.0 1
250 2 vib 463.2588 0.0 1
251 3 vib 487.7643 0.0 1
252 4 vib 591.4112 0.0 1
253 5 vib 643.5134 0.0 1
254 6 vib 894.0580 0.0 1
255 7 vib 975.3989 0.0 1
256 8 vib 1022.1220 0.0 1
257 9 vib 1036.4767 0.0 1
258 10 vib 1322.8171 0.0 1
259 11 vib 1442.5888 0.0 1
260 12 vib 1857.9725 0.0 1
261 13 vib 3168.2281 0.0 1
262 14 vib 3296.8641 0.0 1

```

263	15	kro	46.5724	1.0	1	! K-rotor
264	16	jro	119.6647	1.0	2	! 2D adiabatic rotor
265						
266	ctst	rc-240	0.34	2.4	0.0	
267 C2H2O3						
268 a) (blank comment line)						
269 b) (blank comment line)						
270 c) (blank comment line)						
271	1	1	1			
272	0.0		1			
273	17	'HAR'	AMUA			
274	1	vib	78.6698	0.0	1	
275	2	vib	101.2804	0.0	1	
276	3	vib	206.9209	0.0	1	
277	4	vib	224.0470	0.0	1	
278	5	vib	302.7456	0.0	1	
279	6	vib	439.9100	0.0	1	
280	7	vib	595.9429	0.0	1	
281	8	vib	655.3106	0.0	1	
282	9	vib	991.2270	0.0	1	
283	10	vib	1188.4015	0.0	1	
284	11	vib	1419.1482	0.0	1	
285	12	vib	1603.1880	0.0	1	
286	13	vib	2260.4285	0.0	1	
287	14	vib	3214.3678	0.0	1	
288	15	vib	3318.3945	0.0	1	
289	16	kro	60.7885	1.0	1	! K-rotor
290	17	jro	147.9450	1.0	2	! 2D adiabatic rotor
291						
292	ctst	rc-250	-0.55	2.5	0.0	
293 C2H2O3						
294 a) (blank comment line)						
295 b) (blank comment line)						
296 c) (blank comment line)						
297	1	1	1			
298	0.0		1			
299	17	'HAR'	AMUA			
300	1	vib	86.5574	0.0	1	
301	2	vib	112.5896	0.0	1	
302	3	vib	189.6400	0.0	1	
303	4	vib	194.6879	0.0	1	
304	5	vib	274.0480	0.0	1	
305	6	vib	441.2201	0.0	1	
306	7	vib	597.8937	0.0	1	

307	8	vib	646.4352	0.0	1	
308	9	vib	990.8595	0.0	1	
309	10	vib	1188.3468	0.0	1	
310	11	vib	1418.6532	0.0	1	
311	12	vib	1627.7533	0.0	1	
312	13	vib	2259.7556	0.0	1	
313	14	vib	3214.0132	0.0	1	
314	15	vib	3317.7281	0.0	1	
315	16	kro	61.2086	1.0	1	! K-rotor
316	17	jro	150.8868	1.0	2	! 2D adiabatic rotor
317						
318	ctst	rc-260	-1.16	2.6	0.0	
319	C2H2O3					
320	a) (blank comment line)					
321	b) (blank comment line)					
322	c) (blank comment line)					
323	1	1	1			
324	0.0		1			
325	17	'HAR'	AMUA			
326	1	vib	95.7572	0.0	1	
327	2	vib	113.2189	0.0	1	
328	3	vib	168.5842	0.0	1	
329	4	vib	179.9844	0.0	1	
330	5	vib	247.4917	0.0	1	
331	6	vib	442.7758	0.0	1	
332	7	vib	592.5716	0.0	1	
333	8	vib	642.1746	0.0	1	
334	9	vib	990.8881	0.0	1	
335	10	vib	1187.9100	0.0	1	
336	11	vib	1418.6331	0.0	1	
337	12	vib	1646.1454	0.0	1	
338	13	vib	2257.9098	0.0	1	
339	14	vib	3212.4341	0.0	1	
340	15	vib	3315.7731	0.0	1	
341	16	kro	61.2868	1.0	1	! K-rotor
342	17	jro	154.1488	1.0	2	! 2D adiabatic rotor
343						
344	ctst	rc-270	-1.54	2.7	0.0	
345	C2H2O3					
346	a) (blank comment line)					
347	b) (blank comment line)					
348	c) (blank comment line)					
349	1	1	1			
350	0.0		1			



351	17	'HAR'	AMUA			
352	1	vib	94.7088	0.0	1	
353	2	vib	110.6155	0.0	1	
354	3	vib	156.2284	0.0	1	
355	4	vib	171.1573	0.0	1	
356	5	vib	223.9826	0.0	1	
357	6	vib	443.5970	0.0	1	
358	7	vib	594.0283	0.0	1	
359	8	vib	637.4318	0.0	1	
360	9	vib	990.8128	0.0	1	
361	10	vib	1187.6173	0.0	1	
362	11	vib	1418.3236	0.0	1	
363	12	vib	1663.3110	0.0	1	
364	13	vib	2256.8508	0.0	1	
365	14	vib	3212.5279	0.0	1	
366	15	vib	3315.9058	0.0	1	
367	16	kro	61.0943	1.0	1	! K-rotor
368	17	jro	158.3159	1.0	2	! 2D adiabatic rotor
369						
370	ctst	rc-280	-1.75	2.8	0.0	
371		C2H2O3				
372	a)	(blank comment line)				
373	b)	(blank comment line)				
374	c)	(blank comment line)				
375	1	1	1			
376	0.0		1			
377	17	'HAR'	AMUA			
378	1	vib	94.6352	0.0	1	
379	2	vib	107.5591	0.0	1	
380	3	vib	131.7222	0.0	1	
381	4	vib	160.2442	0.0	1	
382	5	vib	200.1536	0.0	1	
383	6	vib	444.4280	0.0	1	
384	7	vib	589.7787	0.0	1	
385	8	vib	633.6105	0.0	1	
386	9	vib	990.5615	0.0	1	
387	10	vib	1186.8777	0.0	1	
388	11	vib	1418.1262	0.0	1	
389	12	vib	1675.7358	0.0	1	
390	13	vib	2255.2984	0.0	1	
391	14	vib	3212.5877	0.0	1	
392	15	vib	3315.5155	0.0	1	
393	16	kro	60.7339	1.0	1	! K-rotor
394	17	jro	163.0593	1.0	2	! 2D adiabatic rotor

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395
396 ctst rc-290 -1.84 2.9 0.0
397 C2H2O3
398 a) (blank comment line)
399 b) (blank comment line)
400 c) (blank comment line)
401 1 1 1
402 0.0 1
403 17 'HAR' AMUA
404 1 vib 91.4470 0.0 1
405 2 vib 107.8165 0.0 1
406 3 vib 116.1796 0.0 1
407 4 vib 148.6061 0.0 1
408 5 vib 180.4860 0.0 1
409 6 vib 444.5759 0.0 1
410 7 vib 589.7522 0.0 1
411 8 vib 629.4928 0.0 1
412 9 vib 990.4059 0.0 1
413 10 vib 1186.7735 0.0 1
414 11 vib 1418.0141 0.0 1
415 12 vib 1687.4244 0.0 1
416 13 vib 2254.8299 0.0 1
417 14 vib 3213.4627 0.0 1
418 15 vib 3316.3050 0.0 1
419 16 kro 60.2002 1.0 1 ! K-rotor
420 17 jro 168.0164 1.0 2 ! 2D adiabatic rotor
421
422 ctst rc-300 -1.83 3.0 0.0
423 C2H2O3
424 a) (blank comment line)
425 b) (blank comment line)
426 c) (blank comment line)
427 1 1 1
428 0.0 1
429 17 'HAR' AMUA
430 1 vib 86.7727 0.0 1
431 2 vib 88.0163 0.0 1
432 3 vib 113.9716 0.0 1
433 4 vib 144.0897 0.0 1
434 5 vib 163.1046 0.0 1
435 6 vib 444.7222 0.0 1
436 7 vib 588.0758 0.0 1
437 8 vib 627.4670 0.0 1
438 9 vib 990.2480 0.0 1

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439	10	vib	1186.0532	0.0	1	
440	11	vib	1417.1942	0.0	1	
441	12	vib	1698.0122	0.0	1	
442	13	vib	2253.4858	0.0	1	
443	14	vib	3213.0629	0.0	1	
444	15	vib	3315.7835	0.0	1	
445	16	kro	59.7967	1.0	1	! K-rotor
446	17	jro	175.0601	1.0	2	! 2D adiabatic rotor
447						
448	ctst	rc-330	-1.04	3.3	0.0	
449	C2H2O3					
450	a) (blank comment line)					
451	b) (blank comment line)					
452	c) (blank comment line)					
453	1	1	1			
454	0.0		1			
455	16	'HAR'	AMUA			
456	1	vib	43.6270	0.0	1	
457	2	vib	73.5357	0.0	1	
458	3	vib	96.6987	0.0	1	
459	4	vib	132.0331	0.0	1	
460	5	vib	440.3161	0.0	1	
461	6	vib	575.1974	0.0	1	
462	7	vib	596.2242	0.0	1	
463	8	vib	987.3721	0.0	1	
464	9	vib	1187.5375	0.0	1	
465	10	vib	1416.2136	0.0	1	
466	11	vib	1751.3690	0.0	1	
467	12	vib	2256.6697	0.0	1	
468	13	vib	3222.5815	0.0	1	
469	14	vib	3325.4316	0.0	1	
470	15	kro	61.2917	1.0	1	! K-rotor
471	16	jro	191.0352	1.0	2	! 2D adiabatic rotor
472						
473	ctst	rc-340	-1.43	3.4	0.0	
474	C2H2O3					
475	a) (blank comment line)					
476	b) (blank comment line)					
477	c) (blank comment line)					
478	1	1	1			
479	0.0		1			
480	17	'HAR'	AMUA			
481	1	vib	33.5095	0.0	1	
482	2	vib	72.0239	0.0	1	

483	3	vib	105.0161	0.0	1	
484	4	vib	115.2509	0.0	1	
485	5	vib	135.6504	0.0	1	
486	6	vib	444.2914	0.0	1	
487	7	vib	584.0372	0.0	1	
488	8	vib	621.6682	0.0	1	
489	9	vib	989.8608	0.0	1	
490	10	vib	1184.4599	0.0	1	
491	11	vib	1415.3047	0.0	1	
492	12	vib	1722.3427	0.0	1	
493	13	vib	2250.9054	0.0	1	
494	14	vib	3214.2884	0.0	1	
495	15	vib	3317.3000	0.0	1	
496	16	kro	56.6376	1.0	1	! K-rotor
497	17	jro	197.1613	1.0	2	! 2D adiabatic rotor
498						
499	ctst	rc-350	-1.08	3.5	0.0	
500	C2H2O3					
501	a) (blank comment line)					
502	b) (blank comment line)					
503	c) (blank comment line)					
504	1	1	1			
505	0.0		1			
506	17	'HAR'	AMUA			
507	1	vib	32.7323	0.0	1	
508	2	vib	55.9247	0.0	1	
509	3	vib	63.3649	0.0	1	
510	4	vib	83.6348	0.0	1	
511	5	vib	120.8554	0.0	1	
512	6	vib	451.7469	0.0	1	
513	7	vib	580.3361	0.0	1	
514	8	vib	613.3051	0.0	1	
515	9	vib	991.8030	0.0	1	
516	10	vib	1184.2156	0.0	1	
517	11	vib	1417.6672	0.0	1	
518	12	vib	1749.8734	0.0	1	
519	13	vib	2246.8915	0.0	1	
520	14	vib	3204.1906	0.0	1	
521	15	vib	3305.1388	0.0	1	
522	16	kro	60.8026	1.0	1	! K-rotor
523	17	jro	207.4538	1.0	2	! 2D adiabatic rotor
524						
525	ctst	rc-380	-1.00	3.8	0.0	
526	C2H2O3					

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527 a) (blank comment line)
528 b) (blank comment line)
529 c) (blank comment line)
530 1 1 1
531 0.0 1
532 16 'HAR' AMUA
533 1 vib 15.8970 0.0 1
534 2 vib 41.0079 0.0 1
535 3 vib 64.9393 0.0 1
536 4 vib 77.5924 0.0 1
537 5 vib 445.4845 0.0 1
538 6 vib 578.2460 0.0 1
539 7 vib 607.9415 0.0 1
540 8 vib 987.9982 0.0 1
541 9 vib 1184.6945 0.0 1
542 10 vib 1415.7673 0.0 1
543 11 vib 1750.6238 0.0 1
544 12 vib 2246.3046 0.0 1
545 13 vib 3218.2822 0.0 1
546 14 vib 3318.7688 0.0 1
547 15 kro 58.0250 1.0 1 ! K-rotor
548 16 jro 225.3691 1.0 2 ! 2D adiabatic rotor
549
550 ctst rc-440 -0.67 4.4 0.0
551 C2H2O3
552 a) (blank comment line)
553 b) (blank comment line)
554 c) (blank comment line)
555 1 1 1
556 0.0 1
557 16 'HAR' AMUA
558 1 vib -12.5166 0.0 1
559 2 vib 32.3314 0.0 1
560 3 vib 41.6521 0.0 1
561 4 vib 62.9432 0.0 1
562 5 vib 445.9579 0.0 1
563 6 vib 577.4973 0.0 1
564 7 vib 613.2254 0.0 1
565 8 vib 988.3749 0.0 1
566 9 vib 1185.4402 0.0 1
567 10 vib 1415.7856 0.0 1
568 11 vib 1750.7014 0.0 1
569 12 vib 2253.3227 0.0 1
570 13 vib 3216.3932 0.0 1

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571	14	vib	3317.3789	0.0	1	
572	15	kro	28.8646	1.0	1	! K-rotor
573	16	jro	305.1456	1.0	2	! 2D adiabatic rotor
574						
575	ctst	rc-480	-0.12	4.8	0.0	
576 C2H2O3						
577 a) (blank comment line)						
578 b) (blank comment line)						
579 c) (blank comment line)						
580	1	1	1			
581	0.0		1			
582	16	'HAR'	AMUA			
583	1	vib	-29.5427	0.0	1	
584	2	vib	-13.6504	0.0	1	
585	3	vib	9.5630	0.0	1	
586	4	vib	15.6995	0.0	1	
587	5	vib	445.4409	0.0	1	
588	6	vib	575.8558	0.0	1	
589	7	vib	608.2023	0.0	1	
590	8	vib	988.8206	0.0	1	
591	9	vib	1184.6763	0.0	1	
592	10	vib	1415.4482	0.0	1	
593	11	vib	1751.9601	0.0	1	
594	12	vib	2256.7546	0.0	1	
595	13	vib	3216.3793	0.0	1	
596	14	vib	3316.8827	0.0	1	
597	15	kro	58.3864	1.0	1	! K-rotor
598	16	jro	419.3487	1.0	2	! 2D adiabatic rotor
599						
600	ctst	rc-490	0.03	4.9	0.0	
601 C2H2O3						
602 a) (blank comment line)						
603 b) (blank comment line)						
604 c) (blank comment line)						
605	1	1	1			
606	0.0		1			
607	16	'HAR'	AMUA			
608	1	vib	-24.0902	0.0	1	
609	2	vib	6.2468	0.0	1	
610	3	vib	9.2451	0.0	1	
611	4	vib	15.2759	0.0	1	
612	5	vib	446.7848	0.0	1	
613	6	vib	576.7575	0.0	1	
614	7	vib	608.7507	0.0	1	

615	8	vib	989.9390	0.0	1	
616	9	vib	1184.7237	0.0	1	
617	10	vib	1416.3010	0.0	1	
618	11	vib	1750.1384	0.0	1	
619	12	vib	2255.0993	0.0	1	
620	13	vib	3216.0779	0.0	1	
621	14	vib	3317.0761	0.0	1	
622	15	kro	57.0853	1.0	1	! K-rotor
623	16	jro	442.0890	1.0	2	! 2D adiabatic rotor
624						
625	ctst	rc-530	-0.04	5.3	0.0	
626	C2H2O3					
627	a)	(blank comment line)				
628	b)	(blank comment line)				
629	c)	(blank comment line)				
630	1	1	1			
631	0.0		1			
632	16	'HAR'	AMUA			
633	1	vib	13.6299	0.0	1	
634	2	vib	2.4793	0.0	1	
635	3	vib	10.1539	0.0	1	
636	4	vib	25.9838	0.0	1	
637	5	vib	446.7732	0.0	1	
638	6	vib	576.3157	0.0	1	
639	7	vib	609.3841	0.0	1	
640	8	vib	989.9787	0.0	1	
641	9	vib	1184.7971	0.0	1	
642	10	vib	1416.4696	0.0	1	
643	11	vib	1750.1274	0.0	1	
644	12	vib	2256.1002	0.0	1	
645	13	vib	3215.4770	0.0	1	
646	14	vib	3316.3102	0.0	1	
647	15	kro	57.2701	1.0	1	! K-rotor
648	16	jro	502.1917	1.0	2	! 2D adiabatic rotor
649						
650	ctst	rc-540	-0.03	5.4	0.0	
651	C2H2O3					
652	a)	(blank comment line)				
653	b)	(blank comment line)				
654	c)	(blank comment line)				
655	1	1	1			
656	0.0		1			
657	16	'HAR'	AMUA			
658	1	vib	8.2796	0.0	1	

659	2	vib	11.5026	0.0	1	
660	3	vib	16.5436	0.0	1	
661	4	vib	25.9694	0.0	1	
662	5	vib	446.6924	0.0	1	
663	6	vib	576.4410	0.0	1	
664	7	vib	609.2944	0.0	1	
665	8	vib	989.9678	0.0	1	
666	9	vib	1184.8010	0.0	1	
667	10	vib	1416.4402	0.0	1	
668	11	vib	1749.8922	0.0	1	
669	12	vib	2256.1289	0.0	1	
670	13	vib	3215.5917	0.0	1	
671	14	vib	3316.4659	0.0	1	
672	15	kro	57.2157	1.0	1	! K-rotor
673	16	jro	520.8527	1.0	2	! 2D adiabatic rotor
674						
675	ctst	rc-550	-0.02	5.5	0.0	
676	C2H2O3					
677	a) (blank comment line)					
678	b) (blank comment line)					
679	c) (blank comment line)					
680	1	1	1			
681	0.0		1			
682	16	'HAR'	AMUA			
683	1	vib	6.4453	0.0	1	
684	2	vib	7.4243	0.0	1	
685	3	vib	10.2035	0.0	1	
686	4	vib	25.2400	0.0	1	
687	5	vib	446.6548	0.0	1	
688	6	vib	576.5097	0.0	1	
689	7	vib	609.2484	0.0	1	
690	8	vib	989.9604	0.0	1	
691	9	vib	1184.8117	0.0	1	
692	10	vib	1416.4362	0.0	1	
693	11	vib	1749.8871	0.0	1	
694	12	vib	2256.1452	0.0	1	
695	13	vib	3215.6198	0.0	1	
696	14	vib	3316.5033	0.0	1	
697	15	kro	57.1631	1.0	1	! K-rotor
698	16	jro	539.8341	1.0	2	! 2D adiabatic rotor
699						
700	ctst	rc-560	-0.02	5.6	0.0	
701	C2H2O3					
702	a) (blank comment line)					



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703 b) (blank comment line)
704 c) (blank comment line)
705 1 1 1
706 0.0 1
707 16 'HAR' AMUA
708 1 vib 10.8392 0.0 1
709 2 vib 8.2402 0.0 1
710 3 vib 25.0544 0.0 1
711 4 vib 34.0218 0.0 1
712 5 vib 447.6057 0.0 1
713 6 vib 576.9653 0.0 1
714 7 vib 611.7792 0.0 1
715 8 vib 989.8048 0.0 1
716 9 vib 1184.5908 0.0 1
717 10 vib 1416.6586 0.0 1
718 11 vib 1749.7937 0.0 1
719 12 vib 2255.0014 0.0 1
720 13 vib 3214.1797 0.0 1
721 14 vib 3314.3371 0.0 1
722 15 kro 57.5263 1.0 1 ! K-rotor
723 16 jro 562.1324 1.0 2 ! 2D adiabatic rotor
724
725 ctst rc-570 -0.01 5.7 0.0
726 C2H2O3
727 a) (blank comment line)
728 b) (blank comment line)
729 c) (blank comment line)
730 1 1 1
731 0.0 1
732 16 'HAR' AMUA
733 1 vib 12.3174 0.0 1
734 2 vib 6.7288 0.0 1
735 3 vib 9.7290 0.0 1
736 4 vib 23.7084 0.0 1
737 5 vib 446.5902 0.0 1
738 6 vib 576.3762 0.0 1
739 7 vib 609.2093 0.0 1
740 8 vib 989.9439 0.0 1
741 9 vib 1184.8373 0.0 1
742 10 vib 1416.4320 0.0 1
743 11 vib 1749.6731 0.0 1
744 12 vib 2255.9546 0.0 1
745 13 vib 3215.6885 0.0 1
746 14 vib 3316.5915 0.0 1

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747	15	kro	57.1496	1.0	1	! K-rotor
748	16	jro	576.1782	1.0	2	! 2D adiabatic rotor
749						
750	ctst	rc-580	-0.01	5.8	0.0	
751	C2H2O3					
752	a) (blank comment line)					
753	b) (blank comment line)					
754	c) (blank comment line)					
755	1	1	1			
756	0.0		1			
757	15	'HAR'	AMUA			
758	1	vib	39.9014	0.0	1	
759	2	vib	17.2308	0.0	1	
760	3	vib	23.8206	0.0	1	
761	4	vib	445.9114	0.0	1	
762	5	vib	575.8910	0.0	1	
763	6	vib	608.4413	0.0	1	
764	7	vib	989.3311	0.0	1	
765	8	vib	1184.5516	0.0	1	
766	9	vib	1415.6040	0.0	1	
767	10	vib	1750.1002	0.0	1	
768	11	vib	2255.9212	0.0	1	
769	12	vib	3216.9363	0.0	1	
770	13	vib	3317.7695	0.0	1	
771	14	kro	51.3438	1.0	1	! K-rotor
772	15	jro	565.0934	1.0	2	! 2D adiabatic rotor
773						
774	ctst	rc-600	0.00	6.0	0.0	
775	C2H2O3					
776	a) (blank comment line)					
777	b) (blank comment line)					
778	c) (blank comment line)					
779	1	1	1			
780	0.0		1			
781	16	'HAR'	AMUA			
782	1	vib	18.5132	0.0	1	
783	2	vib	7.2983	0.0	1	
784	3	vib	2.9746	0.0	1	
785	4	vib	16.3869	0.0	1	
786	5	vib	446.0252	0.0	1	
787	6	vib	576.5858	0.0	1	
788	7	vib	609.0697	0.0	1	
789	8	vib	989.3770	0.0	1	
790	9	vib	1184.5126	0.0	1	

791	10	vib	1415.5826	0.0	1	
792	11	vib	1749.5646	0.0	1	
793	12	vib	2255.9852	0.0	1	
794	13	vib	3216.9462	0.0	1	
795	14	vib	3317.7995	0.0	1	
796	15	kro	49.1197	1.0	1	! K-rotor
797	16	jro	620.4779	1.0	2	! 2D adiabatic rotor
798						
799	ctst	rc-680	0.00	6.8	0.0	
800	C2H2O3					
801	a) (blank comment line)					
802	b) (blank comment line)					
803	c) (blank comment line)					
804	1	1	1			
805	0.0		1			
806	16	'HAR'	AMUA			
807	1	vib	-4.9877	0.0	1	
808	2	vib	0.7339	0.0	1	
809	3	vib	14.2613	0.0	1	
810	4	vib	32.5332	0.0	1	
811	5	vib	447.0289	0.0	1	
812	6	vib	576.8571	0.0	1	
813	7	vib	610.9045	0.0	1	
814	8	vib	989.9251	0.0	1	
815	9	vib	1184.8010	0.0	1	
816	10	vib	1416.6210	0.0	1	
817	11	vib	1750.6380	0.0	1	
818	12	vib	2256.1450	0.0	1	
819	13	vib	3214.7083	0.0	1	
820	14	vib	3315.1503	0.0	1	
821	15	kro	57.4764	1.0	1	! K-rotor
822	16	jro	826.7412	1.0	2	! 2D adiabatic rotor
823						
824	ctst	rc-710	0.00	7.1	0.0	
825	C2H2O3					
826	a) (blank comment line)					
827	b) (blank comment line)					
828	c) (blank comment line)					
829	1	1	1			
830	0.0		1			
831	16	'HAR'	AMUA			
832	1	vib	-5.6190	0.0	1	
833	2	vib	-1.9075	0.0	1	
834	3	vib	15.1824	0.0	1	

835	4	vib	32.7545	0.0	1	
836	5	vib	447.0081	0.0	1	
837	6	vib	576.8513	0.0	1	
838	7	vib	610.8668	0.0	1	
839	8	vib	989.9205	0.0	1	
840	9	vib	1184.7728	0.0	1	
841	10	vib	1416.5925	0.0	1	
842	11	vib	1750.3295	0.0	1	
843	12	vib	2255.8652	0.0	1	
844	13	vib	3214.7235	0.0	1	
845	14	vib	3315.1721	0.0	1	
846	15	kro	57.3636	1.0	1	! K-rotor
847	16	jro	900.1840	1.0	2	! 2D adiabatic rotor
848						
849	prod	C2H2O-----	0.0	10.0		
850		C2H2O				
851	a)	(blank comment line)				
852	b)	(blank comment line)				
853	c)	(blank comment line)				
854	1	1	1			
855	0.0	1				
856	11	'HAR'	AMUA			
857	1	vib	445.4186	0.0	1	
858	2	vib	576.5236	0.0	1	
859	3	vib	605.5819	0.0	1	
860	4	vib	989.3038	0.0	1	
861	5	vib	1184.8513	0.0	1	
862	6	vib	1415.4176	0.0	1	
863	7	vib	2256.1163	0.0	1	
864	8	vib	3217.5075	0.0	1	
865	9	vib	3318.9177	0.0	1	
866	10	kro	1.7856	1.0	1	! K-rotor
867	11	jro	49.4739	1.0	2	! 2D adiabatic rotor
868						
869	prod	O2-----	0.0	10.0		
870		O2				
871	a)	(blank comment line)				
872	b)	(blank comment line)				
873	c)	(blank comment line)				
874	2	1	1			
875	0.0	3				
876	2	'HAR'	AMUA			
877	1	vib	1681.6328	0.0	1	
878	2	jro	11.6367	1.0	2	! 2D adiabatic rotor

Listing 2: Mesmer input file for  $\text{H}_2\text{C}_2\text{O} + {}^1\text{O}_2$

```

1 <?xml version="1.0" encoding="utf-8" ?>
2 <?xml-stylesheet type='text/xsl' href='../.. / mesmer2.xsl' media='other' ?>
3 <?xml-stylesheet type='text/xsl' href='../.. / mesmer1.xsl' media='screen' ?>
4 <me:mesmer xmlns="http://www.xml-cml.org/schema" xmlns:me="http://www.chem.leeds.ac.
    uk/mesmer"
5 xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xmlns:cml="http://www.xml-cml.
    org/schema">
6 <me:title>MESMER Title</me:title>
7 <moleculeList>
8     <molecule id="N2">
9         <atom elementType="He" />
10        <propertyList>
11            <property dictRef="me:epsilon">
12                <scalar>84.942</scalar>
13            </property>
14            <property dictRef="me:sigma">
15                <scalar>3.707</scalar>
16            </property>
17            <property dictRef="me:MW">
18                <scalar units="amu">28.0</scalar>
19            </property>
20        </propertyList>
21    </molecule>
22    <molecule id="RC">
23        <atomArray>
24            <atom id="a1" elementType="C" x3="-0.60034802558431" y3="0.97348784453155" z3="
                0.00023471289493" />
25            <atom id="a2" elementType="H" x3="-0.72782358392821" y3="1.56764279154758" z3="
                -0.90348943439161" />
26            <atom id="a3" elementType="H" x3="-0.72771479140250" y3="1.56719225104095" z3="
                0.90427236466860" />
27            <atom id="a4" elementType="C" x3="0.60241372768466" y3="0.06269057786815" z3="
                -0.00008596640423" />
28            <atom id="a5" elementType="O" x3="1.78508498488250" y3="0.10865564519820" z3="
                -0.00005074471132" />
29            <atom id="a6" elementType="O" x3="-0.19186338529144" y3="-1.06487091305615" z3="
                -0.00015255573541" />
30            <atom id="a7" elementType="O" x3="-1.42504292636070" y3="-0.21225719713027" z3="
                -0.00000637632096" />
31        </atomArray>
32        <bondArray>
33            <bond atomRefs2="a1 a2" order="1" />
34            <bond atomRefs2="a1 a3" order="1" />

```

```

35 <bond atomRefs2="a1 a4" order="1"/>
36 <bond atomRefs2="a1 a7" order="1"/>
37 <bond atomRefs2="a4 a5" order="1"/>
38 <bond atomRefs2="a4 a6" order="1"/>
39 <bond atomRefs2="a6 a7" order="1"/>
40 </bondArray>
41 <propertyList>
42 <property dictRef="me:ZPE">
43 <scalar units="kcal/mol">81.61</scalar>
44 </property>
45 <property dictRef="me:rotConsts">
46 <array units="cm-1">0.457411 0.176446 0.130578</array>
47 </property>
48 <property dictRef="me:vibFreqs">
49 <array units="cm-1">221.94 484.45 506.35 736.63 819.74 917.58
1020.89 1024.71 1146.46 1153.96 1309.59 1487.84 1941.44 3085.68
3155.69</array>
50 </property>
51 <property dictRef="me:frequenciesScaleFactor">
52 <scalar>1</scalar>
53 </property>
54 <property dictRef="me:symmetryNumber">
55 <scalar>1</scalar>
56 </property>
57 <property dictRef="me:MW">
58 <scalar units="amu">74.03</scalar>
59 </property>
60 <property dictRef="me:spinMultiplicity">
61 <scalar>1</scalar>
62 </property>
63 <property dictRef="me:epsilon">
64 <scalar>483.3418</scalar>
65 </property>
66 <property dictRef="me:sigma">
67 <scalar>4.86</scalar>
68 </property>
69 </propertyList>
70 <me:DOSCMETHOD name="ClassicalRotors"/>
71 <me:energyTransferModel xsi:type="me:ExponentialDown">
72 <me:deltaEDown units="cm-1">200</me:deltaEDown>
73 </me:energyTransferModel>
74 </molecule>
75 <molecule id="TS">
76 <atomArray>

```

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77 <atom id="a1" elementType="C" x3="-0.74382807048935" y3="-0.86769855577965" z3="
    0.00030915393257" />
78 <atom id="a2" elementType="H" x3="-0.80888447000204" y3="-1.46584325280376" z3="
    0.91224544057895" />
79 <atom id="a3" elementType="H" x3="-0.80557363308962" y3="-1.47527338567108" z3="
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80 <atom id="a4" elementType="C" x3="0.53764461267181" y3="-0.01917841264472" z3="
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81 <atom id="a5" elementType="O" x3="1.68687203946410" y3="-0.40804360242030" z3="
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82 <atom id="a6" elementType="O" x3="0.26481183030661" y3="1.23655925641933" z3="
    0.01132945211404" />
83 <atom id="a7" elementType="O" x3="-1.63066630886152" y3="0.20676195290019" z3="
    -0.00554911940995" />
84 </atomArray>
85 <bondArray>
86 <bond atomRefs2="a1 a2" order="1" />
87 <bond atomRefs2="a1 a3" order="1" />
88 <bond atomRefs2="a1 a4" order="1" />
89 <bond atomRefs2="a1 a7" order="1" />
90 <bond atomRefs2="a4 a5" order="1" />
91 <bond atomRefs2="a4 a6" order="1" />
92 </bondArray>
93 <propertyList>
94 <property dictRef="me:ZPE">
95 <scalar units="kcal/mol">100.14</scalar>
96 </property>
97 <property dictRef="me:rotConsts">
98 <array units="cm-1">0.394355 0.164789 0.118958</array>
99 </property>
100 <property dictRef="me:vibFreqs">
101 <array units="cm-1">195.12 450.77 539.34 591.33 729.55 934.62 962.34
    1040.82 1200.81 1285.45 1491.24 1633.05 3015.12 3126.98</array>
102 </property>
103 <property title="ImaginaryFrequency" dictRef="me:imFreqs">
104 <scalar units="cm-1">742.40</scalar>
105 </property>
106 <property dictRef="me:frequenciesScaleFactor">
107 <scalar>1</scalar>
108 </property>
109 <property dictRef="me:symmetryNumber">
110 <scalar>1</scalar>
111 </property>
112 <property dictRef="me:spinMultiplicity">

```

```

113         <scalar>1</scalar>
114     </property>
115 </propertyList>
116 <me:DOSCMMethod name=" ClassicalRotors" />
117 </molecule>
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0.00000083609036" />
121 <atom id="a2" elementType="H" x3="-1.77687215610886" y3="1.21156732452937" z3="
0.00011203508798" />
122 <atom id="a3" elementType="H" x3="-3.22353150671445" y3="0.01112607807650" z3="
0.00002551509760" />
123 <atom id="a4" elementType="C" x3="1.31695680811755" y3="0.16719323513296" z3="
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124 <atom id="a5" elementType="O" x3="1.78988573703196" y3="-0.89273765587214" z3="
0.00007344080807" />
125 <atom id="a6" elementType="O" x3="0.87557297647335" y3="1.24508950048442" z3="
0.00000293873488" />
126 <atom id="a7" elementType="O" x3="-1.36168231205714" y3="-0.76087095521387" z3="
-0.00013891179724" />
127 </atomArray>
128 <bondArray>
129 <bond atomRefs2="a1 a2" order="1" />
130 <bond atomRefs2="a1 a3" order="1" />
131 <bond atomRefs2="a1 a7" order="1" />
132 <bond atomRefs2="a4 a5" order="1" />
133 <bond atomRefs2="a4 a6" order="1" />
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139 <property dictRef="me:rotConsts">
140 <array units="cm-1">0.345509 0.092621 0.073041</array>
141 </property>
142 <property dictRef="me:vibFreqs">
143 <array units="cm-1">41.58 85.71 106.49 149.79 159.13 662.65 678.73
1195.10 1275.73 1352.07 1534.26 1772.59 2392.32 2942.87 3022.18<
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144 </property>
145 <property dictRef="me:frequenciesScaleFactor">
146 <scalar>1</scalar>
147 </property>

```



```

148         <property dictRef="me:symmetryNumber">
149             <scalar>1</scalar>
150         </property>
151         <property dictRef="me:MW">
152             <scalar units="amu">74.03</scalar>
153         </property>
154     </propertyList>
155     <me:DOSCMMethod name="ClassicalRotors"/>
156 </molecule>
157 <molecule id="Ketene">
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160         -0.00000000292172"/>
161     <atom id="a2" elementType="H" x3="-0.94196912661695" y3="-1.73673477024717" z3="
162         0.00000000136923"/>
163     <atom id="a3" elementType="H" x3="0.94259142801765" y3="-1.73639906167143" z3="
164         0.00000000136929"/>
165     <atom id="a4" elementType="C" x3="-0.00001555038755" y3="0.10262415088185" z3="
166         -0.00000000083898"/>
167     <atom id="a5" elementType="O" x3="-0.00022745528336" y3="1.26544619122551" z3="
168         0.00000000102218"/>
169     </atomArray>
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172     <bond atomRefs2="a1 a3" order="1"/>
173     <bond atomRefs2="a1 a4" order="1"/>
174     <bond atomRefs2="a4 a5" order="1"/>
175     </bondArray>
176     <propertyList>
177     <property dictRef="me:ZPE">
178         <scalar units="kcal/mol">133.75</scalar>
179     </property>
180     <property dictRef="me:rotConsts">
181         <array units="cm-1">9.417728 0.342301 0.330296</array>
182     </property>
183     <property dictRef="me:vibFreqs">
184         <array units="cm-1">433.64 511.61 584.74 993.20 1153.78 1415.68
185             2195.26 3196.02 3305.43</array>
186     </property>
187     <property dictRef="me:frequenciesScaleFactor">
188         <scalar>1</scalar>
189     </property>
190     <property dictRef="me:symmetryNumber">
191         <scalar>1</scalar>

```

```

186         </property>
187         <property dictRef="me:spinMultiplicity">
188             <scalar>1</scalar>
189         </property>
190     </propertyList>
191     <me:DOSCMMethod name="ClassicalRotors" />
192 </molecule>
193 <molecule id="O2">
194     <atomArray>
195     <atom id="a1" elementType="C" x3="0.00000000000000" y3="0.00000000000000" z3="
196         0.60991780529370" />
197     <atom id="a2" elementType="H" x3="0.00000000000000" y3="0.00000000000000" z3="
198         -0.60991780529370" />
199 </atomArray>
200 <bondArray>
201     <bond atomRefs2="a1 a2" order="1" />
202 </bondArray>
203     <propertyList>
204         <property dictRef="me:ZPE">
205             <scalar units="kcal/mol">0.0</scalar>
206         </property>
207         <property dictRef="me:rotConsts">
208             <array units="cm-1">0.000000 1.416222 1.416222</array>
209         </property>
210         <property dictRef="me:vibFreqs">
211             <array units="cm-1">1501.35</array>
212         </property>
213         <property dictRef="me:frequenciesScaleFactor">
214             <scalar>1</scalar>
215         </property>
216         <property dictRef="me:symmetryNumber">
217             <scalar>2</scalar>
218         </property>
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220             <scalar>1</scalar>
221         </property>
222     </propertyList>
223     <me:DOSCMMethod name="ClassicalRotors" />
224 </molecule>
225 </moleculeList>
226 <reactionList>
227     <reaction id="R0">
228         <reactant>
229             <molecule ref="Ketene" me:type="deficientReactant" />

```

```

228     </reactant>
229     <reactant>
230         <molecule ref="O2" me:type="excessReactant" />
231     </reactant>
232     <product>
233         <molecule ref="RC" me:type="modelled" />
234     </product>
235     <me:MCRCMethod name="MesmerILT" />
236     <me:preExponential units="cm3molecule-1s-1">4.96E-15</me:preExponential>
237     <me:activationEnergy units="kJ/mol">0.0</me:activationEnergy>
238     <me:TInfinity>298.0</me:TInfinity>
239     <me:nInfinity>0.0</me:nInfinity>
240     <me:excessReactantConc>1.7E8</me:excessReactantConc>
241 </reaction>
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243     <reactant>
244         <molecule ref="RC" me:type="modelled" />
245     </reactant>
246     <product>
247         <molecule ref="PC" me:type="sink" />
248     </product>
249     <me:MCRCMethod name="RRKM" />
250     <me:transitionState>
251         <molecule ref="TS" me:type="transitionState" />
252     </me:transitionState>
253     <me:tunneling>Eckart</me:tunneling>
254 </reaction>
255 </reactionList>
256 <me:conditions>
257     <me:bathGas>N2</me:bathGas>
258     <me:PTs>
259         <!--<me:PTset units="PPCC">-->
260         <!--<me:Prange initial="2.42E18" final="2.82E18" increment="0.40E18"/>-->
261         <!--<me:Trange initial="200" final="350" increment="10"/>-->
262         <!--</me:PTset>-->
263         <!--me:PTpair units="atm" P="1.00" T="298." />-->
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265         <me:PTpair units="atm" P="1.0" T="210." precision="qd"/>
266         <me:PTpair units="atm" P="1.0" T="220." precision="qd"/>
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271         <me:PTpair units="atm" P="1.0" T="270." precision="qd"/>

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272     <me:PTpair units="atm" P="1.0" T="280." precision ="qd" />
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274     <me:PTpair units="atm" P="1.0" T="298." precision ="qd" />
275     <me:PTpair units="atm" P="1.0" T="300." precision ="qd" />
276     <me:PTpair units="atm" P="1.0" T="310." precision ="qd" />
277     <me:PTpair units="atm" P="1.0" T="320." precision ="qd" />
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279 </me:PTs>
280 </me:conditions>
281 <me:modelParameters>
282     <me:grainSize units="cm-1">100</me:grainSize>
283     <me:energyAboveTheTopHill>25.0</me:energyAboveTheTopHill>
284 </me:modelParameters>
285 <me:control>
286     <me:eigenvalues>0</me:eigenvalues>
287     <me:calcMethod>simpleCalc</me:calcMethod>
288     <me:printReactionOperatorColumnSums/>
289     <me:printGrainBoltzmann/>
290     <me:testMicroRates/>
291     <me:testRateConstants/>
292     <me:printGrainDOS/>
293     <me:printGrainkbE/>
294     <me:printGrainkfE/>
295     <me:printTunnellingCoefficients/>
296     <me:testDOS/>
297     <me:printCellDOS/>
298     <me:printSpeciesProfile/>
299 </me:control>
300 </me:mesmer>

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