

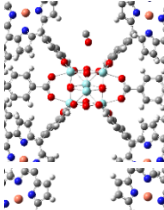
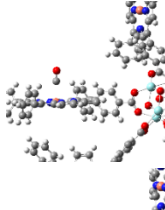
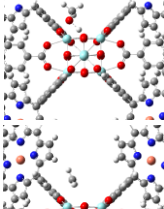
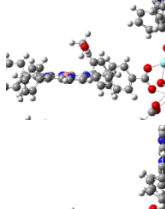
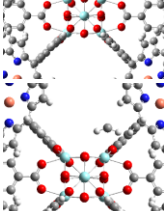
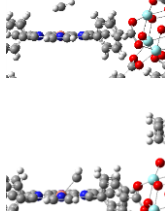
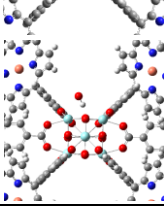
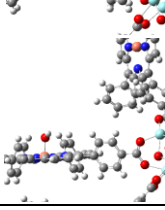


***Supporting Information***

**The cascade catalysis of the porphyrinic zirconium metal-organic framework PCN-224-Cu for CO<sub>2</sub> conversion to alcohols**

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**Table S1.** The energies (in Hartree) of the Zr<sub>6</sub> cluster or TCPP-Cu site chemisorbing intermediates in a Zr<sub>6</sub>O<sub>8</sub>(TCPP-Cu)<sub>6</sub> unit calculated with PM7 semi-empirical method.

Intermediate	Site	Energy	Geometry	Site	Energy	Geometry
CO	Zr <sub>6</sub>	1.3120		TCPP-Cu	1.2796	
CH <sub>3</sub> OH	Zr <sub>6</sub>	1.2126		TCPP-Cu	1.2543	
CH <sub>3</sub>	Zr <sub>6</sub>	1.4101		TCPP-Cu	1.3717	
CH <sub>2</sub>	Zr <sub>6</sub>	1.4712		TCPP-Cu	1.4360	
OH	Zr <sub>6</sub>	1.3178		TCPP-Cu	1.3103	

**Table S2.** The yield and selectivity of CO<sub>2</sub> hydrogenation to alcohols based on recently reported representative catalysts.

Entry	Catalyst	P/MPa	T/°C	Yield/mmol h <sup>-1</sup> g <sup>-1</sup>		Selectivity/%		Ref.
				EtOH	MeOH	EtOH	MeOH	
1	PCN-224-Cu	2	130	4.53	--	~100		This work
2	Cu <sup>II</sup> @Ru-UiO	2	150	0.29	--	>99	<1	[34]
3	Zr <sub>12</sub> -bpdc-CuLi	2	100	3.62	--	66.3	33.7	[38]
4	Cu NPs@Zr <sub>12</sub> -bpdc-Li	2	100	0.09	--	10.1	89.9	[38]
5	Cu <sup>I</sup> @Zr <sub>12</sub> -bpdc	2	100	0.01	--	11.3	88.7	[38]
6	Cu/ZrO <sub>2</sub>	2	100	0.04	--	10.5	89.5	[38]
7	CoAlO <sub>x</sub>	4	140	0.44	0.02	92.1	--	[44]
8	Cu/Na-Beta	1.3	300	1.40	--	64.3	30.1	[45]
9	Cu@Na-ZSM5	1.3	300	1.85	--	85	8.2	[45]
10	Cu@Na-Beta	1.3	300	2.17	--	--	~100	[45]
11	UiO-66(Zr)	1.8	200	--	0.28	--	3.5	[46]
12	UiO-66(Ce/Zr)	1.8	200	--	0.47	--	28.7	[46]
13	Pt <sub>2</sub> Ru <sub>1</sub> /Fe <sub>2</sub> O <sub>3</sub>	18	200	2.6	--	11.8	18.9	[47]
14	Pt <sub>1</sub> Ru <sub>2</sub> /Fe <sub>2</sub> O <sub>3</sub>	18	220	3.2	--	28.4	5.9	[47]

**Table S3.** Ultimate elemental analysis (% wt.) for as-synthesized PCN-224-Cu and that after reusage.

<b>Element</b>	<b>Theoretical</b>	<b>As-synthesized</b>	<b>After reusage</b>
C	40.4	46.7	49.8
H	1.7	2.9	3.0
N	3.9	3.5	3.5
O	23.9	20.7	20.0
Zr	25.6	21.8	19.5
Cu	4.5	4.4	4.2

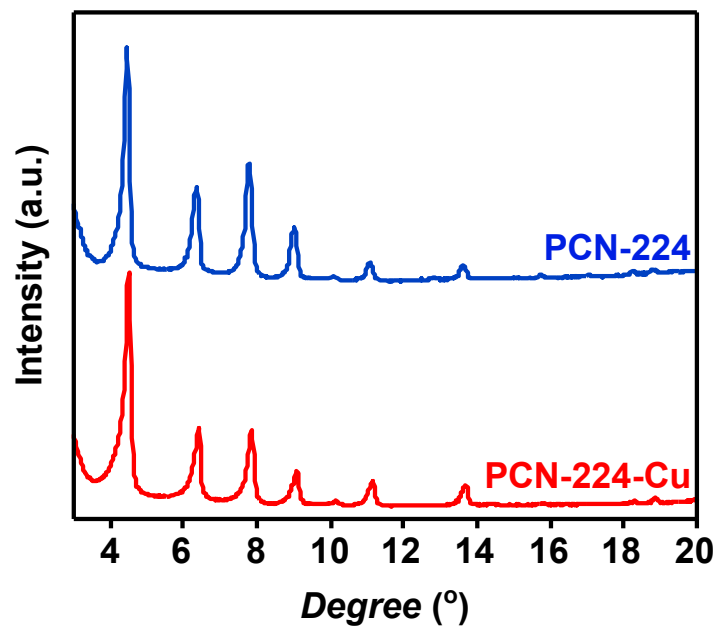


Fig. S1. XRPD patterns of PCN-224 and PCN-224-Cu.

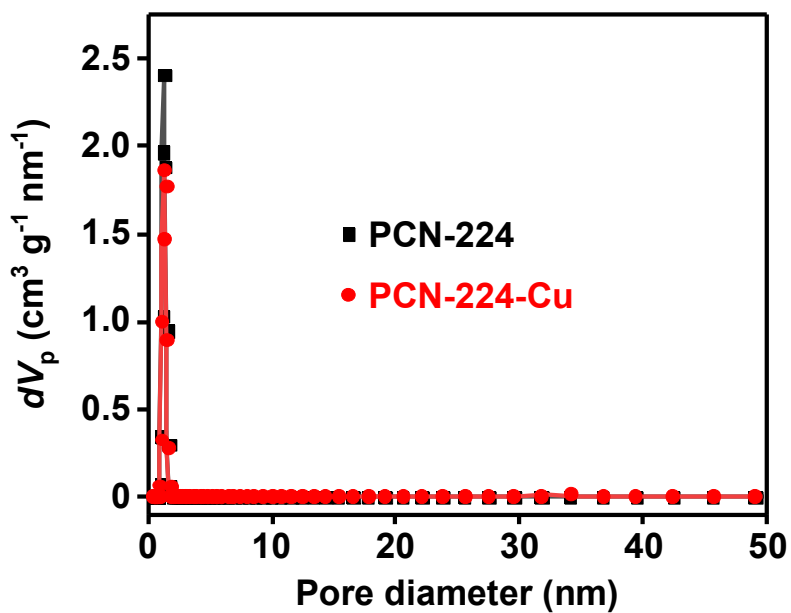
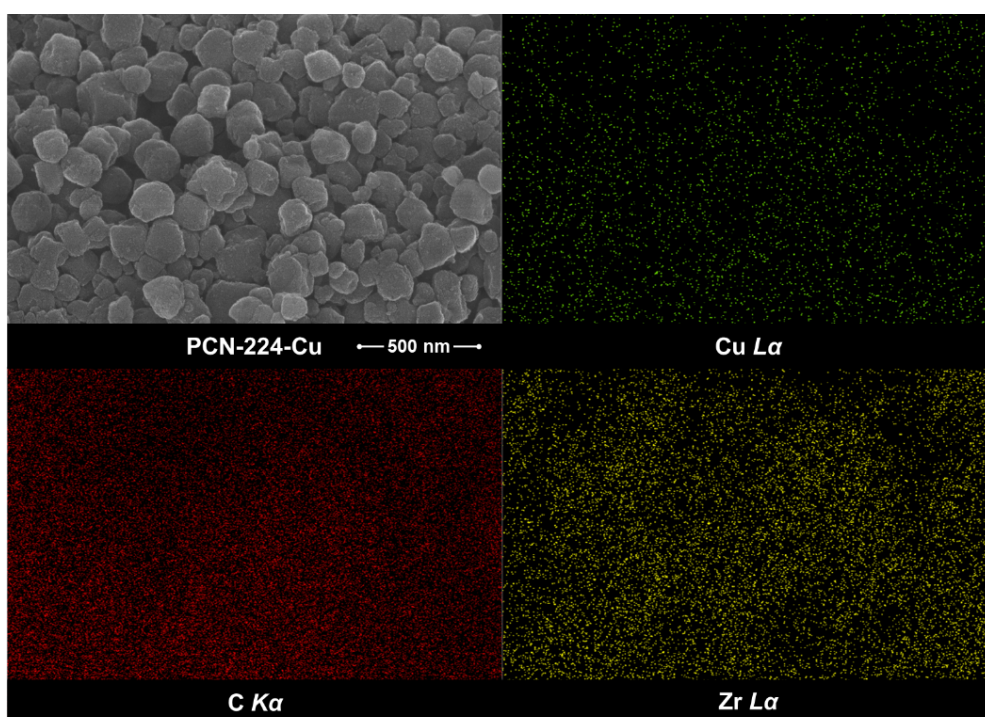
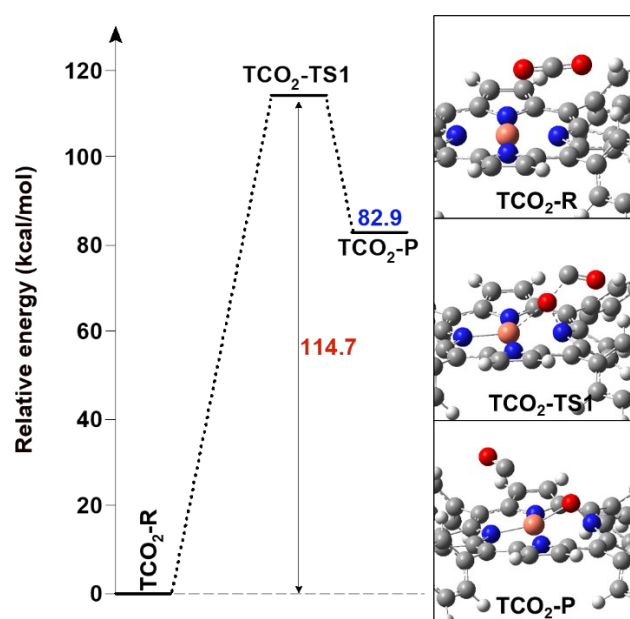


Fig. S2. Pore diameter distributions of PCN-224 and PCN-224-Cu.



**Fig. S3.** Elemental mapping of Cu, C, and Zr for PCN-224-Cu.



**Fig. S4.** Energy profile of CO<sub>2</sub> dissociation to CO over TCPP-Cu unit.

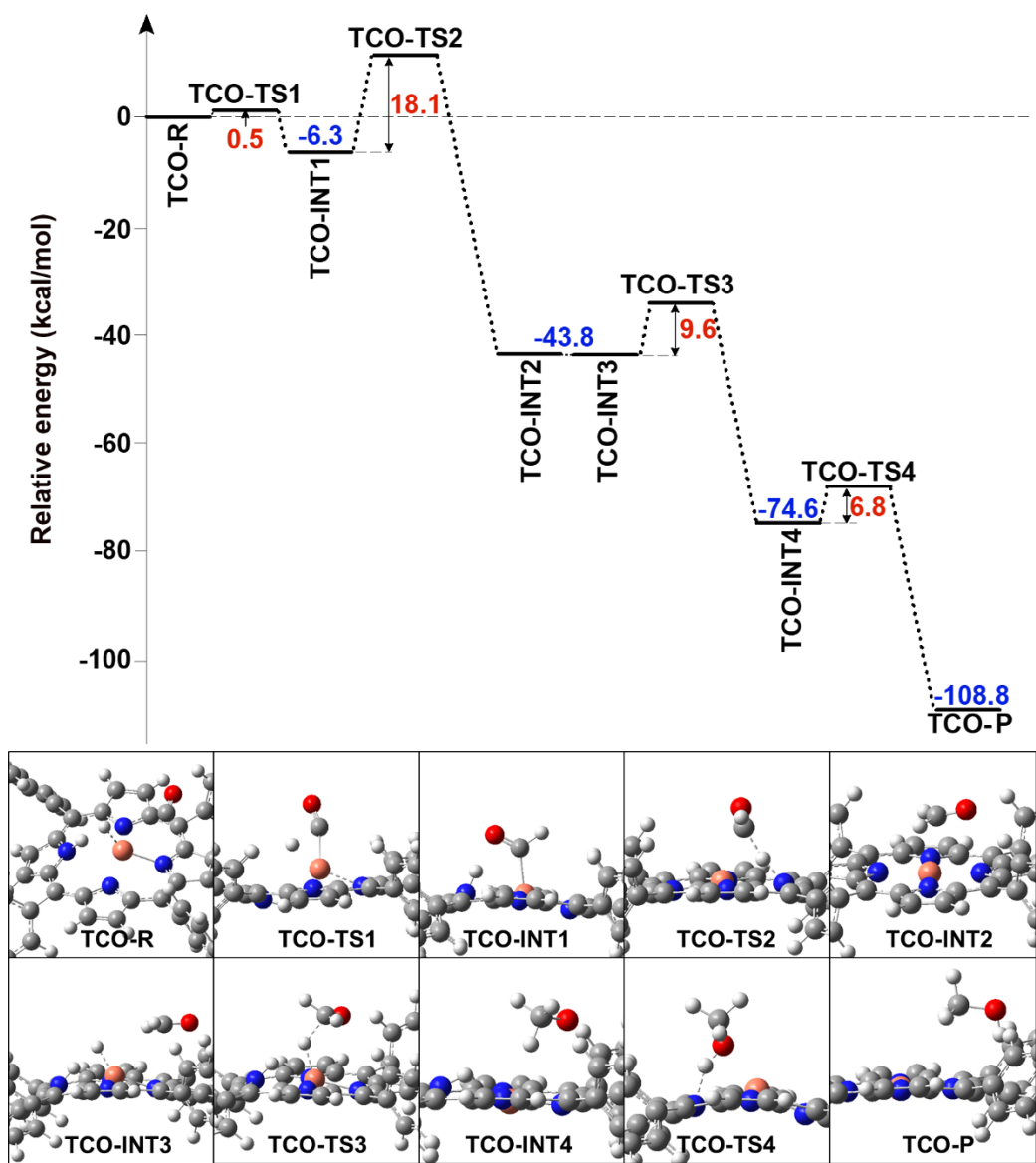
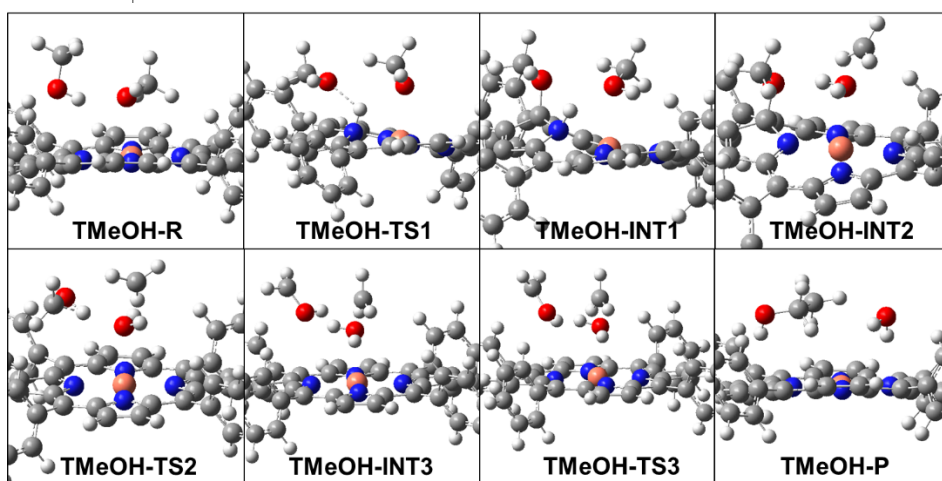
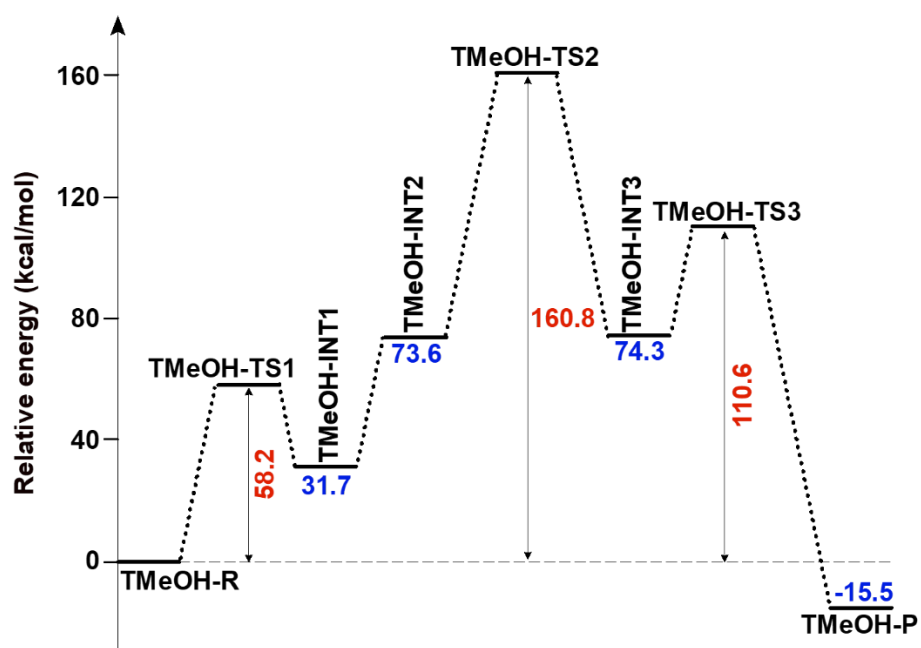
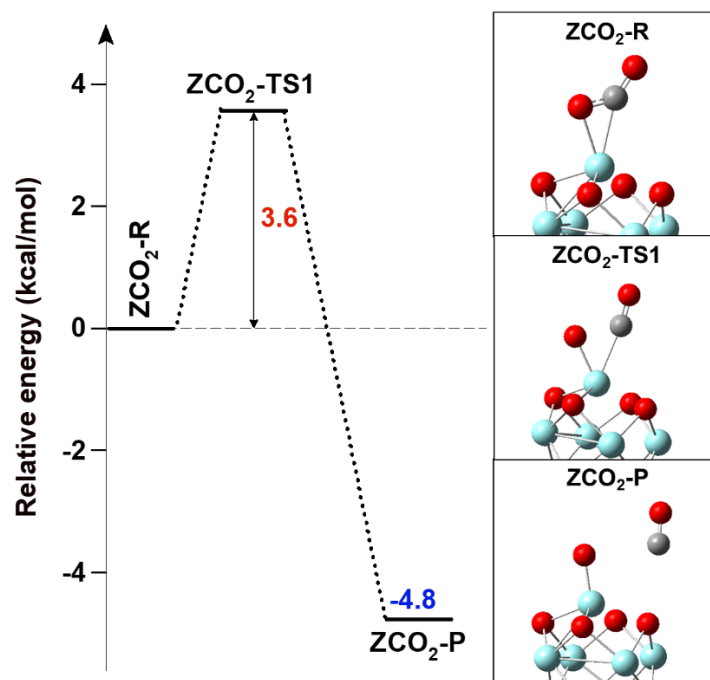


Fig. S5. Energy profile of CO hydrogenation to methanol over TCPP-Cu unit.

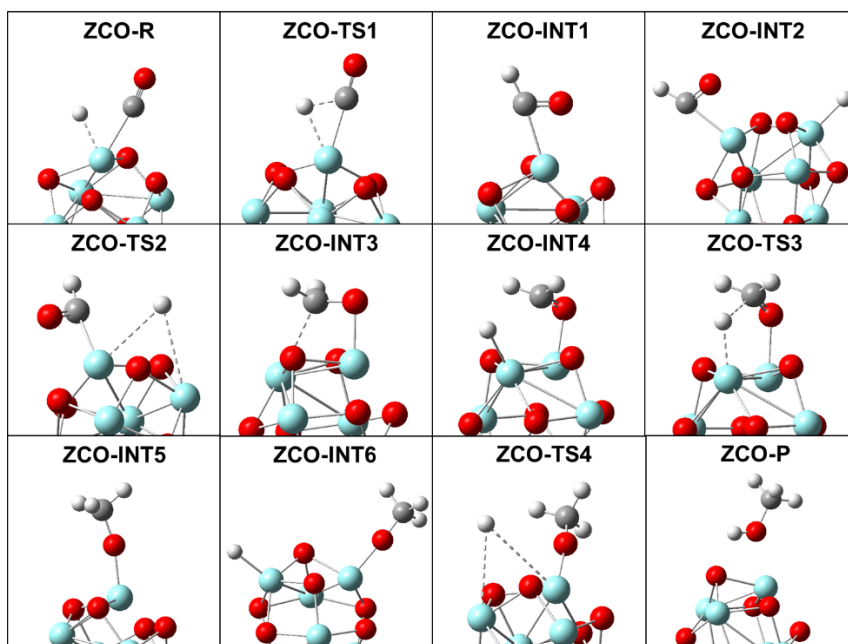
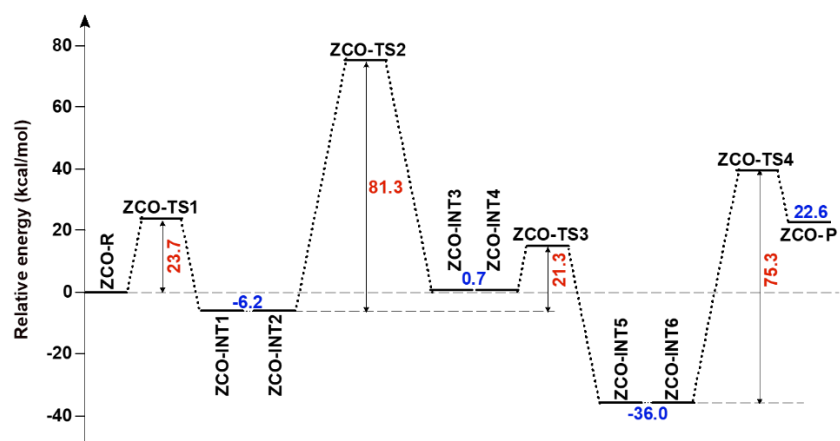




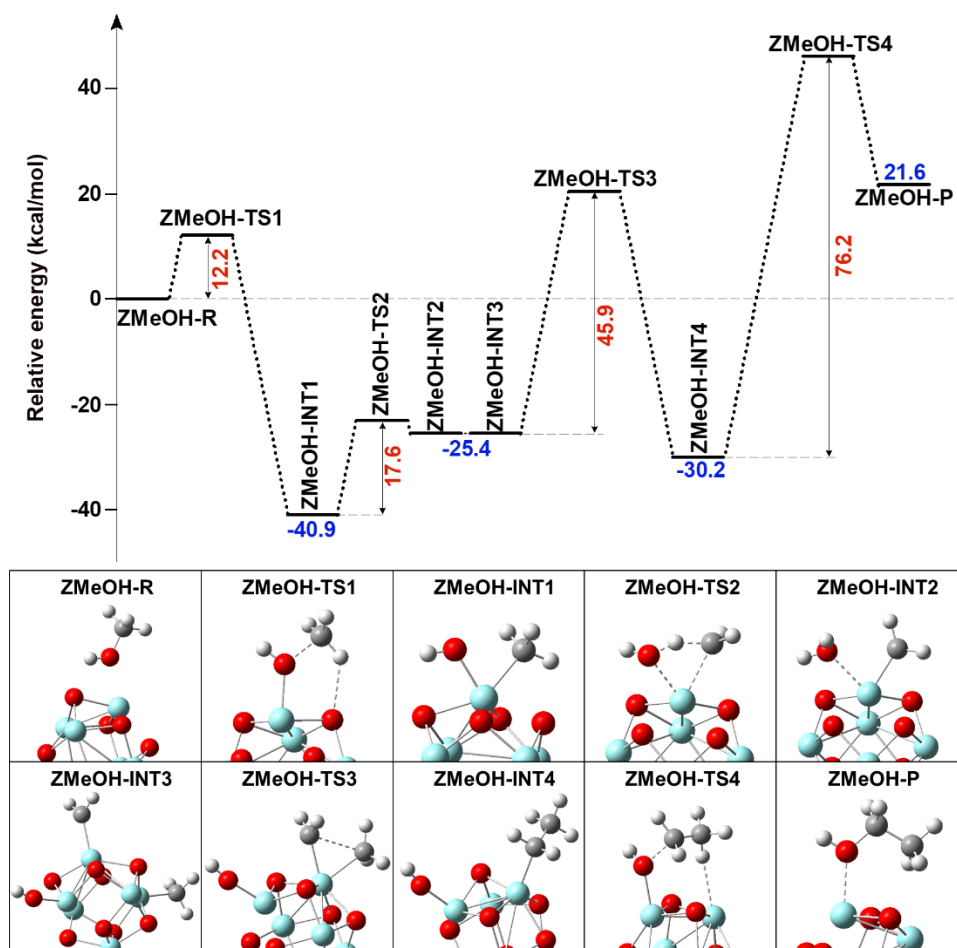
**Fig. S6.** Energy profile of methanol conversion to ethanol over TCPP-Cu unit.



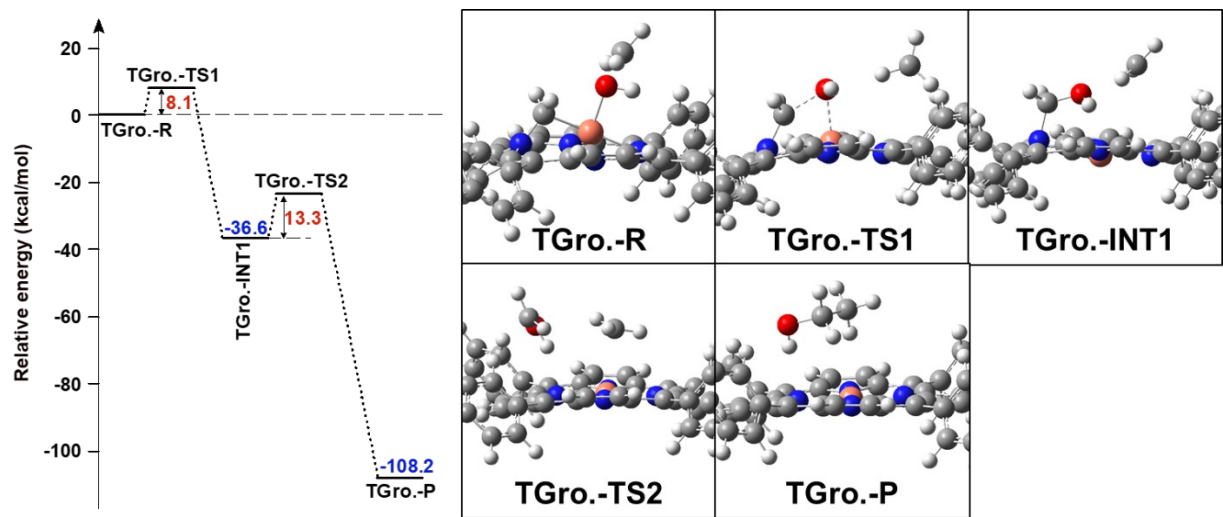
**Fig. S7.** Energy profile of CO<sub>2</sub> dissociation to CO over Zr<sub>6</sub> cluster.



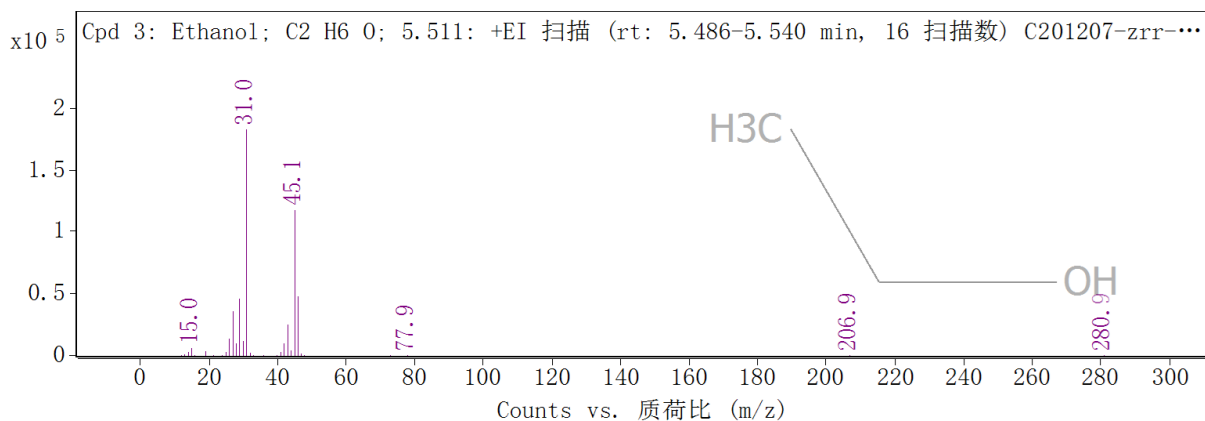
**Fig. S8.** Energy profile of CO hydrogenation to methanol over Zr<sub>6</sub> cluster.



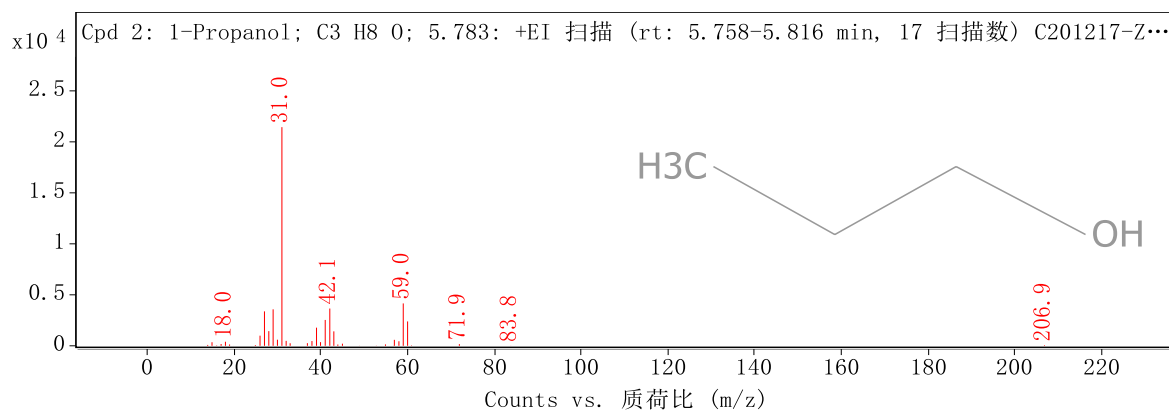
**Fig. S9.** Energy profile of methanol dissociation and re-bonding to ethanol over  $Zr_6$  cluster.



**Fig. S10.** Energy profile of \*CH<sub>3</sub>, \*CH<sub>2</sub>, and \*OH groups bonding to ethanol over TCPP-Cu unit.



**Fig. S11.** MS spectrum of ethanol after catalytic CO<sub>2</sub> hydrogenation (Matching 99.7%).



**Fig. S12.** MS spectrum of *n*-propanol after catalytic methanol conversion (Matching 97.3%).

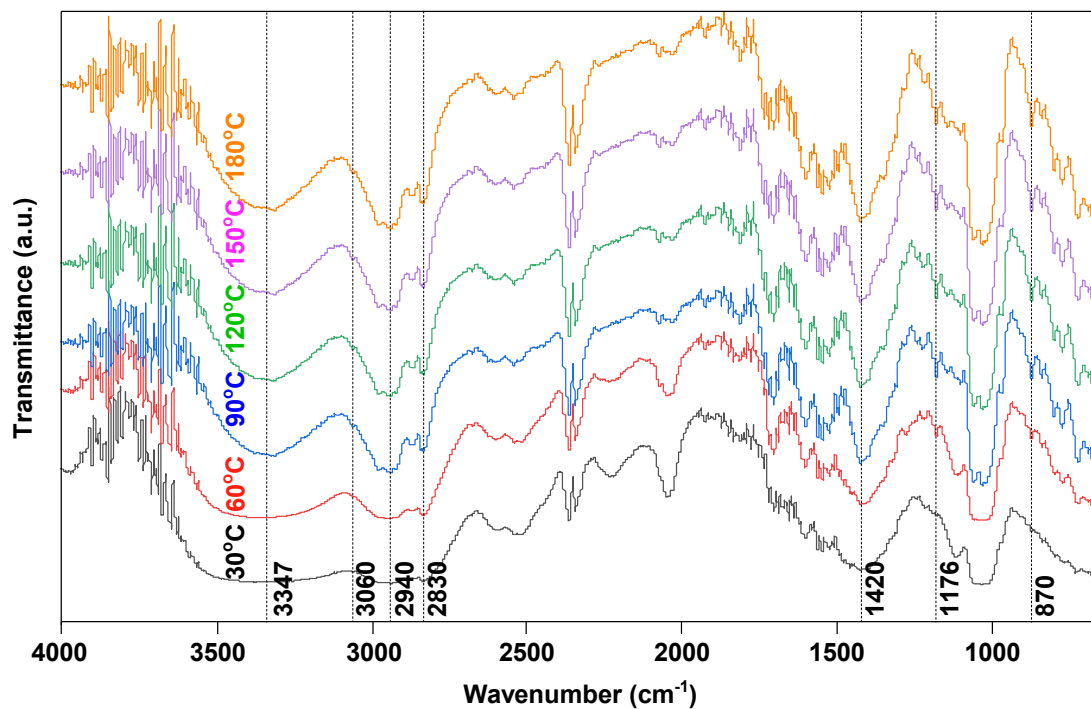


Fig. S13. In-situ DRIFTS for methanol dissociation catalyzed by PCN-224.

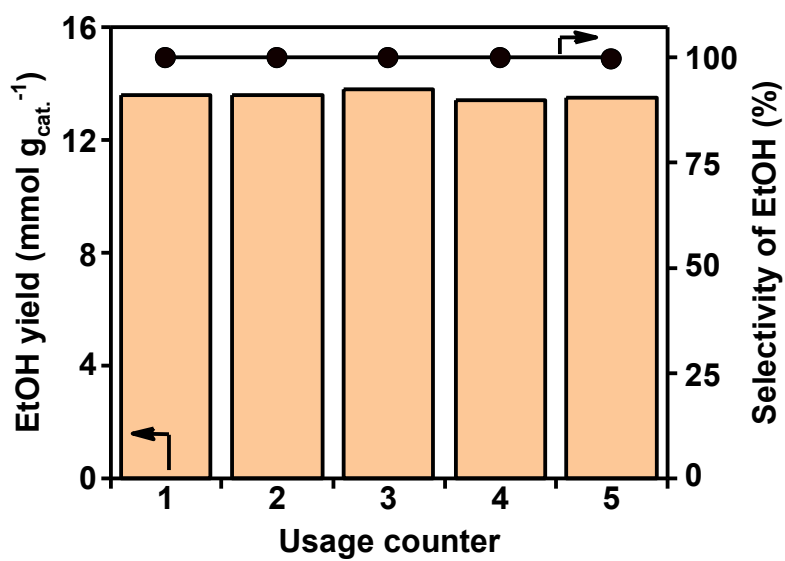


Fig. S14. Reusability test of PCN-224-Cu for CO<sub>2</sub> hydrogenation (403 K, 3h).

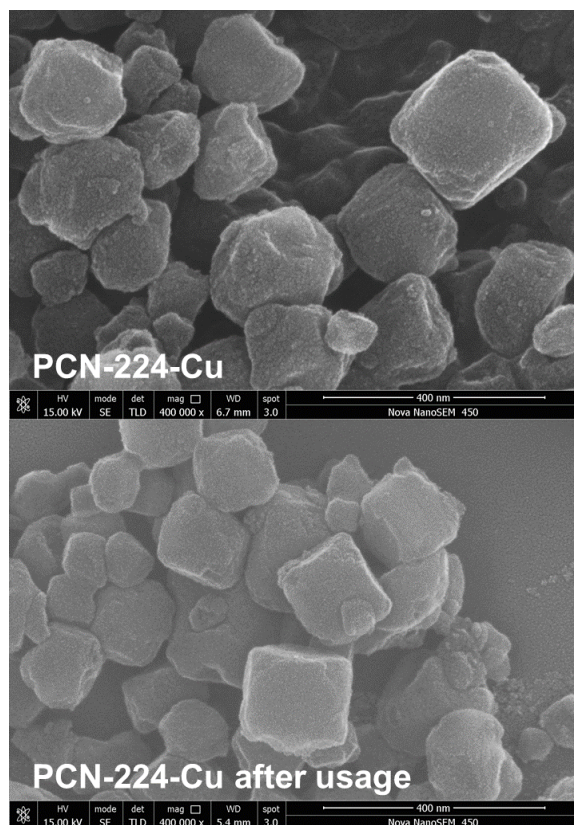


Fig. S15. SEM images of PCN-224-Cu before and after usage.

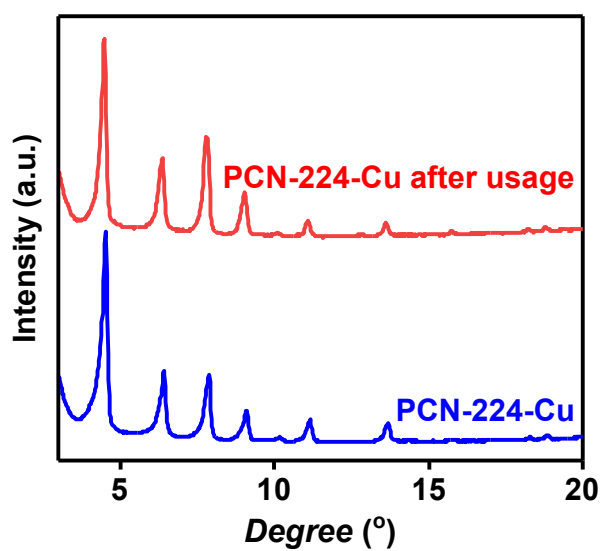


Fig. S16. XRPD patterns of PCN-224-Cu before and after usage.



## Atomic coordinates of optimized geometries and the imaginary frequencies of transition states

TCO<sub>2</sub>-R

-----  
Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z  
-----

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6	6	0	-4.080723	-0.682117	-0.687134
7	6	0	-4.080715	0.682160	-0.687130
8	6	0	-2.720338	1.102855	-0.439738
9	6	0	-2.323292	2.439332	-0.287833
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17	6	0	4.348268	-0.681834	-0.316645
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19	6	0	2.559054	-2.441593	-0.115714
20	6	0	1.215871	-2.844906	-0.073358
21	6	0	0.788359	-4.214151	0.119357
22	6	0	-0.574866	-4.212697	0.082371
23	6	0	-0.987737	-2.843679	-0.141569
24	6	0	-2.323317	-2.439307	-0.287843
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26	1	0	-4.921680	1.350662	-0.847147
27	1	0	-1.247728	5.056317	0.205862
28	1	0	1.451947	5.059009	0.279878
29	1	0	5.199746	1.350480	-0.404387
30	1	0	5.199733	-1.350534	-0.404381
31	1	0	1.451893	-5.059021	0.279885
32	1	0	-1.247782	-5.056304	0.205856
33	29	0	0.126162	0.000000	-0.215997
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35	6	0	4.500811	3.575705	1.018628
36	6	0	3.733545	4.437663	-1.103701

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38 1 0 4.408274 2.854191 1.833110  
39 6 0 4.718206 5.426830 -1.058472  
40 1 0 3.050741 4.380800 -1.954073  
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42 1 0 6.163463 4.615171 1.920270  
43 1 0 4.802371 6.145729 -1.877118  
44 1 0 6.366520 6.268744 0.062901  
45 6 0 3.611997 -3.498441 -0.066355  
46 6 0 3.733504 -4.437701 -1.103684  
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62 1 0 -2.734262 4.474881 -2.056044  
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74 6 0 -5.407760 -5.442741 -0.168447  
75 1 0 -6.071041 -4.450117 1.635940  
76 1 0 -4.516440 -6.210002 -1.984004  
77 1 0 -6.191146 -6.203691 -0.135236  
78 6 0 -1.777331 -0.000003 2.595311  
79 8 0 -0.614365 -0.000005 2.559177  
80 8 0 -2.938283 0.000001 2.664246

TCO<sub>2</sub>-TS1

-----  
Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z  
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7	6	0	-4.413392	0.682913	-0.405006
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41 6 0 5.412162 5.408628 -0.251917  
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78 6 0 2.329860 -0.000003 2.548094  
79 8 0 1.389813 -0.000011 1.334922  
80 8 0 3.482711 0.000012 2.282877

\*\*\*\*\* 1 imaginary frequencies (negative Signs) \*\*\*\*\*

Diagonal vibrational polarizability:

31.5059342 142.6261153 50.3692083

Harmonic frequencies (cm<sup>-1</sup>), IR intensities (KM/Mole), Raman scattering activities (A<sup>4</sup>/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

1 2 3

A A A

Frequencies -- -745.4710 13.4878 21.5548

Red. masses -- 13.9958 6.1569 12.5946

Frc consts -- 4.5826 0.0007 0.0034

IR Inten -- 37.4468 0.0176 2.1535

Atom AN X Y Z X Y Z X Y Z

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3	7	-0.09	0.00	-0.29	0.00	-0.01	0.00	0.00	-0.02	0.00
4	7	0.00	0.00	0.01	-0.00	0.00	0.01	-0.00	-0.02	0.02
5	6	0.00	-0.00	0.00	-0.00	0.01	-0.02	-0.00	-0.01	0.00
6	6	0.00	-0.00	-0.00	-0.00	0.01	-0.02	-0.00	-0.01	-0.00
7	6	0.00	0.00	-0.00	0.00	0.01	0.02	0.00	-0.01	0.00
8	6	0.00	0.00	0.00	0.00	0.01	0.02	0.00	-0.01	-0.00
9	6	-0.00	0.00	0.00	0.00	0.00	0.04	0.00	-0.01	-0.00
10	6	-0.00	-0.00	0.00	0.01	0.00	0.02	0.00	-0.01	-0.02
11	6	0.00	-0.00	-0.00	0.02	0.00	0.01	0.01	-0.01	-0.03
12	6	0.00	-0.00	0.00	0.02	-0.00	-0.02	0.01	-0.01	-0.03
13	6	0.00	0.00	-0.00	0.01	-0.00	-0.03	0.00	-0.02	-0.03
14	6	-0.00	-0.01	-0.02	0.00	-0.01	-0.05	0.00	-0.02	-0.02
15	6	-0.01	-0.02	-0.04	-0.00	-0.01	-0.02	-0.00	-0.03	-0.01
16	6	0.04	-0.00	0.00	-0.00	-0.03	-0.02	-0.00	-0.03	-0.01
17	6	0.04	0.00	0.00	0.00	-0.03	0.02	0.00	-0.03	0.01
18	6	-0.01	0.02	-0.04	0.00	-0.01	0.02	0.00	-0.03	0.01
19	6	-0.00	0.01	-0.02	-0.00	-0.01	0.05	-0.00	-0.02	0.02
20	6	0.00	-0.00	-0.00	-0.01	-0.00	0.03	-0.00	-0.02	0.03
21	6	0.00	0.00	0.00	-0.02	-0.00	0.02	-0.01	-0.01	0.03
22	6	0.00	0.00	-0.00	-0.02	0.00	-0.01	-0.01	-0.01	0.03
23	6	-0.00	0.00	0.00	-0.01	0.00	-0.02	-0.00	-0.01	0.02
24	6	-0.00	-0.00	0.00	-0.00	0.00	-0.04	-0.00	-0.01	0.00
25	1	0.01	-0.00	-0.01	-0.00	0.02	-0.03	-0.00	-0.01	-0.00
26	1	0.01	0.00	-0.01	0.00	0.02	0.03	0.00	-0.01	0.00
27	1	0.00	-0.00	-0.01	0.02	0.00	0.03	0.01	-0.01	-0.03
28	1	0.00	-0.00	-0.00	0.02	-0.00	-0.04	0.01	-0.02	-0.04
29	1	0.08	0.00	0.08	-0.00	-0.04	-0.03	-0.01	-0.03	-0.02
30	1	0.08	-0.00	0.08	0.00	-0.04	0.03	0.01	-0.03	0.02

31 1 0.00 0.00 -0.00 -0.02 -0.00 0.04 -0.01 -0.02 0.04  
32 1 0.00 0.00 -0.01 -0.02 0.00 -0.03 -0.01 -0.01 0.03  
33 29 0.02 0.00 -0.02 0.00 0.00 -0.00 0.00 -0.02 0.00  
34 6 -0.00 -0.00 0.00 -0.00 -0.01 -0.09 0.02 -0.03 0.01  
35 6 -0.00 -0.00 0.00 0.02 0.02 -0.10 -0.01 -0.07 0.03  
36 6 0.00 -0.00 0.00 -0.02 -0.02 -0.11 0.05 -0.02 0.02  
37 6 -0.00 -0.00 0.00 0.01 0.02 -0.15 0.01 -0.08 0.07  
38 1 0.00 -0.00 -0.00 0.03 0.03 -0.09 -0.04 -0.08 0.02  
39 6 -0.00 -0.00 0.00 -0.02 -0.02 -0.15 0.06 -0.03 0.06  
40 1 0.00 -0.00 -0.00 -0.03 -0.04 -0.09 0.07 0.00 0.01  
41 6 -0.00 -0.00 0.00 -0.01 -0.00 -0.17 0.04 -0.06 0.09  
42 1 0.00 -0.00 -0.00 0.03 0.03 -0.16 -0.01 -0.10 0.09  
43 1 -0.00 -0.00 0.00 -0.04 -0.04 -0.17 0.09 -0.02 0.07  
44 1 0.00 -0.00 -0.00 -0.01 -0.00 -0.20 0.05 -0.08 0.11  
45 6 -0.00 0.00 0.00 0.00 -0.01 0.09 -0.02 -0.03 -0.01  
46 6 0.00 0.00 0.00 0.02 -0.02 0.11 -0.05 -0.02 -0.02  
47 6 -0.00 0.00 0.00 -0.02 0.02 0.10 0.01 -0.07 -0.03  
48 6 -0.00 0.00 0.00 0.02 -0.02 0.15 -0.06 -0.03 -0.06  
49 1 0.00 0.00 -0.00 0.03 -0.04 0.09 -0.07 0.00 -0.01  
50 6 -0.00 0.00 0.00 -0.01 0.02 0.15 -0.01 -0.08 -0.07  
51 1 0.00 0.00 -0.00 -0.03 0.03 0.09 0.04 -0.08 -0.02  
52 6 -0.00 0.00 0.00 0.01 -0.00 0.17 -0.04 -0.06 -0.09  
53 1 -0.00 0.00 0.00 0.04 -0.04 0.17 -0.09 -0.02 -0.07  
54 1 0.00 0.00 -0.00 -0.03 0.03 0.16 0.01 -0.10 -0.09  
55 1 0.00 0.00 -0.00 0.01 -0.00 0.20 -0.05 -0.08 -0.11  
56 6 -0.00 -0.00 -0.00 0.00 0.00 0.09 0.00 -0.01 0.01  
57 6 -0.00 0.00 -0.00 0.02 -0.02 0.11 0.01 -0.02 0.02  
58 6 -0.00 0.00 -0.00 -0.02 0.02 0.11 -0.01 -0.01 0.01  
59 6 -0.00 0.00 -0.00 0.02 -0.03 0.16 0.01 -0.02 0.03  
60 1 -0.00 -0.00 -0.00 0.04 -0.04 0.09 0.02 -0.02 0.02  
61 6 -0.00 0.00 0.00 -0.03 0.02 0.16 -0.01 -0.01 0.02  
62 1 -0.00 -0.00 -0.00 -0.04 0.04 0.09 -0.02 -0.01 0.00  
63 6 -0.00 0.00 0.00 -0.00 -0.00 0.18 0.00 -0.02 0.04  
64 1 -0.00 0.00 -0.00 0.04 -0.05 0.17 0.02 -0.02 0.04  
65 1 -0.00 0.00 -0.00 -0.05 0.04 0.17 -0.02 -0.01 0.03  
66 1 -0.00 0.00 -0.00 -0.00 -0.01 0.21 0.00 -0.02 0.05  
67 6 -0.00 0.00 -0.00 -0.00 0.00 -0.09 -0.00 -0.01 -0.01  
68 6 -0.00 -0.00 -0.00 -0.02 -0.02 -0.11 -0.01 -0.02 -0.02  
69 6 -0.00 -0.00 -0.00 0.02 0.02 -0.11 0.01 -0.01 -0.01  
70 6 -0.00 -0.00 -0.00 -0.02 -0.03 -0.16 -0.01 -0.02 -0.03  
71 1 -0.00 0.00 -0.00 -0.04 -0.04 -0.09 -0.02 -0.02 -0.02  
72 6 -0.00 -0.00 0.00 0.03 0.02 -0.16 0.01 -0.01 -0.02  
73 1 -0.00 0.00 -0.00 0.04 0.04 -0.09 0.02 -0.01 -0.00  
74 6 -0.00 -0.00 0.00 0.00 -0.00 -0.18 -0.00 -0.02 -0.04

```

75 1 -0.00 -0.00 -0.00 -0.04 -0.05 -0.17 -0.02 -0.02 -0.04
76 1 -0.00 -0.00 -0.00 0.05 0.04 -0.17 0.02 -0.01 -0.03
77 1 -0.00 -0.00 -0.00 0.00 -0.01 -0.21 -0.00 -0.02 -0.05
78 6 -0.26 -0.00 -0.53 -0.00 0.04 0.00 -0.00 0.39 0.00
79 8 0.16 0.00 0.70 -0.00 0.02 0.00 -0.00 -0.01 0.00
80 8 -0.02 0.00 0.07 -0.00 0.03 0.00 -0.00 0.76 0.00

```

TCO<sub>2</sub>-P

-----  
Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z  
-----

```

1 7 0 -1.571500 -1.301530 -0.249150
2 7 0 -1.189832 1.565459 0.000993
3 7 0 1.894392 1.477940 0.400282
4 7 0 1.307353 -1.558818 0.046138
5 6 0 -1.493466 -2.662353 -0.363781
6 6 0 -2.816487 -3.177709 -0.669356
7 6 0 -3.668611 -2.108831 -0.691561
8 6 0 -2.876886 -0.926671 -0.403772
9 6 0 -3.364133 0.383069 -0.247704
10 6 0 -2.560167 1.522441 -0.010355
11 6 0 -3.087759 2.847784 0.244916
12 6 0 -2.016507 3.683829 0.363734
13 6 0 -0.817194 2.884915 0.181992
14 6 0 0.471082 3.462793 0.065381
15 6 0 1.691426 2.762580 -0.040421
16 6 0 2.902173 3.149308 -0.719630
17 6 0 3.760231 2.074433 -0.707238
18 6 0 3.107635 0.988936 -0.019658
19 6 0 3.520842 -0.353436 0.112456
20 6 0 2.672836 -1.481298 0.242688
21 6 0 3.185476 -2.821692 0.466431
22 6 0 2.134633 -3.684612 0.359567
23 6 0 0.961239 -2.884218 0.068725
24 6 0 -0.325291 -3.423452 -0.175388
25 1 0 -3.056088 -4.221852 -0.851096
26 1 0 -4.736524 -2.113455 -0.892736
27 1 0 -4.141119 3.097420 0.335546
28 1 0 -2.031092 4.750055 0.570452
29 1 0 3.042301 4.102608 -1.222421
30 1 0 4.726401 1.993004 -1.198255
31 1 0 4.219427 -3.065248 0.693264
32 1 0 2.144943 -4.763847 0.482459

```

33 29 0 -0.103257 -0.126670 0.240660  
34 6 0 0.582098 4.939408 -0.093990  
35 6 0 1.466830 5.669094 0.720762  
36 6 0 -0.144285 5.630385 -1.081114  
37 6 0 1.605497 7.049402 0.568011  
38 1 0 2.036213 5.141626 1.488703  
39 6 0 -0.001483 7.009775 -1.237124  
40 1 0 -0.810770 5.071218 -1.740150  
41 6 0 0.870751 7.724817 -0.410777  
42 1 0 2.288273 7.600892 1.218829  
43 1 0 -0.567890 7.528164 -2.014579  
44 1 0 0.980854 8.805014 -0.532652  
45 6 0 4.986814 -0.573874 -0.028760  
46 6 0 5.508824 -1.456321 -0.992270  
47 6 0 5.886758 0.144456 0.779445  
48 6 0 6.886944 -1.625581 -1.132025  
49 1 0 4.821923 -1.996677 -1.646005  
50 6 0 7.264815 -0.029129 0.643127  
51 1 0 5.491453 0.832223 1.529661  
52 6 0 7.769729 -0.915721 -0.312449  
53 1 0 7.274179 -2.309223 -1.891406  
54 1 0 7.947802 0.528150 1.288770  
55 1 0 8.848565 -1.050016 -0.421460  
56 6 0 -4.843144 0.575550 -0.304584  
57 6 0 -5.668208 0.007528 0.680306  
58 6 0 -5.437085 1.323327 -1.334080  
59 6 0 -7.053089 0.181095 0.634913  
60 1 0 -5.208182 -0.559626 1.492030  
61 6 0 -6.822200 1.495463 -1.380586  
62 1 0 -4.801773 1.764251 -2.105276  
63 6 0 -7.634300 0.924488 -0.396394  
64 1 0 -7.680633 -0.261624 1.412265  
65 1 0 -7.269765 2.074985 -2.191732  
66 1 0 -8.717914 1.059900 -0.432408  
67 6 0 -0.456168 -4.909099 -0.231930  
68 6 0 -1.247046 -5.594928 0.705117  
69 6 0 0.204525 -5.651694 -1.224972  
70 6 0 -1.373466 -6.984604 0.651470  
71 1 0 -1.756006 -5.027302 1.486923  
72 6 0 0.077110 -7.041003 -1.280317  
73 1 0 0.815272 -5.126555 -1.962324  
74 6 0 -0.712162 -7.712192 -0.341892  
75 1 0 -1.987358 -7.501919 1.392806  
76 1 0 0.593218 -7.601788 -2.063412



77 1 0 -0.811168 -8.799466 -0.384457  
78 6 0 -1.471937 -0.625852 2.705334  
79 8 0 1.128602 0.877519 1.299919  
80 8 0 -2.566869 -0.415327 2.902356

TCO-R

-----  
Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z  
-----

1 7 0 1.890050 -0.656799 -0.342136  
2 7 0 -0.730645 -1.881807 0.121266  
3 7 0 -2.311351 0.730388 0.349350  
4 7 0 0.507022 1.890488 0.078645  
5 6 0 2.984292 0.147231 -0.443111  
6 6 0 4.164619 -0.684899 -0.620200  
7 6 0 3.740985 -1.984853 -0.591217  
8 6 0 2.298487 -1.954955 -0.398470  
9 6 0 1.453484 -3.063597 -0.188778  
10 6 0 0.057887 -3.005014 0.051871  
11 6 0 -0.776592 -4.187446 0.163266  
12 6 0 -2.064631 -3.756939 0.271125  
13 6 0 -2.042019 -2.304010 0.209467  
14 6 0 -3.232844 -1.537472 0.109581  
15 6 0 -3.317398 -0.131947 0.015408  
16 6 0 -4.364978 0.672176 -0.552740  
17 6 0 -3.934408 1.984592 -0.560264  
18 6 0 -2.612065 2.017392 0.002587  
19 6 0 -1.709890 3.099942 0.081368  
20 6 0 -0.295886 3.010240 0.169417  
21 6 0 0.550039 4.192632 0.215997  
22 6 0 1.840669 3.772971 0.095491  
23 6 0 1.807431 2.326068 -0.010139  
24 6 0 2.961579 1.543661 -0.259082  
25 1 0 5.183092 -0.320138 -0.724928  
26 1 0 4.348899 -2.882431 -0.667600  
27 1 0 -0.420590 -5.213262 0.138512  
28 1 0 -2.957428 -4.366820 0.371222  
29 1 0 -5.290853 0.279951 -0.965388  
30 1 0 -4.449318 2.844864 -0.979991  
31 1 0 0.195320 5.214033 0.316161  
32 1 0 2.737423 4.384933 0.059958  
33 29 0 0.196676 -0.093949 0.489887

34 6 0 -4.533901 -2.252775 -0.044206  
35 6 0 -5.583887 -2.004825 0.856486  
36 6 0 -4.759621 -3.140826 -1.110655  
37 6 0 -6.818162 -2.640478 0.707628  
38 1 0 -5.419329 -1.313495 1.685675  
39 6 0 -5.994950 -3.772484 -1.262696  
40 1 0 -3.959268 -3.321599 -1.830711  
41 6 0 -7.027255 -3.527345 -0.352056  
42 1 0 -7.619285 -2.443663 1.424138  
43 1 0 -6.154726 -4.454459 -2.101354  
44 1 0 -7.993448 -4.023483 -0.470752  
45 6 0 -2.334085 4.446197 -0.078355  
46 6 0 -3.323227 4.874421 0.823652  
47 6 0 -1.993799 5.288787 -1.151340  
48 6 0 -3.941128 6.117030 0.669705  
49 1 0 -3.597152 4.225178 1.657929  
50 6 0 -2.614881 6.528825 -1.308378  
51 1 0 -1.245212 4.955530 -1.872614  
52 6 0 -3.587989 6.948824 -0.396406  
53 1 0 -4.700180 6.437726 1.387279  
54 1 0 -2.342718 7.167654 -2.152056  
55 1 0 -4.072545 7.920380 -0.519107  
56 6 0 2.092528 -4.413481 -0.217680  
57 6 0 2.631588 -4.927767 -1.407673  
58 6 0 2.178824 -5.186121 0.951982  
59 6 0 3.238974 -6.185435 -1.429094  
60 1 0 2.563476 -4.334606 -2.322246  
61 6 0 2.786461 -6.443198 0.930878  
62 1 0 1.771323 -4.786273 1.882961  
63 6 0 3.317979 -6.947101 -0.259889  
64 1 0 3.648685 -6.573699 -2.364796  
65 1 0 2.849798 -7.029820 1.850639  
66 1 0 3.793333 -7.930757 -0.276283  
67 6 0 4.277849 2.249627 -0.299664  
68 6 0 4.833153 2.776718 0.877558  
69 6 0 4.989089 2.380375 -1.502278  
70 6 0 6.069319 3.425711 0.849946  
71 1 0 4.289884 2.659159 1.817244  
72 6 0 6.225642 3.029964 -1.529598  
73 1 0 4.560621 1.973211 -2.420847  
74 6 0 6.768580 3.555382 -0.353742  
75 1 0 6.491168 3.827210 1.774594  
76 1 0 6.765582 3.128937 -2.474500  
77 1 0 7.735714 4.063379 -0.374922

78 1 0 -1.570552 0.492713 1.050415  
79 1 0 -0.450716 0.140914 1.923958  
80 6 0 2.415668 -0.623985 2.736185  
81 8 0 2.898836 0.394560 2.843688

TCO-TS1

-----  
Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z  
-----

1 7 0 -0.575803 -2.039220 -0.114582  
2 7 0 -1.958254 0.512903 -0.114462  
3 7 0 0.545661 2.182787 -0.563495  
4 7 0 1.912916 -0.434399 -0.209037  
5 6 0 0.304522 -3.076941 -0.123473  
6 6 0 -0.433643 -4.330240 -0.091319  
7 6 0 -1.761615 -4.005627 -0.085351  
8 6 0 -1.835171 -2.553934 -0.112195  
9 6 0 -3.003903 -1.768453 -0.155142  
10 6 0 -3.024021 -0.356537 -0.226511  
11 6 0 -4.237412 0.391790 -0.489408  
12 6 0 -3.893413 1.709746 -0.520435  
13 6 0 -2.464341 1.780277 -0.278868  
14 6 0 -1.767863 3.014319 -0.253087  
15 6 0 -0.373079 3.167214 -0.285798  
16 6 0 0.385228 4.334819 0.064984  
17 6 0 1.720327 4.004448 0.033228  
18 6 0 1.827772 2.622215 -0.336432  
19 6 0 2.981079 1.823165 -0.352054  
20 6 0 2.982863 0.406129 -0.379407  
21 6 0 4.196008 -0.363764 -0.607636  
22 6 0 3.841050 -1.676380 -0.552975  
23 6 0 2.409907 -1.715458 -0.292265  
24 6 0 1.704380 -2.936983 -0.187971  
25 1 0 0.006318 -5.323614 -0.077093  
26 1 0 -2.610679 -4.683282 -0.062704  
27 1 0 -5.216772 -0.044118 -0.664427  
28 1 0 -4.535194 2.559831 -0.733301  
29 1 0 -0.052905 5.282836 0.363089  
30 1 0 2.563319 4.634851 0.301036  
31 1 0 5.176011 0.053250 -0.821774  
32 1 0 4.476795 -2.544069 -0.703911  
33 29 0 -0.186720 -0.254459 0.710355

34 6 0 -2.567342 4.267334 -0.147659  
35 6 0 -3.477615 4.452313 0.908283  
36 6 0 -2.417718 5.298474 -1.091653  
37 6 0 -4.217015 5.631124 1.014940  
38 1 0 -3.591416 3.663693 1.654617  
39 6 0 -3.158804 6.476933 -0.986437  
40 1 0 -1.721446 5.161964 -1.921723  
41 6 0 -4.061021 6.647411 0.067493  
42 1 0 -4.914247 5.759702 1.846374  
43 1 0 -3.035658 7.263320 -1.735057  
44 1 0 -4.640765 7.569751 0.150657  
45 6 0 4.285716 2.537023 -0.277924  
46 6 0 5.202763 2.256016 0.750779  
47 6 0 4.619917 3.523020 -1.222931  
48 6 0 6.418388 2.937107 0.828328  
49 1 0 4.946049 1.504541 1.499916  
50 6 0 5.836728 4.203145 -1.146396  
51 1 0 3.919585 3.743236 -2.031355  
52 6 0 6.740402 3.912262 -0.120489  
53 1 0 7.115242 2.710127 1.638764  
54 1 0 6.082932 4.959607 -1.895509  
55 1 0 7.692596 4.444597 -0.059767  
56 6 0 -4.314998 -2.481202 -0.173540  
57 6 0 -4.658622 -3.332863 -1.236695  
58 6 0 -5.232604 -2.313655 0.877104  
59 6 0 -5.885718 -3.999355 -1.248481  
60 1 0 -3.957777 -3.459184 -2.064488  
61 6 0 -6.458502 -2.981913 0.867110  
62 1 0 -4.971723 -1.656888 1.709665  
63 6 0 -6.789153 -3.827160 -0.195927  
64 1 0 -6.139576 -4.652280 -2.087135  
65 1 0 -7.157371 -2.844465 1.695805  
66 1 0 -7.748857 -4.349332 -0.204703  
67 6 0 2.512118 -4.194765 -0.186430  
68 6 0 3.352393 -4.496211 0.897684  
69 6 0 2.447512 -5.097065 -1.260330  
70 6 0 4.106735 -5.671306 0.909165  
71 1 0 3.404988 -3.800053 1.737539  
72 6 0 3.203936 -6.271186 -1.250773  
73 1 0 1.804384 -4.864916 -2.111897  
74 6 0 4.034977 -6.562514 -0.165320  
75 1 0 4.751515 -5.893057 1.763064  
76 1 0 3.147242 -6.959429 -2.097683  
77 1 0 4.626124 -7.481372 -0.157329

78 1 0 0.320261 1.250461 -0.891912  
79 1 0 0.121834 0.890214 1.818783  
80 6 0 0.507575 -0.475243 2.535621  
81 8 0 1.068762 -0.314536 3.534096

\*\*\*\*\* 1 imaginary frequencies (negative Signs) \*\*\*\*\*

Diagonal vibrational polarizability:

49.8564255 29.0063974 54.7253604

Harmonic frequencies (cm<sup>-1</sup>), IR intensities (KM/Mole), Raman scattering activities (A<sup>4</sup>/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

1 2 3

A A A

Frequencies -- -484.0061 11.5591 21.9832

Red. masses -- 1.6517 6.1349 13.5009

Frc consts -- 0.2280 0.0005 0.0038

IR Inten --104.4256 0.0007 0.5297

Atom AN X Y Z X Y Z X Y Z

1 7 -0.00 -0.01 -0.01 0.00 -0.00 -0.00 -0.03 0.01 0.03  
2 7 0.01 0.01 0.02 0.00 -0.00 -0.00 -0.03 -0.01 0.03  
3 7 -0.00 -0.02 0.03 0.01 -0.00 -0.00 -0.01 -0.02 0.02  
4 7 -0.00 0.01 -0.00 0.00 0.00 -0.00 -0.01 0.01 -0.04  
5 6 -0.00 -0.00 -0.00 0.00 0.00 -0.02 -0.02 0.01 0.02  
6 6 -0.00 -0.00 0.00 0.01 -0.00 -0.01 -0.01 0.01 0.02  
7 6 -0.00 -0.01 0.00 0.01 -0.00 0.02 -0.02 -0.00 0.02  
8 6 0.00 -0.00 -0.00 0.00 -0.00 0.03 -0.03 -0.00 0.03  
9 6 0.00 0.00 0.00 0.00 -0.00 0.05 -0.03 -0.01 0.02  
10 6 0.01 0.00 0.00 0.00 -0.01 0.03 -0.03 -0.01 0.01  
11 6 0.00 -0.00 -0.00 -0.00 -0.01 0.02 -0.02 -0.01 -0.01  
12 6 -0.00 -0.00 -0.00 -0.00 -0.01 -0.02 -0.02 -0.01 -0.01  
13 6 -0.00 0.00 0.00 0.00 -0.01 -0.03 -0.02 -0.01 0.01  
14 6 -0.00 0.00 0.00 -0.00 -0.00 -0.05 -0.01 -0.02 0.01  
15 6 -0.00 -0.00 0.01 -0.00 -0.00 -0.03 -0.01 -0.02 0.02  
16 6 -0.00 -0.00 -0.00 -0.01 0.00 -0.02 -0.02 -0.02 0.03  
17 6 -0.00 -0.00 -0.00 -0.01 0.01 0.01 -0.01 -0.01 0.03  
18 6 0.00 -0.00 0.01 -0.00 0.00 0.02 -0.01 -0.01 0.02  
19 6 0.00 0.00 -0.00 0.00 0.01 0.05 -0.00 -0.00 -0.00  
20 6 0.00 -0.00 -0.00 0.00 0.01 0.03 -0.00 -0.00 -0.03  
21 6 0.00 -0.00 -0.00 0.01 0.01 0.02 -0.00 -0.01 -0.02  
22 6 -0.00 -0.00 0.00 0.00 0.01 -0.02 -0.01 -0.00 -0.02  
23 6 -0.00 0.00 0.00 0.00 0.00 -0.02 -0.02 0.01 -0.03  
24 6 -0.00 0.00 -0.00 0.00 0.00 -0.04 -0.02 0.01 -0.00  
25 1 -0.00 -0.00 0.00 0.01 0.00 -0.03 -0.01 0.01 0.01  
26 1 -0.00 -0.01 0.00 0.01 -0.01 0.04 -0.01 -0.01 0.02

27 1 0.01 -0.00 -0.00 -0.00 -0.02 0.04 -0.02 -0.00 -0.03  
28 1 -0.00 -0.00 -0.00 -0.00 -0.02 -0.04 -0.01 -0.01 -0.03  
29 1 0.00 0.00 -0.01 -0.02 0.00 -0.04 -0.02 -0.02 0.04  
30 1 -0.00 0.00 -0.01 -0.02 0.01 0.03 -0.02 -0.01 0.03  
31 1 0.00 -0.00 0.00 0.01 0.02 0.04 0.00 -0.01 -0.01  
32 1 -0.00 -0.00 0.00 0.01 0.01 -0.03 -0.02 -0.01 -0.01  
33 29 0.00 -0.02 -0.01 0.01 0.00 -0.00 -0.07 0.01 0.04  
34 6 -0.00 0.00 -0.00 -0.00 -0.00 -0.09 -0.01 -0.01 -0.00  
35 6 -0.00 0.00 -0.00 -0.02 0.03 -0.10 -0.03 -0.00 -0.02  
36 6 -0.00 0.00 -0.00 0.01 -0.03 -0.11 0.01 -0.02 -0.01  
37 6 -0.00 0.00 0.00 -0.02 0.03 -0.14 -0.03 -0.00 -0.04  
38 1 -0.00 0.00 -0.00 -0.02 0.05 -0.08 -0.04 -0.00 -0.02  
39 6 -0.00 0.00 -0.00 0.01 -0.02 -0.15 0.01 -0.02 -0.02  
40 1 -0.00 0.00 -0.00 0.02 -0.05 -0.10 0.02 -0.02 0.01  
41 6 -0.00 0.00 0.00 -0.00 0.01 -0.17 -0.01 -0.01 -0.04  
42 1 -0.00 0.00 -0.00 -0.02 0.06 -0.15 -0.04 0.00 -0.05  
43 1 -0.00 0.00 0.00 0.02 -0.04 -0.17 0.02 -0.02 -0.03  
44 1 -0.00 0.00 0.00 -0.00 0.01 -0.20 -0.01 -0.01 -0.06  
45 6 0.00 0.00 -0.00 -0.00 0.00 0.09 -0.00 -0.00 0.02  
46 6 0.00 0.00 0.00 -0.03 -0.02 0.11 -0.02 -0.02 0.03  
47 6 0.00 0.00 -0.00 0.03 0.02 0.11 0.01 0.02 0.05  
48 6 0.00 0.00 0.00 -0.03 -0.02 0.15 -0.02 -0.02 0.06  
49 1 0.00 -0.00 -0.00 -0.05 -0.03 0.09 -0.03 -0.04 0.01  
50 6 0.00 0.00 -0.00 0.03 0.01 0.16 0.00 0.02 0.09  
51 1 0.00 -0.00 -0.00 0.05 0.03 0.10 0.02 0.04 0.05  
52 6 0.00 0.00 0.00 -0.00 -0.00 0.18 -0.01 0.00 0.09  
53 1 0.00 -0.00 0.00 -0.05 -0.03 0.17 -0.03 -0.04 0.07  
54 1 0.00 0.00 -0.00 0.05 0.03 0.18 0.01 0.04 0.11  
55 1 0.00 -0.00 0.00 -0.00 -0.01 0.21 -0.01 0.00 0.12  
56 6 0.00 0.00 -0.00 0.00 -0.00 0.09 -0.03 -0.01 -0.01  
57 6 0.00 0.00 0.00 -0.03 -0.02 0.11 -0.00 -0.02 -0.01  
58 6 0.00 0.00 -0.00 0.03 0.02 0.11 -0.06 -0.00 -0.04  
59 6 0.00 0.00 0.00 -0.03 -0.02 0.15 -0.00 -0.02 -0.04  
60 1 0.00 -0.00 0.00 -0.05 -0.03 0.09 0.02 -0.03 0.01  
61 6 0.00 0.00 0.00 0.03 0.02 0.15 -0.06 -0.00 -0.06  
62 1 0.00 -0.00 0.00 0.05 0.03 0.09 -0.08 0.01 -0.04  
63 6 0.00 0.00 -0.00 -0.00 0.00 0.17 -0.03 -0.01 -0.06  
64 1 0.00 0.00 0.00 -0.05 -0.03 0.17 0.02 -0.03 -0.04  
65 1 0.00 -0.00 0.00 0.05 0.03 0.17 -0.08 0.01 -0.09  
66 1 0.00 0.00 0.00 -0.00 0.00 0.21 -0.03 -0.01 -0.09  
67 6 0.00 0.00 -0.00 0.00 0.00 -0.09 -0.03 0.01 0.01  
68 6 -0.00 0.00 0.00 0.02 -0.03 -0.11 -0.05 0.01 0.03  
69 6 -0.00 0.00 -0.00 -0.02 0.03 -0.11 -0.00 0.01 0.01  
70 6 -0.00 0.00 -0.00 0.01 -0.04 -0.15 -0.06 0.01 0.05

71	1	-0.00	0.00	0.00	0.03	-0.06	-0.09	-0.07	0.01	0.03
72	6	-0.00	0.00	-0.00	-0.02	0.03	-0.15	-0.01	0.01	0.02
73	1	-0.00	-0.00	-0.00	-0.03	0.05	-0.09	0.02	0.02	-0.01
74	6	-0.00	0.00	0.00	-0.01	-0.01	-0.17	-0.04	0.01	0.05
75	1	-0.00	0.00	0.00	0.02	-0.06	-0.17	-0.08	0.00	0.06
76	1	-0.00	0.00	0.00	-0.04	0.05	-0.17	0.01	0.01	0.02
77	1	-0.00	0.00	0.00	-0.01	-0.01	-0.21	-0.04	0.00	0.06
78	1	-0.00	0.00	-0.02	0.02	-0.00	-0.00	0.01	-0.02	0.01
79	1	0.33	-0.59	0.70	0.01	0.00	-0.01	-0.03	0.00	0.05
80	6	-0.04	0.21	-0.07	-0.00	0.00	0.00	0.38	0.04	-0.13
81	8	0.00	-0.04	0.01	-0.01	0.00	0.00	0.71	0.08	-0.32

TCO-INT1

-----  
Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

-----

1	7	0	2.138260	0.000038	-0.348918
2	7	0	0.000228	-2.004154	0.079550
3	7	0	-2.281445	-0.000041	0.381133
4	7	0	0.000151	2.004153	0.079552
5	6	0	2.933643	1.102176	-0.308894
6	6	0	4.331795	0.682800	-0.314521
7	6	0	4.331819	-0.682640	-0.314525
8	6	0	2.933683	-1.102068	-0.308900
9	6	0	2.462815	-2.423545	-0.147499
10	6	0	1.112066	-2.814653	0.037054
11	6	0	0.694081	-4.200735	0.146873
12	6	0	-0.666422	-4.202989	0.240065
13	6	0	-1.103567	-2.820046	0.167905
14	6	0	-2.469898	-2.449565	0.058963
15	6	0	-2.960082	-1.133521	-0.033977
16	6	0	-4.142765	-0.690228	-0.709510
17	6	0	-4.142793	0.690070	-0.709510
18	6	0	-2.960125	1.133411	-0.033982
19	6	0	-2.469991	2.449474	0.058952
20	6	0	-1.103674	2.820006	0.167895
21	6	0	-0.666579	4.202964	0.240050
22	6	0	0.693924	4.200758	0.146867
23	6	0	1.111960	2.814691	0.037056
24	6	0	2.462725	2.423633	-0.147491
25	1	0	5.192249	1.345948	-0.280181
26	1	0	5.192298	-1.345758	-0.280189
27	1	0	1.356373	-5.061269	0.133904

28 1 0 -1.319537 -5.064592 0.343057  
29 1 0 -4.847446 -1.348647 -1.210895  
30 1 0 -4.847501 1.348461 -1.210896  
31 1 0 -1.319726 5.064545 0.343033  
32 1 0 1.356185 5.061317 0.133898  
33 29 0 0.226533 0.000003 0.291469  
34 6 0 -3.489961 -3.519433 -0.135890  
35 6 0 -4.609036 -3.585274 0.712521  
36 6 0 -3.390617 -4.446552 -1.188774  
37 6 0 -5.590386 -4.560723 0.526944  
38 1 0 -4.696477 -2.867354 1.530737  
39 6 0 -4.374277 -5.418503 -1.377609  
40 1 0 -2.540375 -4.388061 -1.870814  
41 6 0 -5.475475 -5.481519 -0.518223  
42 1 0 -6.447434 -4.603229 1.203386  
43 1 0 -4.284513 -6.125852 -2.205616  
44 1 0 -6.244134 -6.243868 -0.665821  
45 6 0 -3.490091 3.519304 -0.135906  
46 6 0 -4.609174 3.585104 0.712499  
47 6 0 -3.390777 4.446427 -1.188790  
48 6 0 -5.590559 4.560515 0.526917  
49 1 0 -4.696593 2.867180 1.530715  
50 6 0 -4.374473 5.418340 -1.377630  
51 1 0 -2.540531 4.387967 -1.870827  
52 6 0 -5.475678 5.481316 -0.518249  
53 1 0 -6.447611 4.602990 1.203355  
54 1 0 -4.284730 6.125692 -2.205638  
55 1 0 -6.244363 6.243638 -0.665852  
56 6 0 3.498246 -3.500897 -0.138200  
57 6 0 4.258514 -3.766258 -1.288774  
58 6 0 3.748228 -4.252829 1.021650  
59 6 0 5.238392 -4.761441 -1.282397  
60 1 0 4.069095 -3.187384 -2.195294  
61 6 0 4.729139 -5.246521 1.029398  
62 1 0 3.170221 -4.045092 1.924640  
63 6 0 5.476723 -5.505020 -0.123229  
64 1 0 5.816321 -4.958808 -2.188575  
65 1 0 4.914146 -5.818136 1.942157  
66 1 0 6.244014 -6.282847 -0.117370  
67 6 0 3.498116 3.501025 -0.138184  
68 6 0 3.748063 4.252963 1.021670  
69 6 0 4.258377 3.766420 -1.288754  
70 6 0 4.728937 5.246692 1.029425  
71 1 0 3.170061 4.045201 1.924657



```

72 6 0 5.238217 4.761640 -1.282370
73 1 0 4.068984 3.187540 -2.195276
74 6 0 5.476514 5.505225 -0.123198
75 1 0 4.913920 5.818312 1.942187
76 1 0 5.816142 4.959030 -2.188546
77 1 0 6.243776 6.283079 -0.117335
78 1 0 -1.843550 -0.000032 1.318457
79 1 0 0.982961 0.000028 2.934706
80 6 0 0.041176 0.000003 2.303622
81 8 0 -1.029570 -0.000002 2.870045

```

TCO-TS2

-----  
Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

-----

```

1 7 0 1.993247 -0.804229 -0.242681
2 7 0 -0.738043 -1.824196 -0.033274
3 7 0 -2.032405 0.863105 0.102929
4 7 0 0.788833 1.844273 0.024375
5 6 0 3.153519 -0.089825 -0.238608
6 6 0 4.275235 -1.013904 -0.289686
7 6 0 3.749500 -2.275598 -0.301305
8 6 0 2.303288 -2.130865 -0.257657
9 6 0 1.363703 -3.173713 -0.142721
10 6 0 -0.034857 -3.005846 -0.020126
11 6 0 -0.962507 -4.114972 0.081504
12 6 0 -2.216385 -3.584319 0.127978
13 6 0 -2.080084 -2.142597 0.032836
14 6 0 -3.200960 -1.282750 -0.070681
15 6 0 -3.155229 0.122261 -0.150180
16 6 0 -4.200012 1.023783 -0.569603
17 6 0 -3.671847 2.295410 -0.559446
18 6 0 -2.298278 2.185525 -0.133105
19 6 0 -1.335488 3.208605 -0.033817
20 6 0 0.065243 3.022378 0.077209
21 6 0 0.990849 4.135045 0.167629
22 6 0 2.252914 3.620675 0.123342
23 6 0 2.124027 2.181450 0.028417
24 6 0 3.230527 1.309850 -0.103275
25 1 0 5.324560 -0.731314 -0.287347
26 1 0 4.287469 -3.219773 -0.310651
27 1 0 -0.685276 -5.164687 0.103504

```

28 1 0 -3.157517 -4.118489 0.216278  
29 1 0 -5.197965 0.725786 -0.881720  
30 1 0 -4.163581 3.216855 -0.861482  
31 1 0 0.706236 5.179935 0.246016  
32 1 0 3.191641 4.166514 0.137939  
33 29 0 0.203309 -0.067046 0.144463  
34 6 0 -4.557864 -1.894968 -0.180032  
35 6 0 -5.544002 -1.600838 0.776422  
36 6 0 -4.890920 -2.740074 -1.252380  
37 6 0 -6.825023 -2.146638 0.671097  
38 1 0 -5.292560 -0.946627 1.613850  
39 6 0 -6.172819 -3.282071 -1.360459  
40 1 0 -4.136195 -2.960545 -2.009965  
41 6 0 -7.143351 -2.989066 -0.397673  
42 1 0 -7.576811 -1.915284 1.429538  
43 1 0 -6.416745 -3.932213 -2.204148  
44 1 0 -8.146020 -3.414979 -0.481591  
45 6 0 -1.859027 4.603102 -0.140362  
46 6 0 -2.768128 5.091332 0.812944  
47 6 0 -1.492276 5.438547 -1.209335  
48 6 0 -3.286188 6.384024 0.709064  
49 1 0 -3.060654 4.448403 1.645864  
50 6 0 -2.013109 6.729307 -1.315987  
51 1 0 -0.801035 5.061669 -1.965828  
52 6 0 -2.909709 7.207345 -0.355587  
53 1 0 -3.985282 6.750242 1.464772  
54 1 0 -1.721950 7.363057 -2.157159  
55 1 0 -3.316035 8.218154 -0.438703  
56 6 0 1.901204 -4.567973 -0.126230  
57 6 0 2.489479 -5.119716 -1.275312  
58 6 0 1.843607 -5.344694 1.042336  
59 6 0 3.004286 -6.418112 -1.258364  
60 1 0 2.534515 -4.522439 -2.188647  
61 6 0 2.358610 -6.642602 1.059637  
62 1 0 1.396000 -4.918109 1.942598  
63 6 0 2.940039 -7.183577 -0.090804  
64 1 0 3.454266 -6.834711 -2.162842  
65 1 0 2.309853 -7.232384 1.978234  
66 1 0 3.342902 -8.199103 -0.076974  
67 6 0 4.597157 1.913603 -0.084720  
68 6 0 5.105349 2.506508 1.082546  
69 6 0 5.405633 1.883973 -1.232327  
70 6 0 6.387920 3.058479 1.100813  
71 1 0 4.486730 2.524506 1.982399

72 6 0 6.688408 2.436324 -1.214793  
73 1 0 5.016100 1.428070 -2.145155  
74 6 0 7.183418 3.025615 -0.048177  
75 1 0 6.769746 3.511632 2.018914  
76 1 0 7.302474 2.409395 -2.118276  
77 1 0 8.186988 3.457334 -0.033920  
78 1 0 -1.268314 0.532595 1.073283  
79 1 0 -0.076037 1.135297 2.805790  
80 6 0 -0.568398 0.237665 2.312117  
81 8 0 -0.831199 -0.735460 2.969718

\*\*\*\*\* 1 imaginary frequencies (negative Signs) \*\*\*\*\*

Diagonal vibrational polarizability:

61.6606347 22.8283000 56.7865780

Harmonic frequencies (cm<sup>-1</sup>), IR intensities (KM/Mole), Raman scattering activities (A<sup>4</sup>/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

1 2 3

A A A

Frequencies -- -1872.9858 12.6144 25.5990

Red. masses -- 1.0546 6.1042 6.1985

Frc consts -- 2.1798 0.0006 0.0024

IR Inten -- 1003.3357 0.0151 0.5886

Atom AN X Y Z X Y Z X Y Z

1 7 0.01 -0.00 0.01 0.00 0.00 -0.00 0.00 -0.00 0.09  
2 7 -0.01 0.00 -0.00 0.00 -0.00 -0.00 -0.00 0.00 0.09  
3 7 -0.00 0.00 -0.03 0.00 0.00 0.00 0.01 -0.00 0.07  
4 7 -0.00 0.00 -0.00 -0.00 0.00 0.00 -0.00 0.00 0.08  
5 6 -0.00 -0.01 0.00 0.00 0.00 -0.03 0.00 -0.00 0.06  
6 6 0.00 -0.00 -0.00 0.00 0.00 -0.02 0.01 -0.00 0.01  
7 6 0.00 -0.00 -0.00 0.00 0.00 0.01 0.01 -0.00 0.02  
8 6 0.00 0.00 0.00 0.00 0.00 0.02 0.00 -0.00 0.06  
9 6 -0.00 0.00 0.00 0.00 0.00 0.04 0.00 0.00 0.06  
10 6 -0.00 0.00 -0.00 0.00 -0.00 0.02 -0.00 0.00 0.08  
11 6 -0.00 -0.00 -0.00 0.01 -0.00 0.02 0.00 0.00 0.08  
12 6 -0.00 -0.00 0.00 0.01 -0.00 -0.02 -0.00 -0.00 0.08  
13 6 0.00 -0.00 0.00 0.00 -0.00 -0.02 -0.00 -0.00 0.08  
14 6 -0.00 -0.00 -0.00 0.00 -0.00 -0.04 -0.00 0.00 0.05  
15 6 -0.01 -0.01 -0.00 0.00 -0.00 -0.02 -0.00 0.00 0.05  
16 6 0.01 -0.01 -0.00 -0.00 -0.01 -0.02 -0.01 0.01 0.01  
17 6 0.01 -0.00 -0.00 -0.00 -0.01 0.02 -0.01 0.01 0.01  
18 6 0.00 0.02 -0.00 0.00 -0.00 0.03 -0.00 0.00 0.05  
19 6 -0.00 0.00 -0.00 -0.00 -0.00 0.05 -0.00 0.00 0.05  
20 6 0.00 -0.00 0.00 -0.00 0.00 0.03 -0.00 0.00 0.07

21 6 0.00 0.00 0.00 -0.00 0.00 0.02 -0.00 0.00 0.07  
22 6 -0.00 0.00 -0.00 -0.00 0.00 -0.01 -0.00 -0.00 0.07  
23 6 -0.00 -0.00 -0.00 -0.00 0.00 -0.02 -0.00 0.00 0.07  
24 6 -0.00 -0.00 0.00 0.00 0.00 -0.04 0.00 -0.00 0.05  
25 1 0.00 -0.01 -0.00 0.00 0.00 -0.03 0.01 -0.00 -0.01  
26 1 0.01 0.00 -0.00 0.00 0.00 0.03 0.01 -0.00 -0.01  
27 1 -0.00 -0.00 0.00 0.01 -0.00 0.03 0.00 0.00 0.08  
28 1 0.00 -0.01 -0.00 0.01 -0.00 -0.03 0.00 -0.00 0.07  
29 1 0.01 -0.01 0.01 -0.01 -0.02 -0.03 -0.02 0.01 -0.02  
30 1 0.02 -0.00 0.01 -0.01 -0.02 0.03 -0.02 0.01 -0.02  
31 1 0.00 0.00 -0.00 -0.01 0.00 0.04 0.00 -0.00 0.06  
32 1 -0.00 0.00 0.00 -0.00 0.00 -0.03 -0.00 -0.00 0.06  
33 29 0.00 -0.00 -0.00 0.00 -0.00 -0.00 -0.00 0.00 0.10  
34 6 -0.00 0.00 0.00 -0.00 -0.00 -0.09 -0.01 0.01 -0.01  
35 6 -0.00 -0.00 0.00 0.03 0.01 -0.12 0.04 0.00 -0.07  
36 6 0.00 0.00 0.00 -0.04 -0.01 -0.10 -0.07 0.01 -0.03  
37 6 -0.00 0.00 -0.00 0.02 0.01 -0.16 0.04 0.00 -0.14  
38 1 -0.00 -0.00 -0.00 0.06 0.01 -0.10 0.09 0.00 -0.06  
39 6 0.00 0.00 -0.00 -0.04 -0.00 -0.15 -0.08 0.01 -0.10  
40 1 0.00 -0.00 -0.00 -0.06 -0.01 -0.08 -0.11 0.01 0.01  
41 6 -0.00 0.00 -0.00 -0.01 0.00 -0.18 -0.02 0.01 -0.16  
42 1 -0.00 -0.00 -0.00 0.05 0.02 -0.18 0.08 0.00 -0.18  
43 1 0.00 -0.00 -0.00 -0.07 -0.01 -0.16 -0.12 0.01 -0.12  
44 1 0.00 -0.00 -0.00 -0.02 0.01 -0.21 -0.03 0.00 -0.21  
45 6 -0.00 0.00 0.00 0.00 -0.00 0.09 -0.01 0.00 -0.01  
46 6 0.00 0.00 0.00 -0.01 0.02 0.11 0.02 -0.03 -0.06  
47 6 -0.00 -0.00 0.00 0.02 -0.03 0.10 -0.04 0.04 -0.03  
48 6 -0.00 0.00 -0.00 -0.00 0.02 0.15 0.02 -0.03 -0.12  
49 1 0.00 0.00 -0.00 -0.02 0.05 0.10 0.05 -0.06 -0.05  
50 6 0.00 -0.00 -0.00 0.03 -0.03 0.14 -0.05 0.05 -0.09  
51 1 0.00 -0.00 -0.00 0.03 -0.05 0.08 -0.07 0.07 0.01  
52 6 -0.00 0.00 -0.00 0.01 -0.01 0.17 -0.02 0.01 -0.14  
53 1 0.00 0.00 -0.00 -0.01 0.04 0.17 0.04 -0.05 -0.16  
54 1 0.00 0.00 -0.00 0.04 -0.06 0.16 -0.08 0.08 -0.11  
55 1 0.00 0.00 -0.00 0.02 -0.01 0.20 -0.02 0.02 -0.19  
56 6 -0.00 0.00 -0.00 0.00 0.00 0.09 0.01 0.00 -0.01  
57 6 0.00 0.00 -0.00 -0.01 0.04 0.11 0.06 -0.04 -0.06  
58 6 -0.00 -0.00 0.00 0.02 -0.03 0.11 -0.04 0.05 -0.04  
59 6 -0.00 0.00 -0.00 -0.01 0.04 0.16 0.07 -0.03 -0.13  
60 1 0.00 0.00 -0.00 -0.03 0.06 0.09 0.09 -0.08 -0.04  
61 6 0.00 -0.00 -0.00 0.02 -0.03 0.15 -0.03 0.06 -0.12  
62 1 -0.00 0.00 0.00 0.04 -0.06 0.09 -0.08 0.08 -0.01  
63 6 -0.00 -0.00 -0.00 0.01 0.00 0.18 0.03 0.01 -0.16  
64 1 0.00 0.00 -0.00 -0.03 0.06 0.18 0.11 -0.07 -0.17

```

65 1 0.00 -0.00 -0.00 0.04 -0.06 0.17 -0.06 0.09 -0.14
66 1 0.00 -0.00 -0.00 0.01 0.00 0.21 0.04 0.02 -0.22
67 6 -0.00 0.00 -0.00 0.00 0.00 -0.08 0.00 -0.01 -0.01
68 6 -0.00 0.00 0.00 -0.03 -0.01 -0.10 -0.06 -0.01 -0.04
69 6 -0.00 -0.00 -0.00 0.03 0.01 -0.11 0.06 -0.01 -0.06
70 6 0.00 -0.00 0.00 -0.03 -0.01 -0.14 -0.05 -0.02 -0.11
71 1 -0.00 0.00 0.00 -0.06 -0.01 -0.08 -0.11 -0.01 -0.01
72 6 -0.00 0.00 -0.00 0.03 0.01 -0.15 0.07 -0.02 -0.13
73 1 -0.00 -0.00 -0.00 0.06 0.02 -0.09 0.11 -0.01 -0.04
74 6 0.00 0.00 -0.00 -0.00 0.00 -0.17 0.01 -0.03 -0.16
75 1 0.00 0.00 -0.00 -0.06 -0.01 -0.16 -0.10 -0.02 -0.13
76 1 -0.00 -0.00 -0.00 0.06 0.02 -0.17 0.12 -0.03 -0.16
77 1 0.00 -0.00 -0.00 -0.00 0.00 -0.20 0.01 -0.04 -0.21
78 1 -0.55 0.23 0.80 0.00 0.01 0.00 0.01 -0.01 0.08
79 1 -0.06 0.03 -0.01 0.03 -0.02 -0.00 0.03 -0.02 0.08
80 6 0.03 -0.02 -0.01 -0.01 0.00 -0.00 0.02 -0.02 0.09
81 8 -0.00 0.01 0.00 -0.06 0.01 -0.00 0.03 -0.02 0.09

```

TCO-INT2

-----  
Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z  
-----

```

1 7 0 -1.859789 0.552935 -0.283684
2 7 0 0.624821 1.969906 -0.108911
3 7 0 2.047432 -0.524981 -0.095616
4 7 0 -0.440717 -1.940597 -0.230440
5 6 0 -2.943920 -0.294846 -0.300791
6 6 0 -4.166131 0.472467 -0.354167
7 6 0 -3.808749 1.789876 -0.360394
8 6 0 -2.364005 1.834607 -0.312723
9 6 0 -1.618145 3.017734 -0.233562
10 6 0 -0.220845 3.054939 -0.123401
11 6 0 0.547664 4.276745 -0.029444
12 6 0 1.859953 3.914688 0.051120
13 6 0 1.902965 2.470247 -0.015624
14 6 0 3.088361 1.721909 -0.003225
15 6 0 3.129861 0.322194 -0.068676
16 6 0 4.354519 -0.444628 -0.144532
17 6 0 3.995889 -1.758642 -0.206361
18 6 0 2.550201 -1.802795 -0.162529
19 6 0 1.802303 -2.989027 -0.184941
20 6 0 0.401197 -3.025765 -0.181909

```

21 6 0 -0.374439 -4.245767 -0.093084  
22 6 0 -1.687303 -3.880409 -0.088574  
23 6 0 -1.721174 -2.437419 -0.184259  
24 6 0 -2.903116 -1.690454 -0.220292  
25 1 0 -5.165362 0.046434 -0.376441  
26 1 0 -4.458702 2.659942 -0.383020  
27 1 0 0.128744 5.278900 -0.027489  
28 1 0 2.727633 4.561470 0.143259  
29 1 0 5.354936 -0.022011 -0.165509  
30 1 0 4.644496 -2.626007 -0.288172  
31 1 0 0.043111 -5.245921 -0.021671  
32 1 0 -2.563872 -4.518269 -0.017456  
33 29 0 0.095918 0.011740 -0.189318  
34 6 0 4.386700 2.457944 0.068468  
35 6 0 5.194809 2.370780 1.213273  
36 6 0 4.825495 3.245327 -1.008071  
37 6 0 6.410300 3.055347 1.281326  
38 1 0 4.858733 1.762445 2.055784  
39 6 0 6.041297 3.929377 -0.941313  
40 1 0 4.205892 3.312084 -1.904949  
41 6 0 6.837171 3.836880 0.204026  
42 1 0 7.025131 2.980394 2.181563  
43 1 0 6.370404 4.533984 -1.789953  
44 1 0 7.788254 4.372095 0.256574  
45 6 0 2.539029 -4.287951 -0.197498  
46 6 0 3.308226 -4.687962 0.907171  
47 6 0 2.472420 -5.135886 -1.314841  
48 6 0 3.993816 -5.904539 0.894835  
49 1 0 3.358024 -4.038030 1.783373  
50 6 0 3.159061 -6.351900 -1.328530  
51 1 0 1.879505 -4.829814 -2.179426  
52 6 0 3.921871 -6.739998 -0.223478  
53 1 0 4.583129 -6.203438 1.765130  
54 1 0 3.100582 -6.997596 -2.208130  
55 1 0 4.458416 -7.691735 -0.233404  
56 6 0 -2.360098 4.315058 -0.252499  
57 6 0 -2.986106 4.761969 -1.426722  
58 6 0 -2.450109 5.106844 0.903176  
59 6 0 -3.684760 5.971287 -1.445312  
60 1 0 -2.917246 4.152593 -2.330501  
61 6 0 -3.148344 6.316390 0.885667  
62 1 0 -1.969295 4.763565 1.821909  
63 6 0 -3.767880 6.752142 -0.289034  
64 1 0 -4.163553 6.306636 -2.368530

```

65 1 0 -3.212037 6.919072 1.794933
66 1 0 -4.314493 7.698050 -0.303224
67 6 0 -4.202849 -2.419245 -0.099371
68 6 0 -4.863069 -2.444609 1.139542
69 6 0 -4.774408 -3.080726 -1.195192
70 6 0 -6.078579 -3.119363 1.274233
71 1 0 -4.399488 -1.939175 1.989889
72 6 0 -5.991264 -3.754400 -1.058149
73 1 0 -4.259692 -3.061634 -2.158636
74 6 0 -6.645908 -3.774203 0.176590
75 1 0 -6.583480 -3.137239 2.243272
76 1 0 -6.429940 -4.264249 -1.919457
77 1 0 -7.597075 -4.301390 0.283749
78 1 0 -0.704636 0.364498 2.518850
79 1 0 -2.473330 1.006747 2.413873
80 6 0 -1.797964 0.134917 2.588066
81 8 0 -2.210287 -0.967314 2.838826

```

TCO-INT3

-----  
Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z  
-----

```

1 7 0 1.946873 -0.255823 -0.297406
2 7 0 -0.384833 -1.972451 0.128974
3 7 0 -2.451145 0.274383 0.358538
4 7 0 0.079646 1.964800 0.056140
5 6 0 2.848024 0.750059 -0.473750
6 6 0 4.142537 0.167928 -0.786583
7 6 0 3.988668 -1.190224 -0.746191
8 6 0 2.593128 -1.448254 -0.428963
9 6 0 1.986653 -2.701130 -0.208322
10 6 0 0.611364 -2.917609 0.061188
11 6 0 0.029024 -4.240445 0.192322
12 6 0 -1.318648 -4.073304 0.305885
13 6 0 -1.586515 -2.646165 0.228589
14 6 0 -2.904833 -2.131167 0.120240
15 6 0 -3.264311 -0.769529 0.017836
16 6 0 -4.444643 -0.187435 -0.559688
17 6 0 -4.282129 1.184837 -0.563485
18 6 0 -2.998109 1.477634 0.011015
19 6 0 -2.328129 2.716602 0.112387
20 6 0 -0.923686 2.901522 0.210017

```

21 6 0 -0.321438 4.216650 0.351874  
22 6 0 1.027406 4.060848 0.229855  
23 6 0 1.273033 2.648186 0.005977  
24 6 0 2.556920 2.114358 -0.274620  
25 1 0 5.051533 0.726709 -0.991228  
26 1 0 4.750333 -1.948570 -0.905859  
27 1 0 0.582384 -5.174985 0.175636  
28 1 0 -2.071746 -4.847515 0.418215  
29 1 0 -5.271495 -0.754052 -0.979966  
30 1 0 -4.953871 1.926666 -0.987598  
31 1 0 -0.865628 5.139664 0.529429  
32 1 0 1.791589 4.830658 0.284347  
33 29 0 0.160968 -0.037346 0.486127  
34 6 0 -4.038101 -3.089968 -0.032651  
35 6 0 -5.125364 -3.042034 0.856809  
36 6 0 -4.074248 -4.018564 -1.087920  
37 6 0 -6.208971 -3.909856 0.708154  
38 1 0 -5.108214 -2.321567 1.677290  
39 6 0 -5.159775 -4.882650 -1.239791  
40 1 0 -3.247364 -4.047081 -1.800049  
41 6 0 -6.229079 -4.833818 -0.340245  
42 1 0 -7.040194 -3.865538 1.415961  
43 1 0 -5.174199 -5.593079 -2.069857  
44 1 0 -7.077706 -5.511681 -0.458884  
45 6 0 -3.200167 3.918390 -0.020802  
46 6 0 -4.288242 4.100526 0.850966  
47 6 0 -2.991129 4.865482 -1.039469  
48 6 0 -5.131567 5.205362 0.720544  
49 1 0 -4.460071 3.370514 1.644664  
50 6 0 -3.837127 5.967327 -1.172989  
51 1 0 -2.165577 4.720936 -1.738779  
52 6 0 -4.908104 6.143111 -0.291447  
53 1 0 -5.965132 5.336052 1.414779  
54 1 0 -3.663796 6.688843 -1.975042  
55 1 0 -5.568889 7.006966 -0.395607  
56 6 0 2.872259 -3.902943 -0.282994  
57 6 0 3.419689 -4.314705 -1.508245  
58 6 0 3.182124 -4.633888 0.874893  
59 6 0 4.255620 -5.431813 -1.574597  
60 1 0 3.178603 -3.753843 -2.413908  
61 6 0 4.017681 -5.750879 0.809056  
62 1 0 2.766416 -4.314053 1.832893  
63 6 0 4.556911 -6.153318 -0.416148  
64 1 0 4.670494 -5.741900 -2.536786



65 1 0 4.252966 -6.306046 1.720319  
 66 1 0 5.211283 -7.026737 -0.467732  
 67 6 0 3.710551 3.061138 -0.327400  
 68 6 0 4.732957 2.965061 0.632848  
 69 6 0 3.801102 4.046767 -1.323341  
 70 6 0 5.817900 3.844050 0.595783  
 71 1 0 4.662282 2.197994 1.408193  
 72 6 0 4.889316 4.921283 -1.359599  
 73 1 0 3.014043 4.117241 -2.077364  
 74 6 0 5.899901 4.823214 -0.398614  
 75 1 0 6.603118 3.763488 1.351475  
 76 1 0 4.950384 5.679441 -2.144255  
 77 1 0 6.750769 5.508322 -0.426171  
 78 1 0 -1.682408 0.187986 1.062973  
 79 1 0 -0.498402 0.067510 1.935027  
 80 6 0 2.707070 0.073128 2.601672  
 81 8 0 3.903165 0.187101 2.518949  
 82 1 0 2.006615 0.934280 2.485597  
 83 1 0 2.211554 -0.909359 2.798951

TCO-TS3

-----  
 Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

-----  
 1 7 0 -2.058105 0.225449 -0.528882  
 2 7 0 0.225414 1.995883 0.044641  
 3 7 0 2.361960 -0.195764 0.321536  
 4 7 0 -0.082844 -1.938768 -0.142101  
 5 6 0 -2.942105 -0.807594 -0.495798  
 6 6 0 -4.294901 -0.272821 -0.562494  
 7 6 0 -4.180050 1.088573 -0.593673  
 8 6 0 -2.754796 1.390528 -0.531073  
 9 6 0 -2.172071 2.659676 -0.326643  
 10 6 0 -0.804203 2.910227 -0.051083  
 11 6 0 -0.269263 4.245676 0.125338  
 12 6 0 1.074433 4.121231 0.315710  
 13 6 0 1.395320 2.708534 0.231500  
 14 6 0 2.735315 2.242148 0.208646  
 15 6 0 3.152083 0.901556 0.084423  
 16 6 0 4.378502 0.396161 -0.461764  
 17 6 0 4.267722 -0.977126 -0.567643  
 18 6 0 2.973139 -1.357929 -0.083396

19 6 0 2.347117 -2.619137 -0.113719  
20 6 0 0.948760 -2.853191 -0.056821  
21 6 0 0.387168 -4.189435 0.024005  
22 6 0 -0.968752 -4.061872 -0.022708  
23 6 0 -1.259697 -2.647634 -0.140648  
24 6 0 -2.577800 -2.149699 -0.282430  
25 1 0 -5.206696 -0.864128 -0.549315  
26 1 0 -4.981217 1.822804 -0.609866  
27 1 0 -0.848818 5.163222 0.090701  
28 1 0 1.792214 4.917458 0.487827  
29 1 0 5.200710 1.018558 -0.804808  
30 1 0 4.985763 -1.662951 -1.009375  
31 1 0 0.963112 -5.104888 0.121141  
32 1 0 -1.712919 -4.852247 0.007502  
33 29 0 -0.206432 0.043262 0.125096  
34 6 0 3.841764 3.243729 0.163929  
35 6 0 4.854429 3.217222 1.137813  
36 6 0 3.929660 4.191297 -0.870986  
37 6 0 5.915029 4.124244 1.090830  
38 1 0 4.797723 2.481153 1.942624  
39 6 0 4.992192 5.095011 -0.921055  
40 1 0 3.162009 4.204359 -1.647077  
41 6 0 5.986486 5.066983 0.061638  
42 1 0 6.687766 4.095546 1.862786  
43 1 0 5.048055 5.820357 -1.736325  
44 1 0 6.817076 5.775711 0.022568  
45 6 0 3.258546 -3.780171 -0.319942  
46 6 0 4.333076 -4.003479 0.558723  
47 6 0 3.093642 -4.649315 -1.413352  
48 6 0 5.208905 -5.072169 0.359259  
49 1 0 4.468459 -3.336269 1.412482  
50 6 0 3.971607 -5.715080 -1.615023  
51 1 0 2.275667 -4.472841 -2.114311  
52 6 0 5.030597 -5.931940 -0.728095  
53 1 0 6.031645 -5.236705 1.059173  
54 1 0 3.832205 -6.376128 -2.473769  
55 1 0 5.716345 -6.767776 -0.885672  
56 6 0 -3.101275 3.828877 -0.357306  
57 6 0 -3.763258 4.177571 -1.545643  
58 6 0 -3.354547 4.581863 0.801150  
59 6 0 -4.649301 5.256736 -1.577579  
60 1 0 -3.571746 3.596770 -2.450539  
61 6 0 -4.241712 5.659560 0.770133  
62 1 0 -2.856224 4.307415 1.733326

63 6 0 -4.890827 6.001478 -0.419876  
 64 1 0 -5.151378 5.518290 -2.512217  
 65 1 0 -4.432000 6.231010 1.681861  
 66 1 0 -5.585147 6.844726 -0.443991  
 67 6 0 -3.690597 -3.122580 -0.072502  
 68 6 0 -3.925989 -3.600343 1.227888  
 69 6 0 -4.516728 -3.544760 -1.123201  
 70 6 0 -4.970606 -4.496203 1.464007  
 71 1 0 -3.285967 -3.239543 2.036297  
 72 6 0 -5.559786 -4.443447 -0.882233  
 73 1 0 -4.332819 -3.171058 -2.133257  
 74 6 0 -5.787856 -4.921261 0.411293  
 75 1 0 -5.151350 -4.860799 2.478286  
 76 1 0 -6.194705 -4.772970 -1.708433  
 77 1 0 -6.603988 -5.623266 0.599320  
 78 1 0 1.572465 -0.185597 0.978971  
 79 1 0 0.081479 -0.172466 1.746135  
 80 6 0 -0.988776 -0.463769 2.836367  
 81 8 0 -1.698971 -1.445835 2.573711  
 82 1 0 -0.144509 -0.540323 3.569954  
 83 1 0 -1.383429 0.579507 2.748391

\*\*\*\*\* 1 imaginary frequencies (negative Signs) \*\*\*\*\*

Diagonal vibrational polarizability:

76.4471760 107.4372340 97.3500022

Harmonic frequencies (cm<sup>-1</sup>), IR intensities (KM/Mole), Raman scattering activities (A<sup>4</sup>/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

1 2 3

A A A

Frequencies -- -585.4857 13.9306 24.8941

Red. masses -- 1.3681 6.1101 7.9648

Frc consts -- 0.2763 0.0007 0.0029

IR Inten -- 204.0537 0.0490 2.8801

Atom AN X Y Z X Y Z X Y Z

1 7 0.01 -0.00 -0.00 0.00 0.01 -0.01 0.02 -0.02 -0.01  
 2 7 -0.00 0.01 -0.02 0.00 0.00 -0.00 0.01 -0.01 0.01  
 3 7 0.01 -0.00 -0.00 0.00 0.01 -0.00 0.01 -0.01 0.02  
 4 7 -0.01 -0.01 -0.02 0.00 0.00 -0.01 0.01 -0.01 0.03  
 5 6 0.00 -0.00 -0.00 0.00 0.01 -0.03 0.02 -0.02 -0.01  
 6 6 0.00 -0.00 0.00 0.00 0.00 -0.02 0.02 -0.02 -0.01  
 7 6 0.00 0.00 -0.00 -0.00 0.00 0.01 0.02 -0.02 -0.01  
 8 6 0.00 0.00 -0.00 -0.00 0.01 0.02 0.02 -0.02 -0.00  
 9 6 -0.00 0.00 -0.00 -0.00 0.00 0.04 0.01 -0.02 0.00

10 6 -0.00 0.01 -0.01 0.00 0.00 0.02 0.01 -0.01 0.01  
11 6 0.00 0.00 0.00 0.00 0.00 0.02 0.00 -0.01 0.01  
12 6 -0.00 0.00 0.00 0.01 0.00 -0.01 0.00 -0.01 0.01  
13 6 -0.00 -0.00 -0.01 0.01 0.00 -0.02 0.01 -0.01 0.01  
14 6 -0.00 -0.00 -0.00 0.01 0.00 -0.04 0.01 -0.01 0.01  
15 6 0.00 -0.01 -0.00 0.00 0.00 -0.02 0.01 -0.01 0.01  
16 6 0.01 -0.00 -0.00 0.00 -0.01 -0.01 0.00 -0.01 -0.00  
17 6 0.01 -0.00 -0.00 0.00 -0.02 0.02 0.01 -0.01 -0.00  
18 6 0.00 0.01 -0.00 0.00 -0.00 0.02 0.01 -0.01 0.01  
19 6 0.00 0.00 -0.00 0.00 -0.00 0.04 0.01 -0.01 0.01  
20 6 -0.00 0.00 -0.00 -0.00 -0.00 0.02 0.01 -0.01 0.03  
21 6 0.00 0.00 0.00 -0.00 0.00 0.01 0.02 -0.01 0.03  
22 6 -0.00 -0.00 0.00 -0.00 0.00 -0.02 0.02 -0.01 0.03  
23 6 -0.00 -0.01 -0.01 0.00 0.00 -0.03 0.01 -0.02 0.03  
24 6 -0.00 -0.00 -0.01 0.00 0.00 -0.05 0.02 -0.02 0.01  
25 1 0.00 -0.00 -0.00 0.00 0.00 -0.04 0.02 -0.02 -0.02  
26 1 0.01 0.00 -0.00 -0.00 0.00 0.03 0.02 -0.02 -0.01  
27 1 0.00 0.01 0.01 0.00 0.00 0.04 0.00 -0.01 0.01  
28 1 0.00 -0.00 0.01 0.01 0.00 -0.03 0.00 -0.01 0.01  
29 1 0.01 -0.00 -0.00 0.00 -0.02 -0.03 -0.00 -0.00 -0.01  
30 1 0.01 0.00 -0.00 0.00 -0.03 0.03 0.00 -0.00 -0.01  
31 1 0.00 0.00 0.00 -0.01 0.00 0.03 0.02 -0.01 0.02  
32 1 0.00 -0.01 0.00 -0.00 0.00 -0.03 0.02 -0.02 0.03  
33 29 -0.00 0.00 0.01 0.00 0.00 -0.01 0.00 -0.01 0.03  
34 6 -0.00 -0.00 0.00 0.00 0.00 -0.08 0.01 -0.01 0.00  
35 6 -0.00 -0.00 -0.00 0.03 0.02 -0.11 0.01 -0.01 -0.00  
36 6 -0.00 -0.00 0.00 -0.03 -0.01 -0.10 0.00 -0.01 0.01  
37 6 -0.00 -0.00 -0.00 0.03 0.02 -0.15 0.01 -0.01 -0.01  
38 1 -0.00 -0.00 -0.00 0.05 0.03 -0.10 0.02 -0.01 -0.00  
39 6 -0.00 -0.00 0.00 -0.03 -0.01 -0.14 0.00 -0.01 0.00  
40 1 -0.00 -0.00 0.00 -0.05 -0.02 -0.08 -0.00 -0.00 0.01  
41 6 -0.00 -0.00 0.00 -0.00 0.01 -0.17 0.01 -0.01 -0.00  
42 1 -0.00 -0.00 -0.00 0.05 0.03 -0.17 0.02 -0.02 -0.01  
43 1 -0.00 -0.00 -0.00 -0.05 -0.02 -0.15 -0.00 -0.00 0.00  
44 1 0.00 -0.00 -0.00 -0.00 0.01 -0.20 0.01 -0.01 -0.01  
45 6 -0.00 0.00 0.00 0.01 -0.01 0.09 0.01 -0.01 -0.02  
46 6 -0.00 0.00 -0.00 -0.02 0.01 0.12 0.03 -0.01 -0.04  
47 6 -0.00 0.00 0.00 0.03 -0.03 0.10 -0.01 0.00 -0.02  
48 6 -0.00 0.00 -0.00 -0.01 0.01 0.17 0.03 -0.01 -0.07  
49 1 0.00 0.00 -0.00 -0.04 0.03 0.11 0.05 -0.02 -0.04  
50 6 -0.00 0.00 0.00 0.04 -0.04 0.15 -0.01 0.01 -0.05  
51 1 0.00 0.00 -0.00 0.05 -0.05 0.08 -0.02 0.01 -0.00  
52 6 -0.00 0.00 0.00 0.02 -0.02 0.18 0.01 0.00 -0.08  
53 1 -0.00 0.00 -0.00 -0.03 0.02 0.19 0.05 -0.01 -0.09

54 1 -0.00 0.00 -0.00 0.06 -0.06 0.16 -0.03 0.02 -0.05  
 55 1 0.00 0.00 -0.00 0.02 -0.02 0.22 0.01 0.01 -0.10  
 56 6 -0.00 0.00 0.00 -0.01 0.00 0.09 0.00 -0.02 0.01  
 57 6 -0.00 0.00 0.00 -0.03 0.03 0.11 0.01 -0.01 0.01  
 58 6 -0.00 0.00 -0.00 0.02 -0.03 0.12 -0.00 -0.03 0.01  
 59 6 -0.00 0.00 0.00 -0.04 0.03 0.17 -0.00 -0.02 0.02  
 60 1 0.00 0.00 0.00 -0.05 0.06 0.09 0.01 -0.01 0.00  
 61 6 -0.00 0.00 0.00 0.02 -0.03 0.17 -0.01 -0.04 0.02  
 62 1 0.00 0.00 -0.00 0.04 -0.06 0.10 -0.00 -0.04 0.01  
 63 6 -0.00 0.00 0.00 -0.01 0.00 0.19 -0.01 -0.03 0.02  
 64 1 -0.00 0.00 -0.00 -0.06 0.06 0.18 0.00 -0.01 0.02  
 65 1 0.00 0.00 -0.00 0.04 -0.06 0.19 -0.01 -0.05 0.03  
 66 1 -0.00 0.00 -0.00 -0.01 -0.00 0.23 -0.01 -0.04 0.03  
 67 6 -0.00 -0.00 -0.00 0.00 0.00 -0.08 0.02 -0.02 0.01  
 68 6 -0.00 -0.00 -0.00 -0.03 -0.00 -0.09 0.00 -0.01 0.01  
 69 6 -0.00 -0.00 -0.00 0.03 0.00 -0.11 0.03 -0.03 0.00  
 70 6 -0.00 -0.00 -0.00 -0.04 -0.01 -0.12 0.01 -0.01 0.00  
 71 1 -0.00 -0.01 -0.00 -0.06 -0.01 -0.07 -0.01 0.00 0.01  
 72 6 -0.00 -0.00 0.00 0.02 0.00 -0.14 0.03 -0.03 -0.00  
 73 1 0.00 -0.00 0.00 0.06 0.01 -0.10 0.04 -0.03 -0.00  
 74 6 -0.00 -0.00 -0.00 -0.01 -0.00 -0.14 0.02 -0.02 -0.00  
 75 1 -0.00 -0.00 -0.00 -0.07 -0.01 -0.13 -0.00 -0.00 0.01  
 76 1 -0.00 -0.00 0.00 0.05 0.00 -0.16 0.04 -0.04 -0.01  
 77 1 -0.00 -0.00 -0.00 -0.02 -0.00 -0.17 0.02 -0.02 -0.00  
 78 1 -0.05 0.01 -0.01 0.00 0.02 -0.00 0.01 -0.01 0.02  
 79 1 0.81 0.26 -0.39 -0.01 -0.00 -0.01 0.02 0.02 0.02  
 80 6 -0.12 -0.05 0.11 -0.03 0.00 -0.02 -0.01 0.13 0.03  
 81 8 0.02 0.02 0.00 -0.04 0.01 -0.04 -0.41 0.47 -0.16  
 82 1 0.07 -0.03 -0.12 -0.04 -0.01 -0.02 0.00 -0.38 -0.04  
 83 1 0.09 -0.02 -0.24 -0.01 0.01 -0.02 0.38 0.30 0.30

TCO-INT4

-----  
 Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

-----  
 1 7 0 -0.276075 2.153913 -0.056800  
 2 7 0 1.941099 0.279035 -0.161303  
 3 7 0 0.212377 -2.196939 -0.690413  
 4 7 0 -2.005770 -0.195936 -0.172113  
 5 6 0 -1.467810 2.817216 -0.063402  
 6 6 0 -1.218333 4.245899 0.010298  
 7 6 0 0.138466 4.410175 0.038735

8 6 0 0.722774 3.082484 -0.022306  
9 6 0 2.095655 2.776416 -0.073497  
10 6 0 2.626258 1.474021 -0.203836  
11 6 0 4.028225 1.224517 -0.471739  
12 6 0 4.177348 -0.125225 -0.579441  
13 6 0 2.867960 -0.717343 -0.377940  
14 6 0 2.670601 -2.119034 -0.419420  
15 6 0 1.429853 -2.776635 -0.443215  
16 6 0 1.157291 -4.132965 -0.058070  
17 6 0 -0.207510 -4.295429 -0.011385  
18 6 0 -0.815888 -3.046714 -0.373113  
19 6 0 -2.172905 -2.701496 -0.300103  
20 6 0 -2.687714 -1.381629 -0.302229  
21 6 0 -4.105298 -1.116957 -0.485430  
22 6 0 -4.263480 0.234544 -0.454724  
23 6 0 -2.945995 0.806242 -0.241007  
24 6 0 -2.729094 2.198342 -0.144915  
25 1 0 -1.981941 5.018198 0.040476  
26 1 0 0.693815 5.342103 0.097526  
27 1 0 4.788193 1.990455 -0.596465  
28 1 0 5.082004 -0.676837 -0.818080  
29 1 0 1.918891 -4.854079 0.223774  
30 1 0 -0.757565 -5.173875 0.313022  
31 1 0 -4.866155 -1.872114 -0.660682  
32 1 0 -5.180451 0.801203 -0.588097  
33 29 0 -0.028936 0.282162 0.534187  
34 6 0 3.870679 -2.998036 -0.338015  
35 6 0 4.773098 -2.879621 0.734060  
36 6 0 4.107642 -3.984919 -1.310264  
37 6 0 5.884020 -3.719179 0.826047  
38 1 0 4.584211 -2.129394 1.504293  
39 6 0 5.220769 -4.822856 -1.219899  
40 1 0 3.414554 -4.082370 -2.148559  
41 6 0 6.112809 -4.692315 -0.151648  
42 1 0 6.570817 -3.618304 1.669862  
43 1 0 5.394857 -5.578252 -1.989991  
44 1 0 6.983222 -5.348809 -0.079843  
45 6 0 -3.131521 -3.830049 -0.142799  
46 6 0 -4.006832 -3.877424 0.956995  
47 6 0 -3.164297 -4.883039 -1.073531  
48 6 0 -4.892206 -4.944187 1.116825  
49 1 0 -3.973459 -3.073866 1.695164  
50 6 0 -4.052105 -5.948814 -0.914876  
51 1 0 -2.493873 -4.852103 -1.935005

52 6 0 -4.919245 -5.982696 0.180881  
53 1 0 -5.559765 -4.968739 1.981523  
54 1 0 -4.070526 -6.753789 -1.653590  
55 1 0 -5.613447 -6.817071 0.306197  
56 6 0 3.061113 3.914652 -0.037608  
57 6 0 3.098627 4.863786 -1.072319  
58 6 0 3.955092 4.054461 1.036845  
59 6 0 4.004821 5.925681 -1.032856  
60 1 0 2.416443 4.755645 -1.918150  
61 6 0 4.859851 5.117233 1.077838  
62 1 0 3.929879 3.322321 1.846783  
63 6 0 4.887478 6.056498 0.043029  
64 1 0 4.025131 6.651357 -1.849602  
65 1 0 5.544267 5.213913 1.924154  
66 1 0 5.596057 6.887587 0.074222  
67 6 0 -3.928617 3.088762 -0.152408  
68 6 0 -4.839001 3.066606 0.916872  
69 6 0 -4.167529 3.965968 -1.222681  
70 6 0 -5.958460 3.901306 0.916731  
71 1 0 -4.656993 2.390360 1.754846  
72 6 0 -5.288314 4.799362 -1.224404  
73 1 0 -3.469508 3.982715 -2.062426  
74 6 0 -6.186799 4.770228 -0.154148  
75 1 0 -6.653912 3.875160 1.759169  
76 1 0 -5.462832 5.471301 -2.068293  
77 1 0 -7.063271 5.422603 -0.154934  
78 1 0 0.081239 -1.251556 -1.027343  
79 1 0 0.848971 -1.577297 3.663479  
80 6 0 1.118603 -1.277722 2.626981  
81 8 0 -0.021822 -0.951575 1.924457  
82 1 0 1.852409 -0.445344 2.725409  
83 1 0 1.670575 -2.142425 2.195029

TCO-TS4

-----  
Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z  
-----

1 7 0 0.050181 2.205698 -0.078778  
2 7 0 1.948844 -0.009925 -0.015703  
3 7 0 -0.108567 -2.229611 -0.436934  
4 7 0 -1.988982 0.091794 -0.030805  
5 6 0 -1.038304 3.021806 -0.141170

6 6 0 -0.579006 4.397632 -0.213190  
7 6 0 0.790100 4.364069 -0.199882  
8 6 0 1.178499 2.967238 -0.122121  
9 6 0 2.486352 2.440577 -0.086102  
10 6 0 2.814102 1.062779 -0.077642  
11 6 0 4.170535 0.580093 -0.237848  
12 6 0 4.106796 -0.779995 -0.279427  
13 6 0 2.708311 -1.155635 -0.154848  
14 6 0 2.313651 -2.517713 -0.287748  
15 6 0 1.007510 -3.014475 -0.440109  
16 6 0 0.529792 -4.370409 -0.548370  
17 6 0 -0.849763 -4.338777 -0.526215  
18 6 0 -1.258488 -2.962781 -0.407087  
19 6 0 -2.526731 -2.389634 -0.219584  
20 6 0 -2.826084 -1.001189 -0.102308  
21 6 0 -4.205292 -0.540720 -0.191542  
22 6 0 -4.178774 0.819442 -0.193687  
23 6 0 -2.784772 1.213154 -0.089597  
24 6 0 -2.373251 2.568026 -0.117201  
25 1 0 -1.219371 5.274175 -0.261393  
26 1 0 1.473350 5.208270 -0.234125  
27 1 0 5.050730 1.206669 -0.348538  
28 1 0 4.926733 -1.474185 -0.437191  
29 1 0 1.163584 -5.250084 -0.616216  
30 1 0 -1.525219 -5.188388 -0.574227  
31 1 0 -5.073605 -1.184407 -0.296208  
32 1 0 -5.019632 1.499841 -0.291371  
33 29 0 0.020663 0.416560 0.624739  
34 6 0 3.395711 -3.548306 -0.269488  
35 6 0 4.161951 -3.747808 0.890813  
36 6 0 3.655007 -4.346209 -1.395203  
37 6 0 5.162836 -4.720410 0.923970  
38 1 0 3.959828 -3.133240 1.770611  
39 6 0 4.657350 -5.318638 -1.362738  
40 1 0 3.071477 -4.189324 -2.305048  
41 6 0 5.413615 -5.509087 -0.202900  
42 1 0 5.747098 -4.865977 1.835773  
43 1 0 4.852253 -5.926142 -2.249873  
44 1 0 6.197518 -6.269724 -0.177423  
45 6 0 -3.667837 -3.351275 -0.153189  
46 6 0 -4.414259 -3.483020 1.029595  
47 6 0 -4.004389 -4.151803 -1.256630  
48 6 0 -5.471370 -4.391649 1.105518  
49 1 0 -4.151530 -2.867839 1.892764



50 6 0 -5.062829 -5.060256 -1.180894  
 51 1 0 -3.437339 -4.046192 -2.184143  
 52 6 0 -5.799078 -5.183263 0.000644  
 53 1 0 -6.039610 -4.485084 2.034160  
 54 1 0 -5.317361 -5.669907 -2.051322  
 55 1 0 -6.627149 -5.893561 0.060141  
 56 6 0 3.615550 3.417564 -0.103927  
 57 6 0 3.836226 4.243462 -1.218234  
 58 6 0 4.477796 3.529715 0.999176  
 59 6 0 4.891242 5.158514 -1.228915  
 60 1 0 3.178443 4.153917 -2.085348  
 61 6 0 5.531870 4.445470 0.989368  
 62 1 0 4.310113 2.893812 1.871072  
 63 6 0 5.741814 5.263090 -0.124753  
 64 1 0 5.052878 5.788844 -2.106766  
 65 1 0 6.190142 4.523214 1.858071  
 66 1 0 6.567012 5.979130 -0.132955  
 67 6 0 -3.440546 3.613427 -0.149091  
 68 6 0 -4.276448 3.812988 0.961605  
 69 6 0 -3.622979 4.419719 -1.284088  
 70 6 0 -5.269423 4.794529 0.938010  
 71 1 0 -4.136964 3.192586 1.849487  
 72 6 0 -4.616950 5.400677 -1.308507  
 73 1 0 -2.983268 4.264193 -2.155490  
 74 6 0 -5.442812 5.591508 -0.197203  
 75 1 0 -5.908477 4.939745 1.812393  
 76 1 0 -4.749939 6.015325 -2.202158  
 77 1 0 -6.220255 6.358967 -0.216000  
 78 1 0 -0.102042 -1.341414 0.037489  
 79 1 0 0.542373 -1.597922 3.747746  
 80 6 0 0.865696 -1.377153 2.708290  
 81 8 0 -0.183985 -0.815185 2.006460  
 82 1 0 1.763495 -0.725598 2.788924  
 83 1 0 1.209474 -2.345797 2.280287

\*\*\*\*\* 1 imaginary frequencies (negative Signs) \*\*\*\*\*

Diagonal vibrational polarizability:

20.8432772 25.6343154 67.2658063

Harmonic frequencies (cm<sup>-1</sup>), IR intensities (KM/Mole), Raman scattering  
 activities (A<sup>4</sup>/AMU), depolarization ratios for plane and unpolarized  
 incident light, reduced masses (AMU), force constants (mDyne/A),  
 and normal coordinates:

1 2 3

A A A

Frequencies -- -71.7778 11.9334 27.5563

Red. masses -- 14.7637 6.0938 5.5618

Frc consts -- 0.0448 0.0005 0.0025

IR Inten -- 1.3807 0.0009 0.5509

Atom AN X Y Z X Y Z X Y Z

1	7	0.00	-0.01	-0.05	0.01	0.00	-0.00	0.00	-0.01	-0.07
2	7	0.02	0.02	0.01	-0.00	-0.00	0.00	0.00	0.00	-0.08
3	7	-0.09	0.17	0.11	-0.00	-0.00	-0.00	-0.00	0.01	-0.07
4	7	-0.04	-0.00	0.01	-0.00	0.00	-0.01	-0.00	-0.00	-0.08
5	6	0.00	0.00	-0.05	0.01	0.00	0.02	0.01	-0.01	-0.05
6	6	-0.00	0.00	-0.07	0.01	0.00	0.02	0.01	-0.01	-0.01
7	6	-0.00	0.00	-0.07	0.01	0.01	-0.02	0.01	-0.02	-0.01
8	6	-0.01	-0.01	-0.06	0.01	0.00	-0.02	0.00	-0.01	-0.05
9	6	-0.01	0.01	-0.04	0.00	0.00	-0.04	0.00	-0.00	-0.05
10	6	-0.00	0.02	-0.03	0.00	-0.00	-0.02	0.00	0.00	-0.07
11	6	-0.01	0.04	-0.04	0.00	-0.01	-0.02	0.00	0.00	-0.09
12	6	0.01	0.05	-0.02	0.00	-0.01	0.02	0.00	0.00	-0.09
13	6	0.02	0.05	0.01	-0.00	-0.01	0.03	0.00	0.00	-0.07
14	6	-0.01	0.05	0.01	-0.01	-0.00	0.05	-0.00	0.01	-0.05
15	6	-0.06	0.11	0.00	-0.01	-0.00	0.02	-0.01	0.01	-0.05
16	6	-0.04	0.07	-0.14	-0.02	-0.01	0.02	-0.01	0.03	-0.02
17	6	-0.03	0.07	-0.14	-0.02	-0.01	-0.02	-0.01	0.03	-0.02
18	6	-0.06	0.12	0.00	-0.01	-0.01	-0.03	-0.01	0.01	-0.05
19	6	-0.04	0.04	0.01	-0.01	-0.00	-0.05	-0.01	0.01	-0.05
20	6	-0.06	0.01	0.01	-0.00	0.00	-0.03	-0.00	0.00	-0.07
21	6	-0.05	0.02	-0.01	-0.01	0.01	-0.02	-0.00	0.00	-0.09
22	6	-0.04	0.03	-0.03	-0.00	0.01	0.02	-0.00	0.00	-0.09
23	6	-0.02	0.02	-0.02	-0.00	0.00	0.02	-0.00	0.00	-0.07
24	6	-0.01	0.02	-0.04	0.00	0.00	0.04	0.00	-0.00	-0.05
25	1	-0.00	0.00	-0.08	0.01	0.00	0.03	0.01	-0.02	0.01
26	1	0.00	0.00	-0.09	0.01	0.01	-0.03	0.01	-0.02	0.01
27	1	-0.02	0.05	-0.07	0.00	-0.01	-0.03	-0.00	0.00	-0.09
28	1	0.02	0.06	-0.02	0.00	-0.01	0.04	0.00	0.00	-0.09
29	1	-0.02	0.03	-0.25	-0.03	-0.01	0.03	-0.02	0.03	0.00
30	1	-0.02	0.03	-0.25	-0.02	-0.01	-0.04	-0.02	0.03	0.00
31	1	-0.06	0.02	-0.01	-0.01	0.01	-0.04	-0.00	0.00	-0.09
32	1	-0.03	0.05	-0.06	-0.00	0.01	0.03	-0.00	0.00	-0.09
33	29	0.09	-0.23	0.31	-0.00	0.00	-0.00	0.01	-0.02	-0.05
34	6	-0.02	0.02	-0.01	-0.01	0.00	0.09	-0.00	0.02	0.01
35	6	-0.03	0.03	-0.03	0.02	-0.01	0.12	0.03	-0.03	0.07
36	6	-0.01	-0.00	-0.00	-0.04	0.02	0.10	-0.04	0.07	0.01
37	6	-0.03	0.02	-0.04	0.02	-0.00	0.16	0.02	-0.02	0.14
38	1	-0.03	0.05	-0.03	0.04	-0.03	0.11	0.06	-0.07	0.07
39	6	-0.01	-0.01	-0.02	-0.04	0.03	0.14	-0.04	0.08	0.08
40	1	-0.00	-0.01	0.01	-0.06	0.04	0.08	-0.06	0.11	-0.04

41 6 -0.02 -0.01 -0.03 -0.01 0.02 0.17 -0.01 0.04 0.14  
42 1 -0.04 0.02 -0.05 0.04 -0.01 0.18 0.05 -0.05 0.19  
43 1 -0.01 -0.03 -0.01 -0.06 0.05 0.15 -0.07 0.12 0.08  
44 1 -0.03 -0.02 -0.04 -0.02 0.02 0.20 -0.02 0.04 0.20  
45 6 -0.01 0.03 -0.01 -0.00 -0.01 -0.09 -0.01 0.01 0.01  
46 6 -0.01 0.04 -0.03 0.00 0.02 -0.12 0.00 -0.04 0.07  
47 6 0.01 0.01 -0.00 -0.00 -0.04 -0.10 -0.03 0.07 0.01  
48 6 0.00 0.03 -0.03 0.01 0.02 -0.16 -0.00 -0.03 0.14  
49 1 -0.03 0.06 -0.03 0.00 0.05 -0.11 0.02 -0.09 0.07  
50 6 0.02 0.00 -0.01 0.00 -0.05 -0.14 -0.04 0.08 0.08  
51 1 0.01 -0.00 0.01 -0.00 -0.06 -0.08 -0.04 0.12 -0.04  
52 6 0.02 0.01 -0.02 0.01 -0.02 -0.17 -0.02 0.03 0.14  
53 1 0.00 0.05 -0.05 0.01 0.04 -0.18 0.01 -0.07 0.19  
54 1 0.03 -0.01 -0.01 0.00 -0.07 -0.15 -0.05 0.13 0.08  
55 1 0.03 0.01 -0.03 0.01 -0.02 -0.20 -0.03 0.04 0.20  
56 6 -0.02 0.01 -0.03 0.00 0.00 -0.09 0.01 -0.01 0.01  
57 6 -0.01 -0.00 -0.02 0.01 0.04 -0.11 0.03 -0.07 0.05  
58 6 -0.02 0.03 -0.03 -0.01 -0.03 -0.11 -0.00 0.05 0.04  
59 6 -0.00 -0.00 -0.01 0.01 0.04 -0.15 0.04 -0.08 0.12  
60 1 -0.01 -0.01 -0.03 0.02 0.07 -0.09 0.04 -0.12 0.03  
61 6 -0.01 0.02 -0.01 -0.00 -0.03 -0.15 0.01 0.05 0.10  
62 1 -0.03 0.04 -0.03 -0.01 -0.06 -0.09 -0.02 0.10 0.01  
63 6 -0.01 0.01 -0.00 0.01 0.00 -0.17 0.03 -0.02 0.14  
64 1 0.00 -0.02 0.00 0.02 0.07 -0.17 0.05 -0.13 0.15  
65 1 -0.02 0.03 -0.01 -0.01 -0.06 -0.17 -0.00 0.09 0.12  
66 1 -0.00 0.01 0.01 0.01 0.00 -0.21 0.04 -0.02 0.19  
67 6 -0.01 0.02 -0.03 0.00 -0.00 0.09 0.00 -0.01 0.01  
68 6 -0.02 0.03 -0.02 -0.03 0.01 0.11 -0.04 0.03 0.04  
69 6 0.00 0.01 -0.02 0.04 -0.01 0.11 0.04 -0.06 0.05  
70 6 -0.02 0.03 -0.00 -0.03 0.01 0.15 -0.04 0.02 0.10  
71 1 -0.02 0.04 -0.03 -0.06 0.02 0.09 -0.07 0.07 0.01  
72 6 0.00 0.01 -0.00 0.04 -0.01 0.15 0.04 -0.08 0.11  
73 1 0.01 0.00 -0.02 0.07 -0.02 0.09 0.07 -0.09 0.03  
74 6 -0.01 0.01 0.00 0.01 -0.00 0.17 -0.00 -0.04 0.14  
75 1 -0.02 0.03 0.00 -0.06 0.02 0.17 -0.07 0.05 0.12  
76 1 0.01 -0.01 0.01 0.07 -0.02 0.17 0.07 -0.12 0.14  
77 1 -0.01 0.01 0.02 0.01 -0.00 0.21 -0.01 -0.05 0.19  
78 1 0.09 -0.11 -0.38 0.02 0.01 0.00 0.01 -0.01 -0.10  
79 1 0.11 0.00 -0.15 0.02 0.02 0.01 0.01 0.01 -0.08  
80 6 0.13 0.00 -0.16 0.02 0.02 0.01 0.01 0.00 -0.09  
81 8 0.08 -0.11 -0.24 0.02 0.01 -0.00 0.01 -0.01 -0.09  
82 1 0.05 0.07 -0.08 0.01 0.02 0.01 0.01 0.00 -0.08  
83 1 0.25 0.06 -0.19 0.03 0.03 0.00 0.02 0.01 -0.10

TCO-P

-----  
Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z  
-----

1	7	0	2.195934	0.000005	-0.161703
2	7	0	0.166485	-2.028392	-0.198126
3	7	0	-1.837311	-0.000005	-0.456302
4	7	0	0.166474	2.028391	-0.198125
5	6	0	3.015324	1.102206	-0.106139
6	6	0	4.398667	0.681444	-0.028523
7	6	0	4.398671	-0.681424	-0.028525
8	6	0	3.015330	-1.102193	-0.106141
9	6	0	2.603991	-2.440542	-0.053721
10	6	0	1.262090	-2.847238	-0.068000
11	6	0	0.834538	-4.226015	0.035304
12	6	0	-0.527817	-4.223726	-0.017623
13	6	0	-0.939490	-2.847287	-0.192686
14	6	0	-2.268007	-2.438369	-0.368643
15	6	0	-2.649474	-1.102946	-0.567525
16	6	0	-4.006245	-0.683520	-0.840721
17	6	0	-4.006248	0.683500	-0.840722
18	6	0	-2.649480	1.102933	-0.567527
19	6	0	-2.268019	2.438357	-0.368647
20	6	0	-0.939503	2.847281	-0.192687
21	6	0	-0.527838	4.223722	-0.017624
22	6	0	0.834518	4.226018	0.035306
23	6	0	1.262077	2.847244	-0.067996
24	6	0	2.603979	2.440554	-0.053716
25	1	0	5.250742	1.351691	0.040469
26	1	0	5.250749	-1.351667	0.040465
27	1	0	1.498650	-5.079277	0.138890
28	1	0	-1.200350	-5.074062	0.044995
29	1	0	-4.844496	-1.352491	-1.012090
30	1	0	-4.844502	1.352466	-1.012092
31	1	0	-1.200374	5.074055	0.044993
32	1	0	1.498625	5.079283	0.138893
33	29	0	0.175346	0.000000	-0.253425
34	6	0	-3.354152	-3.458105	-0.285211
35	6	0	-4.283993	-3.389331	0.767544
36	6	0	-3.473993	-4.488103	-1.231098
37	6	0	-5.305070	-4.335816	0.872019
38	1	0	-4.200409	-2.583612	1.501508
39	6	0	-4.497796	-5.432606	-1.125948

40 1 0 -2.762947 -4.538221 -2.058516  
41 6 0 -5.414203 -5.360462 -0.072977  
42 1 0 -6.017635 -4.272664 1.697927  
43 1 0 -4.582899 -6.225438 -1.873111  
44 1 0 -6.214211 -6.100135 0.009235  
45 6 0 -3.354167 3.458089 -0.285218  
46 6 0 -4.284008 3.389315 0.767538  
47 6 0 -3.474013 4.488084 -1.231109  
48 6 0 -5.305089 4.335796 0.872008  
49 1 0 -4.200421 2.583600 1.501504  
50 6 0 -4.497820 5.432583 -1.125963  
51 1 0 -2.762967 4.538202 -2.058527  
52 6 0 -5.414227 5.360438 -0.072991  
53 1 0 -6.017653 4.272644 1.697917  
54 1 0 -4.582927 6.225411 -1.873128  
55 1 0 -6.214238 6.100108 0.009218  
56 6 0 3.659634 -3.494717 0.042300  
57 6 0 4.472767 -3.791657 -1.062511  
58 6 0 3.860060 -4.202042 1.238044  
59 6 0 5.462605 -4.773321 -0.974511  
60 1 0 4.319938 -3.246807 -1.996743  
61 6 0 4.849152 -5.184283 1.326676  
62 1 0 3.235069 -3.971478 2.103591  
63 6 0 5.653325 -5.472781 0.220416  
64 1 0 6.085266 -4.995053 -1.844676  
65 1 0 4.995000 -5.723609 2.265769  
66 1 0 6.427350 -6.240795 0.289623  
67 6 0 3.659617 3.494733 0.042307  
68 6 0 3.860041 4.202055 1.238053  
69 6 0 4.472748 3.791681 -1.062504  
70 6 0 4.849128 5.184301 1.326687  
71 1 0 3.235052 3.971485 2.103600  
72 6 0 5.462581 4.773349 -0.974502  
73 1 0 4.319921 3.246832 -1.996737  
74 6 0 5.653298 5.472807 0.220427  
75 1 0 4.994975 5.723625 2.265781  
76 1 0 6.085240 4.995087 -1.844667  
77 1 0 6.427319 6.240824 0.289636  
78 1 0 -3.847977 -0.000001 1.453076  
79 1 0 -1.850070 0.892948 2.354376  
80 6 0 -2.377150 -0.000002 2.738899  
81 8 0 -3.752366 -0.000002 2.415743  
82 1 0 -1.850070 -0.892953 2.354378  
83 1 0 -2.294958 -0.000001 3.836704

TMeOH-R

-----  
Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z  
-----

1	7	0	2.187124	0.065191	-0.283657
2	7	0	0.204266	-2.017176	-0.401588
3	7	0	-1.848052	-0.028661	-0.661027
4	7	0	0.114627	2.053067	-0.385890
5	6	0	2.983566	1.185947	-0.248480
6	6	0	4.377260	0.793962	-0.260747
7	6	0	4.406576	-0.569984	-0.271854
8	6	0	3.031659	-1.020476	-0.284973
9	6	0	2.647750	-2.368441	-0.236539
10	6	0	1.316562	-2.808595	-0.252376
11	6	0	0.916765	-4.193997	-0.124802
12	6	0	-0.446287	-4.219512	-0.182405
13	6	0	-0.885038	-2.853964	-0.383736
14	6	0	-2.222209	-2.470133	-0.568453
15	6	0	-2.634421	-1.146041	-0.777931
16	6	0	-3.997593	-0.756628	-1.070964
17	6	0	-4.028135	0.605084	-1.067512
18	6	0	-2.683970	1.053673	-0.770593
19	6	0	-2.332960	2.392432	-0.544138
20	6	0	-1.015782	2.836053	-0.345835
21	6	0	-0.646125	4.209755	-0.082953
22	6	0	0.716282	4.247240	-0.003107
23	6	0	1.187312	2.893216	-0.199315
24	6	0	2.540179	2.515908	-0.176663
25	1	0	5.219597	1.479766	-0.260250
26	1	0	5.276418	-1.220902	-0.271252
27	1	0	1.597369	-5.031976	-0.002601
28	1	0	-1.101441	-5.082391	-0.106733
29	1	0	-4.818537	-1.444614	-1.250684
30	1	0	-4.879200	1.256248	-1.244150
31	1	0	-1.343688	5.034331	0.031591
32	1	0	1.350210	5.108239	0.189154
33	29	0	0.157043	0.012295	-0.407603
34	6	0	-3.289516	-3.505186	-0.452300
35	6	0	-4.211275	-3.409314	0.605468
36	6	0	-3.402164	-4.569603	-1.359594
37	6	0	-5.218929	-4.364111	0.752696

38 1 0 -4.118725 -2.573416 1.303874  
39 6 0 -4.413385 -5.522323 -1.211826  
40 1 0 -2.697363 -4.640060 -2.190949  
41 6 0 -5.322394 -5.423380 -0.154551  
42 1 0 -5.926823 -4.281369 1.581151  
43 1 0 -4.494927 -6.342579 -1.929291  
44 1 0 -6.112571 -6.169387 -0.039735  
45 6 0 -3.445735 3.376980 -0.417722  
46 6 0 -3.592390 4.456516 -1.302148  
47 6 0 -4.374462 3.219821 0.626629  
48 6 0 -4.644113 5.362806 -1.145855  
49 1 0 -2.881265 4.575271 -2.122536  
50 6 0 -5.422682 4.128325 0.782736  
51 1 0 -4.255038 2.373843 1.308555  
52 6 0 -5.560221 5.202380 -0.102323  
53 1 0 -4.751637 6.195044 -1.845880  
54 1 0 -6.135363 3.997875 1.600858  
55 1 0 -6.382102 5.912158 0.019276  
56 6 0 3.727001 -3.399973 -0.147123  
57 6 0 3.984920 -4.062935 1.062603  
58 6 0 4.503049 -3.721201 -1.271330  
59 6 0 4.993829 -5.025378 1.147072  
60 1 0 3.386323 -3.815400 1.942214  
61 6 0 5.513900 -4.681794 -1.187813  
62 1 0 4.304886 -3.211237 -2.216686  
63 6 0 5.761833 -5.337053 0.021633  
64 1 0 5.183136 -5.531387 2.096963  
65 1 0 6.107972 -4.922178 -2.072916  
66 1 0 6.551706 -6.089134 0.086948  
67 6 0 3.563632 3.596578 -0.057328  
68 6 0 4.383520 3.691616 1.079199  
69 6 0 3.722790 4.545139 -1.081029  
70 6 0 5.336571 4.706339 1.189763  
71 1 0 4.263323 2.962797 1.883677  
72 6 0 4.676295 5.559576 -0.972296  
73 1 0 3.093338 4.475844 -1.970732  
74 6 0 5.486290 5.643654 0.163749  
75 1 0 5.962215 4.767695 2.083599  
76 1 0 4.789925 6.285507 -1.781112  
77 1 0 6.232067 6.437540 0.249400  
78 6 0 -2.954744 -0.069324 3.608827  
79 1 0 -3.966971 -0.106070 4.042327  
80 1 0 -2.463514 0.851607 3.981635  
81 1 0 -2.389289 -0.934110 4.012172

82 8 0 -3.074806 -0.097005 2.210956  
83 1 0 -2.176912 -0.023088 1.842529  
84 6 0 0.628618 -0.725291 2.727510  
85 1 0 0.196202 -1.724368 2.581471  
86 1 0 0.661859 -0.506437 3.809290  
87 1 0 1.651995 -0.730041 2.318128  
88 8 0 -0.206169 0.189263 2.032303  
89 1 0 0.184845 1.074622 2.032613

TMeOH-TS1

-----  
Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z  
-----

1 7 0 -0.379597 1.918121 -0.250846  
2 7 0 2.166385 0.565221 -0.220683  
3 7 0 0.739834 -1.941574 -0.104730  
4 7 0 -1.789959 -0.616143 0.062993  
5 6 0 -1.664557 2.401614 -0.086817  
6 6 0 -1.625204 3.856929 -0.084494  
7 6 0 -0.330845 4.225999 -0.269427  
8 6 0 0.452853 3.006343 -0.367136  
9 6 0 1.849267 2.997962 -0.476427  
10 6 0 2.640672 1.833056 -0.377829  
11 6 0 4.089389 1.813264 -0.352173  
12 6 0 4.463950 0.519909 -0.120762  
13 6 0 3.250291 -0.265733 -0.052181  
14 6 0 3.195867 -1.648666 0.152014  
15 6 0 2.013226 -2.417587 0.118846  
16 6 0 1.983082 -3.855082 0.192783  
17 6 0 0.682780 -4.238891 -0.016009  
18 6 0 -0.081826 -3.036425 -0.209435  
19 6 0 -1.473995 -3.014089 -0.504732  
20 6 0 -2.245013 -1.867552 -0.469467  
21 6 0 -3.591567 -1.699991 -0.907078  
22 6 0 -4.013455 -0.434872 -0.589272  
23 6 0 -2.939027 0.256906 0.068829  
24 6 0 -2.850629 1.676407 0.034444  
25 1 0 -2.486463 4.500759 0.065747  
26 1 0 0.078262 5.231785 -0.304178  
27 1 0 4.730848 2.680979 -0.476319  
28 1 0 5.471233 0.127186 -0.014187  
29 1 0 2.847048 -4.492307 0.358966



30 1 0 0.278988 -5.247386 -0.031107  
31 1 0 -4.156891 -2.463625 -1.435836  
32 1 0 -4.971369 0.020352 -0.823849  
33 29 0 0.249279 0.021726 -0.122247  
34 6 0 4.481149 -2.375454 0.380306  
35 6 0 4.768672 -2.931586 1.636795  
36 6 0 5.419078 -2.522535 -0.653670  
37 6 0 5.967056 -3.614475 1.855782  
38 1 0 4.043632 -2.819426 2.445826  
39 6 0 6.617528 -3.206029 -0.435486  
40 1 0 5.197360 -2.100964 -1.636398  
41 6 0 6.895437 -3.753445 0.820103  
42 1 0 6.178042 -4.037142 2.841143  
43 1 0 7.335559 -3.315115 -1.251955  
44 1 0 7.832894 -4.288013 0.990937  
45 6 0 -2.141890 -4.292783 -0.876035  
46 6 0 -1.677093 -5.061056 -1.957523  
47 6 0 -3.255999 -4.752311 -0.152766  
48 6 0 -2.311497 -6.253894 -2.307643  
49 1 0 -0.816294 -4.708539 -2.529210  
50 6 0 -3.888409 -5.947459 -0.501275  
51 1 0 -3.615881 -4.167756 0.696685  
52 6 0 -3.418781 -6.701402 -1.580299  
53 1 0 -1.942378 -6.835137 -3.156090  
54 1 0 -4.748566 -6.293758 0.076737  
55 1 0 -3.913823 -7.636209 -1.853934  
56 6 0 2.544650 4.309228 -0.645863  
57 6 0 3.343132 4.842197 0.379514  
58 6 0 2.401900 5.041873 -1.835328  
59 6 0 3.983392 6.072843 0.218926  
60 1 0 3.450964 4.285117 1.312698  
61 6 0 3.040908 6.273427 -1.996916  
62 1 0 1.784480 4.633407 -2.638419  
63 6 0 3.834659 6.792385 -0.970396  
64 1 0 4.596513 6.474824 1.029295  
65 1 0 2.920855 6.828301 -2.930662  
66 1 0 4.334931 7.755605 -1.095947  
67 6 0 -4.152577 2.400129 0.094987  
68 6 0 -4.993654 2.219632 1.207079  
69 6 0 -4.577778 3.236545 -0.951459  
70 6 0 -6.225667 2.873660 1.272004  
71 1 0 -4.639284 1.565184 2.005797  
72 6 0 -5.811575 3.886855 -0.884066  
73 1 0 -3.938495 3.362618 -1.828061

```

74 6 0 -6.638621 3.708636 0.229370
75 1 0 -6.867066 2.732355 2.145635
76 1 0 -6.131822 4.529799 -1.707735
77 1 0 -7.604381 4.217436 0.281563
78 6 0 -4.034701 -1.078351 2.408383
79 1 0 -4.291427 -1.066822 3.492208
80 1 0 -3.686861 -2.117269 2.180425
81 1 0 -5.006001 -0.965735 1.866574
82 8 0 -3.123802 -0.102408 2.088912
83 1 0 -1.601583 -0.706051 1.081138
84 6 0 -0.330470 1.061740 3.032365
85 1 0 -0.088719 1.978196 2.478072
86 1 0 0.159626 1.111552 4.020549
87 1 0 -1.423993 0.980600 3.139185
88 8 0 0.179000 -0.026942 2.260830
89 1 0 -0.001902 -0.856664 2.721416

```

\*\*\*\*\* 1 imaginary frequencies (negative Signs) \*\*\*\*\*

Diagonal vibrational polarizability:

193.7512982 38.7190229 130.5960101

Harmonic frequencies (cm<sup>-1</sup>), IR intensities (KM/Mole), Raman scattering activities (A<sup>4</sup>/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

1 2 3

A A A

Frequencies -- -248.0637 11.2514 24.3694

Red. masses -- 5.3032 6.0832 4.4481

Frc consts -- 0.1923 0.0005 0.0016

IR Inten -- 200.2605 0.0956 0.4204

Atom AN X Y Z X Y Z X Y Z

```

1 7 -0.00 0.02 0.01 0.00 0.00 -0.00 0.01 0.01 -0.05
2 7 -0.01 -0.00 -0.00 0.00 0.00 0.00 0.00 0.00 -0.03
3 7 -0.00 0.00 0.00 0.00 -0.00 -0.00 0.00 0.01 -0.04
4 7 -0.03 0.05 0.06 -0.00 0.00 0.00 -0.00 0.01 -0.01
5 6 0.02 0.04 -0.01 -0.00 0.00 0.02 0.01 0.01 -0.07
6 6 0.01 0.02 -0.04 -0.00 0.00 0.01 0.02 0.01 -0.11
7 6 0.02 0.02 -0.01 -0.00 0.00 -0.03 0.02 0.01 -0.11
8 6 0.00 0.01 0.00 0.00 0.01 -0.03 0.01 0.01 -0.06
9 6 0.01 -0.00 0.00 0.00 0.01 -0.05 0.01 0.00 -0.02
10 6 -0.00 0.00 0.00 0.00 0.01 -0.02 0.01 -0.00 0.01
11 6 -0.00 -0.00 0.00 0.00 0.01 -0.00 0.01 -0.01 0.06
12 6 -0.00 -0.00 0.00 0.01 0.00 0.03 0.01 -0.01 0.06
13 6 -0.01 0.00 0.00 0.01 -0.00 0.03 0.00 -0.00 0.00
14 6 -0.01 -0.00 0.00 0.01 -0.00 0.04 0.00 0.00 -0.02

```

15 6 -0.01 0.01 0.01 0.01 -0.00 0.02 -0.00 0.01 -0.06  
16 6 -0.01 -0.00 0.00 0.01 0.00 -0.00 -0.01 0.01 -0.10  
17 6 -0.00 -0.00 0.00 0.00 -0.00 -0.04 -0.01 0.01 -0.10  
18 6 -0.01 0.01 -0.00 0.00 -0.00 -0.04 -0.00 0.01 -0.06  
19 6 -0.00 0.00 -0.03 -0.00 -0.01 -0.05 0.01 0.01 -0.02  
20 6 -0.02 0.01 -0.00 -0.00 -0.01 -0.02 0.01 0.01 0.01  
21 6 -0.02 -0.05 -0.01 0.00 -0.02 -0.01 0.03 0.02 0.07  
22 6 -0.01 0.01 0.13 0.00 -0.01 0.03 0.02 0.02 0.07  
23 6 0.03 0.09 0.41 -0.00 0.00 0.03 0.00 0.01 0.02  
24 6 -0.00 0.02 0.09 -0.01 0.00 0.05 0.00 0.01 -0.03  
25 1 0.01 0.02 -0.04 -0.01 -0.00 0.02 0.02 0.01 -0.14  
26 1 0.02 0.02 -0.00 -0.00 0.00 -0.05 0.02 0.01 -0.13  
27 1 0.00 -0.00 0.00 0.00 0.01 -0.01 0.01 -0.02 0.10  
28 1 -0.01 -0.00 0.00 0.01 -0.00 0.06 0.01 -0.02 0.10  
29 1 -0.01 -0.00 0.00 0.01 0.00 0.01 -0.01 0.01 -0.12  
30 1 -0.00 0.00 -0.00 0.00 -0.00 -0.06 -0.01 0.01 -0.12  
31 1 -0.04 -0.11 -0.12 0.01 -0.03 -0.02 0.05 0.03 0.10  
32 1 -0.03 -0.03 0.14 0.01 -0.01 0.05 0.04 0.03 0.10  
33 29 -0.03 -0.01 -0.03 0.00 0.00 0.00 0.00 0.01 -0.04  
34 6 -0.00 -0.00 0.00 0.02 -0.00 0.09 0.01 -0.00 0.00  
35 6 -0.00 0.00 -0.00 0.06 -0.01 0.10 0.06 0.06 -0.01  
36 6 -0.00 0.00 0.00 -0.02 -0.00 0.12 -0.05 -0.06 0.05  
37 6 -0.00 0.00 0.00 0.07 -0.01 0.14 0.07 0.06 0.02  
38 1 -0.00 0.00 -0.00 0.09 -0.01 0.07 0.11 0.11 -0.04  
39 6 -0.00 0.00 0.00 -0.01 -0.00 0.16 -0.05 -0.07 0.07  
40 1 -0.00 -0.00 0.00 -0.05 0.00 0.11 -0.10 -0.11 0.05  
41 6 -0.00 0.00 0.00 0.03 -0.00 0.17 0.01 -0.01 0.06  
42 1 -0.00 0.00 -0.00 0.10 -0.01 0.15 0.12 0.11 0.01  
43 1 -0.00 0.00 0.00 -0.04 0.00 0.19 -0.09 -0.12 0.11  
44 1 -0.00 0.00 0.00 0.04 -0.00 0.21 0.01 -0.01 0.08  
45 6 0.00 -0.00 -0.02 -0.01 -0.02 -0.09 0.02 0.01 -0.00  
46 6 0.00 0.01 -0.01 -0.02 -0.05 -0.10 0.07 -0.01 -0.04  
47 6 -0.00 -0.00 -0.02 -0.00 0.01 -0.11 -0.03 0.03 0.06  
48 6 0.00 0.01 -0.00 -0.03 -0.06 -0.14 0.08 -0.01 -0.02  
49 1 -0.00 0.01 -0.01 -0.03 -0.07 -0.08 0.11 -0.03 -0.08  
50 6 0.00 -0.00 -0.00 -0.01 -0.00 -0.15 -0.02 0.03 0.08  
51 1 -0.00 -0.01 -0.02 0.01 0.03 -0.10 -0.08 0.05 0.09  
52 6 0.00 0.00 -0.00 -0.02 -0.03 -0.17 0.03 0.01 0.04  
53 1 0.00 0.02 -0.00 -0.04 -0.08 -0.15 0.13 -0.03 -0.05  
54 1 -0.00 -0.00 -0.00 -0.00 0.02 -0.17 -0.06 0.05 0.13  
55 1 0.00 0.01 0.01 -0.03 -0.04 -0.20 0.04 0.01 0.06  
56 6 0.01 -0.00 0.00 0.01 0.01 -0.09 0.00 -0.00 0.02  
57 6 0.00 -0.00 -0.00 -0.00 -0.02 -0.11 0.09 -0.01 0.08  
58 6 0.00 -0.00 0.00 0.02 0.05 -0.11 -0.08 0.01 0.00

59 6 -0.00 0.00 -0.00 0.00 -0.02 -0.15 0.09 -0.02 0.12  
60 1 0.00 -0.00 -0.00 -0.01 -0.05 -0.09 0.16 -0.02 0.09  
61 6 0.00 -0.00 0.00 0.03 0.05 -0.15 -0.09 0.01 0.04  
62 1 0.00 -0.00 0.00 0.03 0.07 -0.09 -0.15 0.02 -0.04  
63 6 -0.00 -0.00 -0.00 0.02 0.02 -0.17 -0.00 -0.01 0.10  
64 1 -0.00 0.00 -0.00 -0.01 -0.04 -0.17 0.15 -0.03 0.16  
65 1 -0.00 -0.00 -0.00 0.04 0.08 -0.16 -0.16 0.01 0.03  
66 1 -0.00 0.00 -0.00 0.02 0.02 -0.20 -0.00 -0.01 0.13  
67 6 -0.00 0.01 0.04 -0.01 0.00 0.08 0.00 0.01 -0.01  
68 6 0.03 -0.02 0.02 -0.04 0.01 0.10 -0.04 -0.04 0.03  
69 6 -0.01 0.02 0.02 0.02 -0.00 0.10 0.05 0.06 -0.03  
70 6 0.03 -0.02 -0.00 -0.04 0.01 0.14 -0.04 -0.04 0.05  
71 1 0.06 -0.05 0.05 -0.06 0.01 0.09 -0.07 -0.07 0.04  
72 6 -0.02 0.01 -0.00 0.02 -0.00 0.13 0.05 0.06 -0.01  
73 1 -0.02 0.04 0.02 0.05 -0.01 0.08 0.08 0.09 -0.06  
74 6 0.01 -0.01 -0.02 -0.01 0.00 0.15 0.00 0.01 0.03  
75 1 0.04 -0.04 -0.01 -0.06 0.02 0.15 -0.08 -0.07 0.08  
76 1 -0.04 0.02 -0.02 0.04 -0.01 0.15 0.08 0.10 -0.03  
77 1 0.00 -0.02 -0.04 -0.01 0.00 0.18 0.00 0.01 0.05  
78 6 0.02 -0.04 -0.12 -0.03 0.03 0.02 -0.08 -0.07 0.08  
79 1 -0.19 -0.12 -0.09 -0.07 0.07 0.03 -0.15 -0.07 0.10  
80 1 -0.09 -0.09 -0.12 0.01 0.03 -0.03 -0.03 -0.06 0.06  
81 1 0.09 0.05 0.02 -0.01 -0.01 0.06 -0.04 -0.10 0.15  
82 8 0.13 -0.16 -0.22 -0.04 0.04 0.03 -0.08 -0.04 0.02  
83 1 -0.54 0.17 -0.10 -0.00 0.03 0.00 -0.01 -0.00 -0.01  
84 6 0.00 0.01 0.00 -0.03 -0.00 -0.00 -0.11 -0.07 -0.07  
85 1 0.03 0.02 -0.03 -0.04 0.00 -0.01 -0.15 -0.04 -0.09  
86 1 -0.05 -0.01 -0.02 -0.03 -0.00 -0.00 -0.10 -0.07 -0.06  
87 1 -0.00 -0.01 0.06 -0.03 -0.01 -0.01 -0.10 -0.12 -0.07  
88 8 0.04 0.02 -0.00 -0.03 0.00 0.00 -0.06 -0.02 -0.03  
89 1 -0.33 0.00 0.17 0.01 0.00 -0.01 0.01 -0.04 -0.02

TMeOH-INT1

-----  
Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

-----  
1 7 0 -0.773770 1.704488 -0.269496  
2 7 0 1.977213 0.945470 -0.141031  
3 7 0 1.093459 -1.767396 -0.120258  
4 7 0 -1.572156 -1.019450 0.473255  
5 6 0 -2.147301 1.895502 -0.149484  
6 6 0 -2.438331 3.295982 -0.474340

7 6 0 -1.258814 3.912143 -0.724625  
8 6 0 -0.204748 2.916425 -0.573687  
9 6 0 1.159432 3.222672 -0.608846  
10 6 0 2.176850 2.279795 -0.322121  
11 6 0 3.584034 2.577744 -0.157438  
12 6 0 4.209196 1.401736 0.159110  
13 6 0 3.204646 0.362778 0.131138  
14 6 0 3.432847 -1.009706 0.260876  
15 6 0 2.438595 -2.005379 0.082687  
16 6 0 2.687427 -3.411796 -0.023484  
17 6 0 1.480116 -4.014175 -0.316703  
18 6 0 0.499348 -2.976008 -0.359046  
19 6 0 -0.907457 -3.172244 -0.569388  
20 6 0 -1.854914 -2.243914 -0.217691  
21 6 0 -3.276599 -2.309127 -0.431222  
22 6 0 -3.888192 -1.275283 0.183821  
23 6 0 -2.874126 -0.369307 0.845452  
24 6 0 -3.105161 1.027372 0.323711  
25 1 0 -3.426073 3.745761 -0.447650  
26 1 0 -1.090571 4.961266 -0.952410  
27 1 0 4.031541 3.562727 -0.256663  
28 1 0 5.264264 1.248519 0.368812  
29 1 0 3.658693 -3.887730 0.080173  
30 1 0 1.282001 -5.072271 -0.467531  
31 1 0 -3.756569 -3.086991 -1.021118  
32 1 0 -4.950580 -1.048281 0.184480  
33 29 0 0.216532 0.027150 -0.108417  
34 6 0 4.821945 -1.478662 0.538215  
35 6 0 5.115161 -2.163506 1.729182  
36 6 0 5.857973 -1.263302 -0.385323  
37 6 0 6.410915 -2.609759 1.995905  
38 1 0 4.314486 -2.341976 2.450258  
39 6 0 7.153923 -1.711716 -0.120489  
40 1 0 5.635303 -0.749581 -1.322599  
41 6 0 7.435324 -2.384211 1.071852  
42 1 0 6.621953 -3.134689 2.930823  
43 1 0 7.946601 -1.539884 -0.852802  
44 1 0 8.449272 -2.734617 1.279131  
45 6 0 -1.342882 -4.469166 -1.158631  
46 6 0 -0.832767 -4.891843 -2.398557  
47 6 0 -2.254673 -5.303133 -0.489940  
48 6 0 -1.234600 -6.104978 -2.959155  
49 1 0 -0.118629 -4.253804 -2.923114  
50 6 0 -2.657195 -6.517775 -1.050011

51 1 0 -2.636524 -4.997742 0.486594  
52 6 0 -2.149899 -6.921757 -2.287676  
53 1 0 -0.833238 -6.413723 -3.927490  
54 1 0 -3.363253 -7.155512 -0.512430  
55 1 0 -2.462773 -7.872421 -2.726069  
56 6 0 1.564329 4.628609 -0.911134  
57 6 0 2.104522 5.457489 0.086235  
58 6 0 1.404486 5.155975 -2.202954  
59 6 0 2.477094 6.772885 -0.199452  
60 1 0 2.223143 5.061791 1.097476  
61 6 0 1.770414 6.473411 -2.489831  
62 1 0 0.989631 4.517824 -2.986517  
63 6 0 2.310259 7.285916 -1.489128  
64 1 0 2.892519 7.403066 0.590989  
65 1 0 1.638313 6.865120 -3.501546  
66 1 0 2.599044 8.315732 -1.712813  
67 6 0 -4.527384 1.480748 0.362160  
68 6 0 -5.245393 1.539776 1.570688  
69 6 0 -5.194104 1.837472 -0.824853  
70 6 0 -6.581003 1.948553 1.588234  
71 1 0 -4.738298 1.265560 2.495166  
72 6 0 -6.527343 2.249892 -0.806189  
73 1 0 -4.654166 1.773651 -1.771901  
74 6 0 -7.227860 2.306632 0.402370  
75 1 0 -7.118344 1.994751 2.538961  
76 1 0 -7.024249 2.519454 -1.741539  
77 1 0 -8.272558 2.626406 0.418945  
78 6 0 -3.131050 -1.522906 2.959508  
79 1 0 -3.111867 -1.284873 4.031577  
80 1 0 -2.322778 -2.246692 2.749580  
81 1 0 -4.095457 -1.995864 2.708555  
82 8 0 -2.947505 -0.299471 2.271095  
83 1 0 -1.021448 -1.155693 1.331959  
84 6 0 0.111251 1.052271 2.994563  
85 1 0 -0.981540 1.152885 3.037050  
86 1 0 0.514619 1.858982 2.360164  
87 1 0 0.521499 1.147655 4.015613  
88 8 0 0.375954 -0.232255 2.443484  
89 1 0 1.326078 -0.336882 2.292194

TMeOH-INT2

-----  
Center Atomic Atomic Coordinates (Angstroms)

S62

Number Number Type X Y Z

-----  
1 7 0 -0.637709 1.737437 -0.291852  
2 7 0 2.037226 0.701732 -0.159060  
3 7 0 0.945115 -1.915949 -0.090859  
4 7 0 -1.627005 -0.870173 0.277834  
5 6 0 -1.997974 2.009790 -0.373389  
6 6 0 -2.167996 3.374096 -0.868744  
7 6 0 -0.924711 3.897315 -1.031824  
8 6 0 0.028781 2.867731 -0.639102  
9 6 0 1.428915 3.060910 -0.566478  
10 6 0 2.338899 2.036430 -0.262842  
11 6 0 3.752404 2.227762 0.000481  
12 6 0 4.279267 0.994072 0.259182  
13 6 0 3.197191 0.038199 0.127329  
14 6 0 3.338251 -1.369085 0.202889  
15 6 0 2.274504 -2.260964 0.020635  
16 6 0 2.410269 -3.693264 -0.183072  
17 6 0 1.163977 -4.179389 -0.445940  
18 6 0 0.242483 -3.054671 -0.367463  
19 6 0 -1.158996 -3.157650 -0.471794  
20 6 0 -2.011619 -2.092800 -0.109734  
21 6 0 -3.481381 -2.208973 -0.027723  
22 6 0 -3.955390 -1.075467 0.505669  
23 6 0 -2.789183 -0.130229 0.753701  
24 6 0 -3.020490 1.206718 0.081363  
25 1 0 -3.122557 3.866411 -1.029947  
26 1 0 -0.661104 4.895563 -1.369853  
27 1 0 4.261864 3.187398 0.013578  
28 1 0 5.306289 0.749783 0.515371  
29 1 0 3.348447 -4.241105 -0.156472  
30 1 0 0.876345 -5.206925 -0.652208  
31 1 0 -4.048916 -3.082089 -0.340277  
32 1 0 -4.989945 -0.822583 0.722015  
33 29 0 0.194598 -0.062018 0.036805  
34 6 0 4.698784 -1.939210 0.418974  
35 6 0 4.964916 -2.735708 1.545519  
36 6 0 5.737136 -1.709969 -0.500001  
37 6 0 6.232780 -3.284087 1.750472  
38 1 0 4.165867 -2.915785 2.267817  
39 6 0 7.004770 -2.258367 -0.296302  
40 1 0 5.537687 -1.105620 -1.387229  
41 6 0 7.257519 -3.046494 0.830414  
42 1 0 6.422099 -3.896148 2.635740

43 1 0 7.797939 -2.074668 -1.025217  
44 1 0 8.249835 -3.475093 0.989900  
45 6 0 -1.742120 -4.465855 -0.886073  
46 6 0 -1.497447 -4.975107 -2.173387  
47 6 0 -2.525233 -5.233117 -0.005977  
48 6 0 -2.024137 -6.205784 -2.570910  
49 1 0 -0.889610 -4.388833 -2.866153  
50 6 0 -3.058956 -6.461100 -0.403457  
51 1 0 -2.702704 -4.863891 1.006758  
52 6 0 -2.810367 -6.951981 -1.688298  
53 1 0 -1.824331 -6.581300 -3.577569  
54 1 0 -3.663064 -7.042508 0.297576  
55 1 0 -3.224953 -7.913859 -1.999273  
56 6 0 1.965078 4.431105 -0.801075  
57 6 0 1.592401 5.500117 0.032473  
58 6 0 2.861549 4.680104 -1.854280  
59 6 0 2.099697 6.782323 -0.185046  
60 1 0 0.913834 5.304864 0.866006  
61 6 0 3.367805 5.963230 -2.072324  
62 1 0 3.152184 3.856130 -2.509431  
63 6 0 2.987732 7.018922 -1.238856  
64 1 0 1.805742 7.600213 0.477479  
65 1 0 4.059042 6.139967 -2.900090  
66 1 0 3.384136 8.022936 -1.408671  
67 6 0 -4.419108 1.700256 0.031520  
68 6 0 -5.161977 1.854260 1.217835  
69 6 0 -5.036771 2.010270 -1.192625  
70 6 0 -6.479647 2.311045 1.176551  
71 1 0 -4.682138 1.620987 2.169695  
72 6 0 -6.355878 2.467371 -1.231339  
73 1 0 -4.475366 1.873555 -2.119120  
74 6 0 -7.082330 2.619811 -0.047452  
75 1 0 -7.038518 2.434684 2.107598  
76 1 0 -6.820489 2.698616 -2.193044  
77 1 0 -8.114565 2.976552 -0.077741  
78 6 0 -2.704552 -0.929817 3.051641  
79 1 0 -2.356130 -0.579688 4.033674  
80 1 0 -2.066562 -1.767786 2.720782  
81 1 0 -3.741178 -1.293185 3.144762  
82 8 0 -2.612547 0.178125 2.170488  
83 1 0 -0.745454 0.494674 2.408502  
84 6 0 -0.307564 3.617789 2.585486  
85 1 0 -1.189706 3.752767 1.958829  
86 1 0 0.276248 2.700346 2.509318



87 1 0 -0.054455 4.373291 3.331312  
88 8 0 0.217213 0.327160 2.452474  
89 1 0 0.282447 -0.615983 2.652328

TMeOH-TS2

-----  
Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z  
-----

1 7 0 -0.088853 -1.927443 -0.455510  
2 7 0 -2.150251 0.069741 -0.265924  
3 7 0 -0.149427 2.137968 -0.255642  
4 7 0 1.912957 0.145370 -0.443098  
5 6 0 1.028404 -2.725691 -0.484894  
6 6 0 0.633766 -4.116445 -0.556432  
7 6 0 -0.730537 -4.139996 -0.588191  
8 6 0 -1.176422 -2.764787 -0.497337  
9 6 0 -2.522328 -2.377461 -0.408904  
10 6 0 -2.950422 -1.047685 -0.275634  
11 6 0 -4.332021 -0.661175 -0.079681  
12 6 0 -4.350401 0.697178 0.042791  
13 6 0 -2.980786 1.149941 -0.085964  
14 6 0 -2.589616 2.496776 -0.021128  
15 6 0 -1.259770 2.935338 -0.121781  
16 6 0 -0.863663 4.328636 -0.118400  
17 6 0 0.494431 4.354295 -0.240139  
18 6 0 0.935135 2.977817 -0.329483  
19 6 0 2.279266 2.592027 -0.441890  
20 6 0 2.713028 1.259066 -0.487956  
21 6 0 4.103609 0.859073 -0.572625  
22 6 0 4.124099 -0.504502 -0.542946  
23 6 0 2.746434 -0.943092 -0.464018  
24 6 0 2.359272 -2.289254 -0.450647  
25 1 0 1.319751 -4.958220 -0.587087  
26 1 0 -1.382459 -5.006040 -0.657883  
27 1 0 -5.171490 -1.348645 -0.026368  
28 1 0 -5.208369 1.340590 0.215575  
29 1 0 -1.543598 5.172029 -0.039028  
30 1 0 1.147156 5.222219 -0.267426  
31 1 0 4.946566 1.540048 -0.648131  
32 1 0 4.985560 -1.164952 -0.587525  
33 29 0 -0.111234 0.104411 -0.309653  
34 6 0 -3.656030 3.529271 0.150417

35 6 0 -3.744408 4.280542 1.333433  
36 6 0 -4.590407 3.770463 -0.869806  
37 6 0 -4.740744 5.246043 1.493867  
38 1 0 -3.023482 4.098712 2.133564  
39 6 0 -5.587099 4.735779 -0.710995  
40 1 0 -4.524597 3.195774 -1.796126  
41 6 0 -5.665748 5.476517 0.471747  
42 1 0 -4.796795 5.818472 2.423024  
43 1 0 -6.303023 4.913362 -1.517236  
44 1 0 -6.445335 6.231833 0.596299  
45 6 0 3.315691 3.667822 -0.487329  
46 6 0 3.447667 4.489866 -1.617357  
47 6 0 4.175774 3.876355 0.602525  
48 6 0 4.416453 5.495394 -1.657340  
49 1 0 2.784581 4.330454 -2.470476  
50 6 0 5.145054 4.881128 0.563557  
51 1 0 4.073991 3.243863 1.487189  
52 6 0 5.268184 5.693832 -0.567028  
53 1 0 4.508923 6.124112 -2.546314  
54 1 0 5.804588 5.032274 1.421635  
55 1 0 6.026331 6.479993 -0.598315  
56 6 0 -3.563941 -3.448625 -0.419447  
57 6 0 -3.683558 -4.342498 0.657058  
58 6 0 -4.447433 -3.577663 -1.502793  
59 6 0 -4.659766 -5.341164 0.649944  
60 1 0 -3.005026 -4.244334 1.507078  
61 6 0 -5.424041 -4.576221 -1.511214  
62 1 0 -4.358467 -2.888105 -2.345059  
63 6 0 -5.533026 -5.461249 -0.434905  
64 1 0 -4.741137 -6.026088 1.497507  
65 1 0 -6.100576 -4.665716 -2.364673  
66 1 0 -6.296741 -6.242584 -0.441322  
67 6 0 3.438386 -3.318517 -0.358008  
68 6 0 4.102030 -3.504762 0.865562  
69 6 0 3.803757 -4.101969 -1.462259  
70 6 0 5.114450 -4.460633 0.977147  
71 1 0 3.800680 -2.893790 1.719858  
72 6 0 4.817571 -5.056902 -1.347827  
73 1 0 3.291116 -3.953832 -2.415552  
74 6 0 5.475065 -5.238191 -0.127704  
75 1 0 5.622908 -4.601218 1.934336  
76 1 0 5.097126 -5.658873 -2.216042  
77 1 0 6.268001 -5.984858 -0.038446  
78 6 0 2.873041 0.037065 2.959171

79 1 0 2.929845 0.460269 3.977673  
80 1 0 1.666229 -0.290154 2.537569  
81 1 0 3.552305 0.448850 2.195730  
82 8 0 2.440325 -1.246556 2.812482  
83 1 0 -0.637537 0.494286 2.481631  
84 6 0 -0.388282 -3.001531 3.014831  
85 1 0 -0.460414 -3.533101 2.064361  
86 1 0 0.583699 -2.626260 3.344399  
87 1 0 -1.236726 -3.015349 3.702782  
88 8 0 0.000094 -0.129273 2.105819  
89 1 0 -0.362845 -1.027025 2.257604

\*\*\*\*\* 1 imaginary frequencies (negative Signs) \*\*\*\*\*

Diagonal vibrational polarizability:

49.4772770 51.7081180 117.2462883

Harmonic frequencies (cm<sup>-1</sup>), IR intensities (KM/Mole), Raman scattering activities (A<sup>4</sup>/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

1 2 3

A A A

Frequencies -- -1960.6807 10.0068 24.2420

Red. masses -- 1.1286 6.1428 4.5147

Frc consts -- 2.5562 0.0004 0.0016

IR Inten -- 86.4669 0.0621 0.0747

Atom AN X Y Z X Y Z X Y Z

1 7 -0.00 -0.00 -0.00 0.00 -0.00 0.00 -0.01 -0.01 -0.00  
2 7 -0.00 0.00 -0.00 0.00 -0.00 -0.00 -0.01 -0.01 -0.03  
3 7 0.00 0.00 -0.00 0.00 -0.01 -0.00 -0.00 -0.01 -0.01  
4 7 0.00 0.00 -0.00 0.00 -0.00 0.00 -0.01 -0.01 -0.04  
5 6 -0.00 0.00 0.00 0.00 -0.00 0.03 -0.01 -0.02 0.02  
6 6 -0.00 -0.00 -0.00 0.01 -0.00 0.02 -0.01 -0.02 0.07  
7 6 0.00 -0.00 -0.00 0.01 -0.00 -0.02 -0.01 -0.02 0.07  
8 6 0.00 0.00 0.00 0.00 -0.00 -0.03 -0.01 -0.01 0.02  
9 6 0.00 0.00 -0.00 0.00 -0.00 -0.05 -0.01 -0.01 -0.01  
10 6 0.00 0.00 0.00 0.00 -0.00 -0.03 -0.01 -0.00 -0.05  
11 6 -0.00 0.00 0.00 0.00 -0.01 -0.02 -0.02 0.00 -0.09  
12 6 -0.00 -0.00 0.00 0.01 -0.01 0.02 -0.01 -0.00 -0.09  
13 6 0.00 -0.00 -0.00 0.01 -0.01 0.03 -0.01 -0.01 -0.04  
14 6 0.00 -0.00 0.00 0.01 -0.01 0.05 -0.00 -0.01 -0.01  
15 6 0.00 -0.00 0.00 0.01 -0.01 0.03 -0.00 -0.01 0.02  
16 6 -0.00 0.00 0.00 0.00 -0.01 0.02 0.00 -0.01 0.07  
17 6 0.00 0.00 0.00 0.00 -0.01 -0.02 0.00 -0.01 0.07  
18 6 -0.00 0.00 -0.00 0.00 -0.00 -0.03 -0.00 -0.01 0.02  
19 6 -0.00 0.00 0.00 0.00 -0.00 -0.05 -0.00 -0.01 -0.01

20 6 -0.00 -0.00 -0.00 0.00 -0.00 -0.02 -0.01 -0.01 -0.05  
21 6 0.00 0.00 0.00 0.00 -0.01 -0.01 -0.01 -0.02 -0.09  
22 6 -0.00 -0.00 0.00 0.00 -0.00 0.03 -0.01 -0.01 -0.09  
23 6 -0.00 0.00 0.00 0.00 -0.00 0.03 -0.01 -0.01 -0.05  
24 6 -0.00 0.00 0.00 0.00 -0.00 0.05 -0.01 -0.01 -0.01  
25 1 -0.00 -0.00 0.00 0.01 -0.00 0.03 -0.02 -0.02 0.11  
26 1 0.00 -0.00 0.00 0.01 -0.00 -0.04 -0.02 -0.02 0.11  
27 1 -0.00 0.00 0.00 0.00 -0.01 -0.04 -0.02 0.00 -0.12  
28 1 -0.00 -0.00 0.00 0.01 -0.01 0.04 -0.02 0.00 -0.11  
29 1 -0.00 0.00 -0.00 0.01 -0.01 0.04 0.01 -0.01 0.10  
30 1 -0.00 0.00 -0.00 -0.00 -0.00 -0.04 0.01 -0.01 0.10  
31 1 0.00 0.00 -0.00 0.00 -0.01 -0.03 -0.01 -0.02 -0.12  
32 1 0.00 -0.00 -0.00 0.00 -0.01 0.05 -0.01 -0.01 -0.11  
33 29 0.00 -0.00 0.00 0.00 -0.00 -0.00 -0.01 -0.01 -0.02  
34 6 0.00 -0.00 -0.00 0.01 -0.01 0.09 -0.00 -0.01 0.01  
35 6 -0.00 0.00 -0.00 0.05 -0.03 0.11 -0.04 -0.07 0.05  
36 6 -0.00 0.00 0.00 -0.01 0.01 0.12 0.04 0.05 -0.01  
37 6 0.00 0.00 -0.00 0.05 -0.03 0.15 -0.04 -0.07 0.06  
38 1 -0.00 -0.00 -0.00 0.07 -0.05 0.08 -0.07 -0.12 0.06  
39 6 -0.00 0.00 0.00 -0.00 0.01 0.16 0.04 0.05 0.01  
40 1 0.00 -0.00 0.00 -0.04 0.03 0.11 0.06 0.10 -0.04  
41 6 -0.00 0.00 0.00 0.03 -0.01 0.18 0.00 -0.01 0.04  
42 1 -0.00 -0.00 0.00 0.08 -0.05 0.16 -0.06 -0.12 0.09  
43 1 -0.00 -0.00 0.00 -0.02 0.03 0.18 0.07 0.10 -0.01  
44 1 -0.00 0.00 0.00 0.03 -0.01 0.21 0.00 -0.01 0.06  
45 6 -0.00 -0.00 0.00 -0.00 -0.00 -0.09 -0.00 -0.02 0.02  
46 6 0.00 0.00 0.00 -0.03 -0.02 -0.11 -0.03 0.05 0.06  
47 6 0.00 0.00 -0.00 0.02 0.03 -0.11 0.03 -0.08 0.01  
48 6 0.00 -0.00 0.00 -0.04 -0.02 -0.15 -0.02 0.04 0.09  
49 1 -0.00 -0.00 0.00 -0.05 -0.04 -0.09 -0.05 0.10 0.07  
50 6 0.00 0.00 0.00 0.01 0.03 -0.16 0.03 -0.08 0.04  
51 1 0.00 0.00 0.00 0.04 0.04 -0.10 0.05 -0.13 -0.03  
52 6 0.00 0.00 0.00 -0.02 0.01 -0.18 0.01 -0.02 0.08  
53 1 0.00 0.00 0.00 -0.06 -0.04 -0.17 -0.04 0.09 0.12  
54 1 0.00 0.00 -0.00 0.03 0.05 -0.17 0.05 -0.13 0.03  
55 1 0.00 -0.00 0.00 -0.02 0.01 -0.21 0.01 -0.02 0.10  
56 6 0.00 0.00 -0.00 0.00 0.00 -0.09 -0.01 -0.01 -0.01  
57 6 0.00 0.00 0.00 -0.02 -0.02 -0.11 -0.07 0.05 0.03  
58 6 -0.00 0.00 0.00 0.02 0.03 -0.11 0.04 -0.06 -0.05  
59 6 0.00 0.00 -0.00 -0.03 -0.02 -0.15 -0.07 0.05 0.03  
60 1 0.00 0.00 -0.00 -0.04 -0.04 -0.09 -0.11 0.09 0.06  
61 6 -0.00 -0.00 -0.00 0.01 0.03 -0.15 0.04 -0.06 -0.05  
62 1 -0.00 0.00 0.00 0.04 0.05 -0.09 0.09 -0.10 -0.08  
63 6 -0.00 -0.00 -0.00 -0.01 0.01 -0.17 -0.01 -0.00 -0.01

64 1 0.00 0.00 0.00 -0.05 -0.03 -0.16 -0.11 0.09 0.06  
65 1 -0.00 -0.00 -0.00 0.03 0.05 -0.16 0.08 -0.10 -0.08  
66 1 -0.00 -0.00 -0.00 -0.01 0.01 -0.20 -0.01 -0.00 -0.01  
67 6 -0.00 0.00 0.00 0.00 -0.00 0.08 -0.01 -0.01 0.00  
68 6 0.00 -0.00 -0.00 -0.02 0.02 0.10 0.05 0.07 -0.02  
69 6 0.00 0.00 0.00 0.02 -0.02 0.10 -0.06 -0.09 0.04  
70 6 -0.00 0.00 -0.00 -0.02 0.02 0.13 0.06 0.08 -0.00  
71 1 -0.00 0.00 -0.00 -0.03 0.03 0.08 0.10 0.13 -0.04  
72 6 0.00 -0.00 0.00 0.02 -0.01 0.13 -0.06 -0.08 0.05  
73 1 -0.00 0.00 0.00 0.04 -0.03 0.09 -0.11 -0.15 0.05  
74 6 0.00 -0.00 -0.00 0.00 0.01 0.15 0.00 0.00 0.03  
75 1 0.00 -0.00 0.00 -0.03 0.04 0.14 0.10 0.14 -0.02  
76 1 0.00 -0.00 0.00 0.04 -0.03 0.15 -0.10 -0.14 0.08  
77 1 -0.00 -0.00 0.00 0.00 0.01 0.17 0.00 0.01 0.05  
78 6 -0.07 -0.03 -0.02 -0.04 0.04 0.01 0.05 0.14 -0.07  
79 1 -0.00 -0.01 -0.02 -0.03 0.06 0.00 0.04 0.17 -0.08  
80 1 0.13 0.98 0.05 -0.04 0.03 0.02 0.06 0.11 -0.06  
81 1 -0.01 -0.01 0.01 -0.04 0.02 0.00 0.05 0.14 -0.08  
82 8 0.04 -0.04 0.02 -0.04 0.03 0.04 0.08 0.13 -0.05  
83 1 -0.02 -0.01 -0.01 -0.04 0.02 -0.03 0.05 0.09 -0.05  
84 6 0.00 -0.00 0.00 -0.04 0.02 -0.01 0.09 0.10 0.05  
85 1 -0.00 0.00 0.00 -0.03 0.02 -0.01 0.02 0.10 0.06  
86 1 0.00 0.01 -0.00 -0.04 0.02 0.00 0.11 0.10 -0.02  
87 1 -0.00 -0.00 -0.00 -0.05 0.02 -0.02 0.14 0.10 0.11  
88 8 -0.00 0.00 -0.00 -0.03 0.02 0.00 0.04 0.07 -0.02  
89 1 0.02 -0.00 0.01 -0.03 0.02 0.00 0.04 0.08 0.04

TMeOH-INT3

-----  
Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z  
-----

1 7 0 1.133895 -1.529971 -0.426377  
2 7 0 -1.732950 -1.289661 -0.266296  
3 7 0 -1.496470 1.583553 -0.222721  
4 7 0 1.370416 1.337644 -0.376831  
5 6 0 2.500769 -1.441622 -0.529505  
6 6 0 3.070223 -2.771425 -0.602096  
7 6 0 2.028287 -3.651853 -0.552999  
8 6 0 0.819110 -2.865534 -0.427766  
9 6 0 -0.465448 -3.416478 -0.304594  
10 6 0 -1.642154 -2.658369 -0.218398  
11 6 0 -2.961462 -3.231693 -0.044232

12 6 0 -3.840984 -2.191558 0.000546  
13 6 0 -3.063040 -0.976711 -0.141348  
14 6 0 -3.619746 0.312034 -0.121913  
15 6 0 -2.868299 1.495858 -0.176229  
16 6 0 -3.441688 2.824548 -0.184625  
17 6 0 -2.400996 3.706923 -0.216167  
18 6 0 -1.185160 2.923022 -0.250192  
19 6 0 0.106742 3.469440 -0.291470  
20 6 0 1.283859 2.708169 -0.354100  
21 6 0 2.609370 3.284091 -0.460500  
22 6 0 3.486593 2.243966 -0.540181  
23 6 0 2.703129 1.027675 -0.480637  
24 6 0 3.255823 -0.258969 -0.543385  
25 1 0 4.130130 -2.994321 -0.684355  
26 1 0 2.066477 -4.736655 -0.595842  
27 1 0 -3.174803 -4.292981 0.045951  
28 1 0 -4.917957 -2.231729 0.136143  
29 1 0 -4.504881 3.046635 -0.168853  
30 1 0 -2.445545 4.792265 -0.220127  
31 1 0 2.827471 4.347816 -0.491070  
32 1 0 4.566664 2.286536 -0.647222  
33 29 0 -0.173005 0.013824 -0.249714  
34 6 0 -5.106240 0.430481 -0.030327  
35 6 0 -5.714993 0.954193 1.121550  
36 6 0 -5.923270 0.017796 -1.095153  
37 6 0 -7.104747 1.063032 1.206848  
38 1 0 -5.087090 1.270196 1.957402  
39 6 0 -7.313075 0.127099 -1.011304  
40 1 0 -5.456952 -0.386766 -1.996072  
41 6 0 -7.908187 0.650160 0.140199  
42 1 0 -7.562242 1.467999 2.112835  
43 1 0 -7.933830 -0.194525 -1.851152  
44 1 0 -8.995473 0.735307 0.206425  
45 6 0 0.238123 4.958361 -0.278180  
46 6 0 -0.149216 5.722680 -1.390194  
47 6 0 0.755625 5.619834 0.846660  
48 6 0 -0.024044 7.113740 -1.377264  
49 1 0 -0.546041 5.214494 -2.271745  
50 6 0 0.881718 7.010810 0.860678  
51 1 0 1.057640 5.032021 1.716366  
52 6 0 0.491646 7.762127 -0.251481  
53 1 0 -0.326601 7.693405 -2.252798  
54 1 0 1.283366 7.510147 1.745829  
55 1 0 0.590010 8.850252 -0.241225

56 6 0 -0.582794 -4.904571 -0.243222  
 57 6 0 -0.114304 -5.607324 0.878663  
 58 6 0 -1.162864 -5.626201 -1.298195  
 59 6 0 -0.222389 -6.998187 0.943326  
 60 1 0 0.329221 -5.048862 1.706077  
 61 6 0 -1.270321 -7.017467 -1.234572  
 62 1 0 -1.525861 -5.085704 -2.175108  
 63 6 0 -0.800283 -7.707503 -0.113595  
 64 1 0 0.142254 -7.530019 1.825568  
 65 1 0 -1.720265 -7.565245 -2.066215  
 66 1 0 -0.884801 -8.795718 -0.063435  
 67 6 0 4.743956 -0.377757 -0.603027  
 68 6 0 5.524771 -0.032546 0.512164  
 69 6 0 5.387730 -0.835309 -1.763299  
 70 6 0 6.916190 -0.144526 0.467138  
 71 1 0 5.027939 0.322636 1.416651  
 72 6 0 6.779441 -0.946877 -1.808290  
 73 1 0 4.786520 -1.098294 -2.636417  
 74 6 0 7.547932 -0.602435 -0.692687  
 75 1 0 7.509667 0.125200 1.344294  
 76 1 0 7.265896 -1.300226 -2.720794  
 77 1 0 8.636560 -0.689349 -0.727830  
 78 6 0 3.348830 0.685432 3.617414  
 79 1 0 2.361096 -0.556877 2.509612  
 80 1 0 3.633905 1.735709 3.695766  
 81 1 0 3.997991 -0.108737 3.998035  
 82 8 0 2.528745 0.407296 2.569956  
 83 1 0 0.646395 0.731551 2.302262  
 84 6 0 1.482930 -2.407725 2.841013  
 85 1 0 2.071020 -2.949617 2.098534  
 86 1 0 0.610469 -1.828932 2.530325  
 87 1 0 1.674504 -2.568878 3.904126  
 88 8 0 -0.239797 0.340435 2.190593  
 89 1 0 -0.814073 1.074585 1.930495

TMeOH-TS3

-----  
 Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

-----  
 1 7 0 1.261494 -1.422322 -0.399889  
 2 7 0 -1.618678 -1.403589 -0.279091  
 3 7 0 -1.603279 1.478271 -0.215030

4 7 0 1.275740 1.451483 -0.358742  
5 6 0 2.619407 -1.231059 -0.501227  
6 6 0 3.288040 -2.513910 -0.569346  
7 6 0 2.315020 -3.470088 -0.526809  
8 6 0 1.049067 -2.778407 -0.408589  
9 6 0 -0.190721 -3.426172 -0.304926  
10 6 0 -1.423232 -2.761065 -0.234094  
11 6 0 -2.696553 -3.435513 -0.080415  
12 6 0 -3.654074 -2.466578 -0.042490  
13 6 0 -2.970066 -1.194581 -0.168132  
14 6 0 -3.623928 0.047496 -0.143769  
15 6 0 -2.964835 1.285768 -0.178995  
16 6 0 -3.637435 2.566974 -0.175760  
17 6 0 -2.666652 3.526224 -0.190379  
18 6 0 -1.394552 2.837536 -0.226994  
19 6 0 -0.147553 3.480523 -0.263296  
20 6 0 1.083648 2.811408 -0.334363  
21 6 0 2.359528 3.488446 -0.452029  
22 6 0 3.314454 2.520293 -0.539018  
23 6 0 2.628720 1.247142 -0.472783  
24 6 0 3.281101 0.007047 -0.526843  
25 1 0 4.362242 -2.654901 -0.647643  
26 1 0 2.434770 -4.548945 -0.569658  
27 1 0 -2.827839 -4.510635 0.002410  
28 1 0 -4.726381 -2.590025 0.079109  
29 1 0 -4.714517 2.707372 -0.164093  
30 1 0 -2.793754 4.604956 -0.181983  
31 1 0 2.493908 4.565872 -0.483414  
32 1 0 4.387384 2.645693 -0.652444  
33 29 0 -0.164724 0.015706 -0.238679  
34 6 0 -5.115923 0.050950 -0.066012  
35 6 0 -5.773573 0.510835 1.086170  
36 6 0 -5.888628 -0.408838 -1.144451  
37 6 0 -7.168316 0.511696 1.158386  
38 1 0 -5.179576 0.862467 1.932516  
39 6 0 -7.283454 -0.407324 -1.073666  
40 1 0 -5.384121 -0.764653 -2.045371  
41 6 0 -7.927632 0.053044 0.078196  
42 1 0 -7.664024 0.867998 2.064703  
43 1 0 -7.869832 -0.764273 -1.923871  
44 1 0 -9.018808 0.053738 0.134240  
45 6 0 -0.128927 4.974897 -0.238596  
46 6 0 -0.582495 5.717059 -1.340560  
47 6 0 0.347945 5.663905 0.887720



48 6 0 -0.561877 7.113415 -1.316229  
49 1 0 -0.947568 5.187893 -2.223478  
50 6 0 0.369109 7.060233 0.913143  
51 1 0 0.702143 5.093139 1.749030  
52 6 0 -0.086408 7.789298 -0.188905  
53 1 0 -0.914617 7.675967 -2.184102  
54 1 0 0.740456 7.580956 1.799182  
55 1 0 -0.069881 8.881610 -0.169746  
56 6 0 -0.194971 -4.919304 -0.249843  
57 6 0 0.295590 -5.587478 0.883556  
58 6 0 -0.689805 -5.678424 -1.321620  
59 6 0 0.292419 -6.982849 0.942271  
60 1 0 0.671380 -4.998630 1.723442  
61 6 0 -0.691800 -7.074105 -1.263585  
62 1 0 -1.070074 -5.163661 -2.206717  
63 6 0 -0.200464 -7.730212 -0.131395  
64 1 0 0.672654 -7.488664 1.833187  
65 1 0 -1.076046 -7.651593 -2.107983  
66 1 0 -0.202532 -8.821910 -0.085558  
67 6 0 4.773999 0.003126 -0.599761  
68 6 0 5.539639 0.399485 0.508892  
69 6 0 5.435234 -0.397000 -1.771455  
70 6 0 6.935043 0.392951 0.445049  
71 1 0 5.033296 0.707697 1.426722  
72 6 0 6.830572 -0.402021 -1.834845  
73 1 0 4.844197 -0.700280 -2.638482  
74 6 0 7.584662 -0.007385 -0.726017  
75 1 0 7.517224 0.699940 1.317430  
76 1 0 7.330639 -0.711765 -2.755788  
77 1 0 8.676231 -0.011305 -0.775061  
78 6 0 3.292598 0.536621 3.541070  
79 1 0 2.364778 -0.197513 2.021252  
80 1 0 3.302023 1.398800 4.210005  
81 1 0 3.575757 -0.458588 3.896063  
82 8 0 2.383373 0.628680 2.533311  
83 1 0 0.478869 0.719265 2.433807  
84 6 0 1.489440 -2.437151 2.879772  
85 1 0 2.183054 -2.855309 2.149170  
86 1 0 0.628731 -1.851645 2.552671  
87 1 0 1.646411 -2.626431 3.943103  
88 8 0 -0.361236 0.275333 2.216451  
89 1 0 -0.961778 0.981461 1.938059

\*\*\*\*\* 1 imaginary frequencies (negative Signs) \*\*\*\*\*

Diagonal vibrational polarizability:

58.8603604 40.0506754 182.5204725

Harmonic frequencies (cm<sup>-1</sup>), IR intensities (KM/Mole), Raman scattering activities (A<sup>4</sup>/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

1 2 3

A A A

Frequencies -- -89.7162 8.3886 24.3202

Red. masses -- 1.6542 5.9194 5.0820

Frc consts -- 0.0078 0.0002 0.0018

IR Inten -- 6.4776 0.0171 0.1431

Atom AN X Y Z X Y Z X Y Z

1	7	0.00	0.00	0.01	-0.00	-0.00	0.01	-0.01	-0.01	-0.06
2	7	-0.00	0.00	-0.00	-0.00	-0.00	-0.00	-0.01	-0.01	-0.06
3	7	-0.00	0.00	-0.00	-0.00	-0.00	0.00	-0.00	-0.01	-0.05
4	7	0.00	0.00	-0.01	-0.00	-0.00	0.00	-0.00	-0.01	-0.07
5	6	0.00	0.00	0.01	-0.00	-0.00	-0.02	-0.00	-0.01	-0.04
6	6	0.00	0.00	0.01	-0.01	-0.00	-0.01	-0.00	-0.02	-0.01
7	6	0.00	0.00	0.01	-0.00	-0.00	0.03	-0.01	-0.01	-0.01
8	6	0.00	0.00	0.01	-0.00	-0.00	0.03	-0.01	-0.01	-0.04
9	6	0.00	0.00	0.00	-0.00	-0.00	0.05	-0.01	-0.01	-0.04
10	6	0.00	0.00	-0.00	-0.00	-0.00	0.03	-0.01	-0.01	-0.06
11	6	0.00	0.00	-0.00	-0.01	0.00	0.02	-0.01	-0.01	-0.07
12	6	0.00	0.00	-0.00	-0.01	0.00	-0.02	-0.01	-0.01	-0.06
13	6	0.00	0.00	-0.00	-0.00	-0.00	-0.03	-0.01	-0.01	-0.05
14	6	0.00	0.00	-0.00	-0.01	0.00	-0.05	-0.00	-0.01	-0.03
15	6	0.00	0.00	-0.00	-0.00	-0.00	-0.03	-0.00	-0.01	-0.02
16	6	-0.00	0.00	0.00	-0.00	0.00	-0.02	-0.00	-0.01	0.02
17	6	-0.00	0.00	0.00	0.00	-0.00	0.02	0.00	-0.01	0.03
18	6	-0.00	0.00	-0.00	-0.00	-0.00	0.03	-0.00	-0.01	-0.02
19	6	-0.00	0.00	-0.00	0.00	-0.00	0.05	0.00	-0.01	-0.03
20	6	0.00	0.00	-0.01	-0.00	-0.00	0.03	-0.00	-0.01	-0.07
21	6	-0.00	0.00	-0.02	-0.00	-0.00	0.03	-0.00	-0.01	-0.09
22	6	-0.00	0.01	-0.02	-0.00	-0.00	-0.01	-0.00	-0.01	-0.09
23	6	0.00	0.01	-0.01	-0.00	-0.00	-0.02	-0.00	-0.01	-0.07
24	6	0.00	0.00	0.00	-0.01	-0.00	-0.04	-0.00	-0.01	-0.04
25	1	0.00	0.00	0.02	-0.01	-0.00	-0.03	-0.00	-0.02	0.02
26	1	0.00	0.00	0.02	-0.00	-0.00	0.04	-0.01	-0.01	0.01
27	1	0.00	0.00	-0.00	-0.01	0.00	0.03	-0.01	-0.01	-0.07
28	1	0.00	0.00	-0.00	-0.01	0.00	-0.04	-0.01	-0.00	-0.07
29	1	-0.00	0.00	0.01	-0.00	0.00	-0.04	0.00	-0.00	0.05
30	1	-0.00	0.00	0.01	0.00	-0.00	0.04	0.00	-0.01	0.05
31	1	-0.00	0.00	-0.02	-0.00	-0.00	0.05	-0.00	-0.01	-0.10
32	1	-0.00	0.01	-0.02	-0.01	-0.00	-0.02	-0.01	-0.01	-0.10

33 29 -0.00 0.00 0.01 -0.00 -0.00 0.00 -0.00 -0.01 -0.06  
34 6 0.00 0.00 -0.00 -0.01 -0.00 -0.09 -0.00 -0.00 0.01  
35 6 0.00 0.00 -0.00 -0.04 -0.00 -0.11 0.03 -0.05 0.05  
36 6 0.00 0.00 -0.00 0.02 -0.00 -0.11 -0.03 0.04 0.01  
37 6 0.00 -0.00 0.00 -0.04 -0.01 -0.15 0.04 -0.05 0.09  
38 1 0.00 -0.00 -0.00 -0.07 -0.00 -0.09 0.06 -0.08 0.04  
39 6 0.00 0.00 -0.00 0.02 -0.01 -0.15 -0.03 0.04 0.06  
40 1 -0.00 0.00 -0.00 0.05 -0.00 -0.09 -0.06 0.08 -0.01  
41 6 0.00 -0.00 0.00 -0.01 -0.01 -0.17 0.00 -0.00 0.09  
42 1 0.00 -0.00 0.00 -0.07 -0.01 -0.16 0.06 -0.09 0.12  
43 1 0.00 0.00 0.00 0.05 -0.01 -0.17 -0.06 0.08 0.06  
44 1 0.00 -0.00 0.00 -0.01 -0.01 -0.20 0.01 -0.01 0.13  
45 6 -0.00 0.00 -0.00 0.01 -0.00 0.09 0.01 -0.01 0.02  
46 6 -0.00 0.00 0.00 0.01 0.03 0.11 -0.05 0.03 0.07  
47 6 0.00 0.00 -0.00 0.01 -0.04 0.11 0.07 -0.05 0.02  
48 6 -0.00 0.00 0.00 0.02 0.03 0.15 -0.04 0.03 0.12  
49 1 -0.00 0.00 0.00 0.01 0.06 0.09 -0.09 0.07 0.07  
50 6 0.00 0.00 -0.00 0.01 -0.04 0.15 0.07 -0.06 0.07  
51 1 0.00 -0.00 -0.00 0.00 -0.07 0.10 0.11 -0.09 -0.02  
52 6 -0.00 0.00 0.00 0.02 -0.01 0.17 0.02 -0.01 0.13  
53 1 -0.00 0.00 0.00 0.03 0.06 0.17 -0.08 0.07 0.16  
54 1 0.00 -0.00 -0.00 0.01 -0.07 0.17 0.12 -0.09 0.08  
55 1 0.00 0.00 0.00 0.02 -0.01 0.21 0.02 -0.01 0.17  
56 6 0.00 0.00 0.00 0.00 0.00 0.08 -0.01 -0.01 -0.01  
57 6 0.00 0.00 0.00 0.01 0.03 0.10 -0.02 0.03 0.02  
58 6 0.00 0.00 0.00 0.00 -0.03 0.10 0.01 -0.04 0.01  
59 6 0.00 0.00 0.00 0.01 0.03 0.13 -0.02 0.03 0.06  
60 1 0.01 0.01 0.00 0.01 0.05 0.08 -0.03 0.05 0.01  
61 6 0.00 0.00 0.00 0.01 -0.03 0.14 0.01 -0.04 0.05  
62 1 -0.00 0.00 0.00 0.00 -0.05 0.09 0.02 -0.07 -0.01  
63 6 0.00 0.00 0.00 0.01 0.00 0.15 -0.01 -0.00 0.08  
64 1 0.00 0.00 0.00 0.01 0.05 0.14 -0.04 0.05 0.08  
65 1 -0.00 0.00 0.01 0.01 -0.05 0.15 0.02 -0.06 0.06  
66 1 0.00 0.00 0.01 0.02 0.00 0.18 -0.01 -0.00 0.11  
67 6 0.00 0.00 -0.00 -0.01 -0.01 -0.08 -0.00 -0.01 0.01  
68 6 0.01 0.01 -0.01 0.02 -0.01 -0.10 -0.05 0.06 0.02  
69 6 0.00 -0.01 0.00 -0.04 -0.00 -0.09 0.05 -0.08 0.06  
70 6 0.01 0.01 -0.01 0.02 -0.02 -0.13 -0.04 0.05 0.08  
71 1 0.01 0.03 -0.01 0.05 -0.01 -0.08 -0.08 0.12 -0.02  
72 6 0.00 -0.01 0.00 -0.04 -0.01 -0.13 0.05 -0.09 0.12  
73 1 -0.00 -0.01 0.01 -0.07 -0.00 -0.08 0.09 -0.14 0.05  
74 6 0.00 -0.00 -0.00 -0.01 -0.01 -0.15 0.01 -0.02 0.13  
75 1 0.01 0.02 -0.01 0.05 -0.02 -0.15 -0.08 0.11 0.08  
76 1 -0.00 -0.01 0.00 -0.07 -0.01 -0.15 0.09 -0.14 0.16

```

77 1 0.00 -0.00 -0.00 -0.01 -0.02 -0.18 0.01 -0.02 0.17
78 6 -0.05 -0.13 -0.01 0.06 0.06 -0.10 -0.10 0.16 0.06
79 1 0.19 0.35 -0.39 -0.03 0.05 -0.05 0.08 0.12 -0.03
80 1 -0.22 -0.38 0.32 0.08 0.05 -0.09 -0.18 0.18 0.04
81 1 0.03 -0.23 -0.35 0.12 0.07 -0.14 -0.14 0.17 0.12
82 8 -0.00 0.13 -0.03 -0.02 0.04 -0.03 0.02 0.14 -0.05
83 1 0.03 -0.09 0.04 -0.03 0.01 0.02 0.02 0.04 -0.09
84 6 -0.02 -0.08 0.05 0.04 0.04 0.02 0.09 0.08 -0.04
85 1 0.08 0.09 0.05 0.04 0.03 0.02 0.08 0.08 -0.05
86 1 0.06 0.05 0.08 0.03 0.01 0.02 0.09 0.08 -0.03
87 1 -0.14 -0.30 0.03 0.07 0.07 0.03 0.09 0.06 -0.04
88 8 0.01 -0.03 -0.02 -0.02 -0.01 0.01 0.03 0.01 -0.06
89 1 0.04 0.02 0.06 -0.03 -0.02 0.00 0.00 -0.01 -0.05

```

TMeOH-P

-----  
Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

-----

```

1 7 0 0.297962 2.061078 -0.337908
2 7 0 2.125458 -0.146121 -0.362743
3 7 0 -0.080369 -1.976222 -0.489379
4 7 0 -1.903407 0.233367 -0.523973
5 6 0 -0.726337 2.971728 -0.215527
6 6 0 -0.183482 4.287403 0.043779
7 6 0 1.174157 4.162245 0.046887
8 6 0 1.469199 2.767116 -0.199660
9 6 0 2.769110 2.244144 -0.275450
10 6 0 3.050081 0.876640 -0.396999
11 6 0 4.378521 0.326742 -0.542217
12 6 0 4.248780 -1.032108 -0.559564
13 6 0 2.840290 -1.321680 -0.441562
14 6 0 2.308439 -2.614084 -0.357045
15 6 0 0.936340 -2.894104 -0.353471
16 6 0 0.382503 -4.222074 -0.204988
17 6 0 -0.974136 -4.095175 -0.271986
18 6 0 -1.257478 -2.689116 -0.459147
19 6 0 -2.548588 -2.157477 -0.570854
20 6 0 -2.818380 -0.785095 -0.660864
21 6 0 -4.144422 -0.231378 -0.817180
22 6 0 -4.021005 1.126199 -0.733677
23 6 0 -2.617004 1.409610 -0.531971
24 6 0 -2.095450 2.695347 -0.327374

```

25 1 0 -0.773286 5.183786 0.211921  
26 1 0 1.916943 4.935561 0.220032  
27 1 0 5.289403 0.912634 -0.624677  
28 1 0 5.030569 -1.780812 -0.652832  
29 1 0 0.966317 -5.126959 -0.061316  
30 1 0 -1.725253 -4.875551 -0.191000  
31 1 0 -5.048317 -0.814375 -0.967472  
32 1 0 -4.803881 1.875270 -0.809108  
33 29 0 0.106444 0.045632 -0.434801  
34 6 0 3.265863 -3.739885 -0.151019  
35 6 0 3.926668 -3.843388 1.084592  
36 6 0 3.513005 -4.698281 -1.143908  
37 6 0 4.823461 -4.887748 1.317853  
38 1 0 3.707522 -3.101416 1.856764  
39 6 0 4.413929 -5.740494 -0.909424  
40 1 0 2.999425 -4.618100 -2.104696  
41 6 0 5.070670 -5.836803 0.320847  
42 1 0 5.328448 -4.962995 2.283933  
43 1 0 4.605293 -6.479093 -1.691658  
44 1 0 5.774083 -6.652831 0.503188  
45 6 0 -3.709686 -3.092711 -0.507253  
46 6 0 -3.960394 -4.017074 -1.532671  
47 6 0 -4.562851 -3.057254 0.609483  
48 6 0 -5.047933 -4.889768 -1.448064  
49 1 0 -3.300125 -4.042774 -2.402526  
50 6 0 -5.646856 -3.933958 0.691730  
51 1 0 -4.355896 -2.341493 1.409854  
52 6 0 -5.893018 -4.850455 -0.335247  
53 1 0 -5.237546 -5.600898 -2.255802  
54 1 0 -6.300864 -3.902867 1.566604  
55 1 0 -6.742755 -5.534253 -0.268653  
56 6 0 3.916787 3.195842 -0.207689  
57 6 0 4.816001 3.157116 0.870630  
58 6 0 4.117146 4.149060 -1.219508  
59 6 0 5.888088 4.049475 0.935631  
60 1 0 4.661957 2.424699 1.665936  
61 6 0 5.190777 5.039729 -1.156097  
62 1 0 3.425556 4.181494 -2.064105  
63 6 0 6.079161 4.992868 -0.077960  
64 1 0 6.574695 4.010411 1.784698  
65 1 0 5.336199 5.771216 -1.954676  
66 1 0 6.918513 5.690477 -0.027516  
67 6 0 -3.061900 3.824305 -0.191578  
68 6 0 -3.937065 3.871335 0.906335

69 6 0 -3.116734 4.852541 -1.145642  
70 6 0 -4.844496 4.923112 1.047041  
71 1 0 -3.893866 3.077182 1.655298  
72 6 0 -4.026337 5.903223 -1.006081  
73 1 0 -2.443914 4.817862 -2.005197  
74 6 0 -4.891953 5.941726 0.090764  
75 1 0 -5.514620 4.948678 1.909614  
76 1 0 -4.061810 6.693376 -1.759973  
77 1 0 -5.602720 6.764270 0.200066  
78 6 0 -1.849456 -0.657099 2.747824  
79 1 0 -1.799321 -1.292606 3.646555  
80 1 0 1.846042 -0.788408 1.758268  
81 1 0 -1.365124 -1.221708 1.929093  
82 8 0 -3.230914 -0.467461 2.482777  
83 1 0 -3.313839 0.038726 1.663591  
84 6 0 -1.092026 0.640790 2.982660  
85 1 0 -1.118924 1.279057 2.085118  
86 1 0 -0.038175 0.415091 3.206699  
87 1 0 -1.529518 1.206175 3.820474  
88 8 0 1.726640 -1.321270 2.560577  
89 1 0 1.146649 -2.033522 2.257642

ZCO<sub>2</sub>-R

-----  
Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

-----  
1 40 0 -0.008162 0.010592 -2.044058  
2 8 0 -1.626423 -1.378856 -1.381508  
3 40 0 1.765312 0.000454 -0.125109  
4 8 0 0.911524 -1.395870 1.406623  
5 40 0 -0.319749 2.258287 -0.002204  
6 8 0 -1.778954 1.351002 1.316268  
7 40 0 -0.415607 -0.011382 2.150052  
8 8 0 0.911645 1.380715 1.421185  
9 40 0 -0.319953 -2.258359 -0.025885  
10 8 0 1.122031 -1.687203 -1.340867  
11 40 0 -2.493031 0.000627 -0.121388  
12 8 0 -1.626291 1.393161 -1.366980  
13 8 0 1.122186 1.700822 -1.323103  
14 8 0 -1.779068 -1.364821 1.302036  
15 6 0 3.985024 -0.005695 0.490428  
16 8 0 4.923230 -0.021474 1.225706  
17 8 0 3.787301 0.025705 -0.784218

ZCO<sub>2</sub>-TS1

-----  
Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

-----  
1 40 0 0.007035 -0.002991 -2.042125  
2 8 0 -1.613996 -1.386870 -1.376512  
3 40 0 1.774085 0.000259 -0.116934  
4 8 0 0.914141 -1.387253 1.420396  
5 40 0 -0.311084 2.258437 -0.015222  
6 8 0 -1.775017 1.359907 1.303824  
7 40 0 -0.415076 0.001746 2.150672  
8 8 0 0.915104 1.389319 1.417867  
9 40 0 -0.312685 -2.258100 -0.010967  
10 8 0 1.134028 -1.695605 -1.324403  
11 40 0 -2.484588 0.000766 -0.127951  
12 8 0 -1.613121 1.385215 -1.379194  
13 8 0 1.135239 1.692430 -1.327619  
14 8 0 -1.776014 -1.355988 1.306343  
15 6 0 3.865589 -0.000025 0.787334  
16 8 0 4.987922 -0.000304 1.095029  
17 8 0 3.504089 -0.001416 -0.913596

\*\*\*\*\* 1 imaginary frequencies (negative Signs) \*\*\*\*\*

Diagonal vibrational polarizability:

41.2400896 20.0457063 37.8007498

Harmonic frequencies (cm<sup>-1</sup>), IR intensities (KM/Mole), Raman scattering activities (A<sup>4</sup>/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

1 2 3

A A A

Frequencies -- -401.3504 47.1907 61.0022

Red. masses -- 13.4994 15.0119 15.1631

Frc consts -- 1.2812 0.0197 0.0332

IR Inten -- 139.8313 1.1088 3.6610

Atom AN X Y Z X Y Z X Y Z

15 6 0.07 0.00 0.79 0.00 0.50 -0.00 -0.23 0.00 0.40  
16 8 0.14 -0.00 0.07 0.00 0.87 -0.00 -0.31 0.00 0.72  
17 8 -0.44 -0.00 -0.39 -0.00 0.03 -0.00 0.19 0.00 0.38

ZCO<sub>2</sub>-P

-----  
Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

-----  
1 40 0 -0.746698 -0.004385 2.006108  
2 8 0 -2.024701 1.383928 0.811565  
3 40 0 1.589861 -0.001737 0.836501  
4 8 0 1.333769 1.390630 -0.901815  
5 40 0 -0.321445 -2.258410 -0.008110  
6 8 0 -1.220106 -1.354364 -1.759131  
7 40 0 0.352024 0.004850 -2.061949  
8 8 0 1.334407 -1.385973 -0.907882  
9 40 0 -0.322502 2.258313 0.001635  
10 8 0 0.561816 1.690499 1.742303  
11 40 0 -2.393272 0.000940 -0.669588  
12 8 0 -2.024093 -1.388198 0.805489  
13 8 0 0.562589 -1.697597 1.735161  
14 8 0 -1.220739 1.361469 -1.753237  
15 6 0 4.331909 0.003291 -1.193331  
16 8 0 5.440483 0.002368 -0.971543  
17 8 0 3.217803 -0.003091 1.571104

ZCO-R

-----  
Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

-----  
1 40 0 0.144348 0.552022 -1.956737  
2 8 0 -0.817972 -1.454436 -1.771178  
3 40 0 1.685771 0.797996 0.138860  
4 8 0 1.385850 -1.115905 1.268918  
5 40 0 -1.128021 2.011728 0.403289  
6 8 0 -2.166448 0.356403 1.336339  
7 40 0 -0.414336 -0.535161 2.075666  
8 8 0 0.283208 1.378652 1.788637  
9 40 0 0.665926 -2.046237 -0.441758  
10 8 0 1.821753 -0.700310 -1.435475  
11 40 0 -2.218431 -0.815709 -0.402512  
12 8 0 -1.918903 1.036552 -1.252500  
13 8 0 0.476354 2.343917 -0.801671  
14 8 0 -1.087908 -2.083685 0.828038  
15 6 0 3.902917 0.187260 0.499864  
16 8 0 5.025567 0.043140 0.644561  
17 1 0 3.160226 1.856241 -0.516857

ZCO-TS1



-----  
Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z  
-----

1 40 0 0.381333 0.120566 -1.970741  
2 8 0 -1.178339 -1.437085 -1.613550  
3 40 0 1.827485 0.190685 0.204419  
4 8 0 0.883464 -1.342641 1.541407  
5 40 0 -0.460179 2.241240 0.057624  
6 8 0 -2.012376 1.149578 1.100736  
7 40 0 -0.670530 -0.118281 2.102504  
8 8 0 0.613268 1.419123 1.633515  
9 40 0 -0.020431 -2.251426 -0.091796  
10 8 0 1.546759 -1.495749 -1.144311  
11 40 0 -2.359898 -0.197227 -0.469428  
12 8 0 -1.447971 1.320607 -1.521884  
13 8 0 1.217258 1.874423 -1.032330  
14 8 0 -1.748114 -1.551832 1.010715  
15 6 0 4.030880 0.013557 0.349882  
16 8 0 5.184720 -0.042443 0.538847  
17 1 0 3.434139 1.344503 0.492308

\*\*\*\*\* 1 imaginary frequencies (negative Signs) \*\*\*\*\*

Diagonal vibrational polarizability:

66.4693852 9.4479952 12.8016727

Harmonic frequencies (cm<sup>-1</sup>), IR intensities (KM/Mole), Raman scattering activities (A<sup>4</sup>/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

1 2 3

A A A

Frequencies -- -68.1634 51.1627 226.8148

Red. masses -- 10.2964 14.0308 6.1678

Frc consts -- 0.0282 0.0216 0.1869

IR Inten -- 2.7638 2.0664 19.7751

Atom AN X Y Z X Y Z X Y Z

15 6 0.00 0.56 -0.20 -0.03 0.20 0.40 0.22 -0.36 0.21

16 8 0.03 0.56 -0.21 -0.09 0.24 0.81 0.27 0.33 -0.06

17 1 -0.06 0.16 0.51 -0.09 0.09 0.25 -0.23 0.05 -0.74

ZCO-INT1  
-----

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z  
-----

```

1 40 0 0.571557 0.280314 -1.897283
2 8 0 -0.919746 -1.377878 -1.778976
3 40 0 1.811874 0.285018 0.402509
4 8 0 0.845340 -1.379082 1.552620
5 40 0 -0.569190 2.217486 0.167814
6 8 0 -2.141281 0.979575 0.996696
7 40 0 -0.821525 -0.277363 2.040310
8 8 0 0.406584 1.352822 1.784253
9 40 0 0.144462 -2.226569 -0.208877
10 8 0 1.751871 -1.322386 -1.065044
11 40 0 -2.268715 -0.279192 -0.676485
12 8 0 -1.357826 1.349644 -1.547730
13 8 0 1.216629 2.011235 -0.782629
14 8 0 -1.712154 -1.692561 0.770166
15 6 0 4.040473 0.510656 0.065739
16 8 0 3.901510 -0.398660 0.908097
17 1 0 5.091196 0.766669 -0.213601

```

ZCO-INT2

-----  
Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z  
-----

```

1 40 0 -0.565683 -0.272432 -1.901294
2 8 0 0.916633 1.391832 -1.759612
3 40 0 -1.809636 -0.312778 0.395963
4 8 0 -0.854357 1.342265 1.568449
5 40 0 0.581732 -2.229257 0.141597
6 8 0 2.145764 -0.993437 0.988810
7 40 0 0.817378 0.243741 2.045529
8 8 0 -0.401503 -1.389883 1.766992
9 40 0 -0.154954 2.215573 -0.180980
10 8 0 -1.755950 1.313305 -1.051363
11 40 0 2.269461 0.286685 -0.668422
12 8 0 1.368815 -1.335928 -1.561518
13 8 0 -1.203522 -2.020620 -0.809467
14 8 0 1.702885 1.678901 0.794540
15 6 0 -4.041409 -0.566203 0.084992
16 8 0 -3.905477 0.373837 0.891975
17 1 0 -5.091174 -0.842319 -0.179566
18 1 0 -0.298585 4.096050 -0.256552

```

ZCO-TS2  
-----

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

-----  
1 40 0 0.565851 -0.174188 -1.911107  
2 8 0 -1.323833 -1.322634 -1.599217  
3 40 0 1.815596 -0.226950 0.382752  
4 8 0 0.454314 -1.398704 1.724524  
5 40 0 0.059990 2.246830 -0.121720  
6 8 0 -1.772795 1.609802 0.840731  
7 40 0 -0.828291 0.175466 2.050056  
8 8 0 0.797402 1.353834 1.602226  
9 40 0 -0.498202 -2.231109 0.077665  
10 8 0 1.275149 -1.924807 -0.869038  
11 40 0 -2.286601 0.237331 -0.660188  
12 8 0 -0.981352 1.425484 -1.721449  
13 8 0 1.693961 1.433907 -1.018647  
14 8 0 -2.108432 -1.082470 0.960278  
15 6 0 4.024464 -0.345373 -0.021954  
16 8 0 3.882052 0.470391 0.911978  
17 1 0 5.072081 -0.569440 -0.332593  
18 1 0 2.315693 -2.971933 1.114909

\*\*\*\*\* 1 imaginary frequencies (negative Signs) \*\*\*\*\*

Diagonal vibrational polarizability:

17.0645428 5.7435150 9.7740356

Harmonic frequencies (cm<sup>-1</sup>), IR intensities (KM/Mole), Raman scattering activities (A<sup>4</sup>/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

1 2 3

A A A

Frequencies -- -504.0134 66.6718 81.6491

Red. masses -- 1.0105 6.6457 7.7389

Frc consts -- 0.1512 0.0174 0.0304

IR Inten -- 73.1278 0.3248 0.3963

Atom AN X Y Z X Y Z X Y Z

15 6 -0.01 0.00 -0.00 0.09 -0.04 0.49 0.05 0.44 0.06

16 8 -0.01 -0.00 0.00 -0.10 -0.01 0.43 -0.16 0.53 -0.06

17 1 -0.02 -0.03 0.01 0.15 -0.08 0.73 0.11 0.69 0.07

18 1 0.59 0.80 -0.01 0.01 0.01 0.02 -0.01 0.02 0.04

ZCO-INT3

-----  
Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

```

-----
1 40 0 -1.124161 0.000583 -1.574216
2 8 0 0.605414 1.386113 -1.852999
3 40 0 -1.626968 0.001102 0.989749
4 8 0 -0.091976 1.388280 1.852199
5 40 0 0.204897 -2.258406 -0.009883
6 8 0 2.141937 -1.359087 0.350934
7 40 0 1.423307 -0.001142 1.782331
8 8 0 -0.093551 -1.388243 1.852037
9 40 0 0.207527 2.258595 -0.009417
10 8 0 -1.711802 1.695205 -0.374755
11 40 0 1.999912 -0.000851 -1.241344
12 8 0 0.604027 -1.385950 -1.853271
13 8 0 -1.713871 -1.692841 -0.375205
14 8 0 2.143500 1.356701 0.351221
15 6 0 -3.583710 0.001023 -0.453716
16 8 0 -3.623849 -0.000701 0.928073
17 1 0 -3.978028 -0.930682 -0.897419
18 1 0 -3.978870 0.933476 -0.894948

```

ZCO-INT4

```

-----
Center Atomic Atomic Coordinates (Angstroms)

```

```

Number Number Type X Y Z
-----

```

```

1 40 0 -1.007995 -0.000480 -1.653298
2 8 0 0.734718 1.386065 -1.824433
3 40 0 -1.669043 0.000169 0.874497
4 8 0 -0.191404 1.388437 1.830309
5 40 0 0.222720 -2.258385 -0.008983
6 8 0 2.133075 -1.357814 0.471231
7 40 0 1.326130 -0.000066 1.854959
8 8 0 -0.191293 -1.388087 1.830630
9 40 0 0.222595 2.258617 -0.009298
10 8 0 -1.670004 1.693986 -0.492995
11 40 0 2.089379 0.000062 -1.127076
12 8 0 0.735021 -1.385999 -1.824212
13 8 0 -1.670000 -1.694061 -0.492865
14 8 0 2.132981 1.357974 0.471048
15 6 0 -3.886651 -0.000057 -0.223964
16 8 0 -3.685536 0.000085 1.101842
17 1 0 -4.192839 -0.945761 -0.690616
18 1 0 -4.192969 0.945513 -0.690800
19 1 0 -2.266173 -0.000803 -3.071293

```

ZCO-TS3

-----  
Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z  
-----

1 40 0 1.116677 0.001418 -1.556213  
2 8 0 -0.607671 -1.386580 -1.856803  
3 40 0 1.587618 0.000040 1.014216  
4 8 0 0.043151 -1.388362 1.856773  
5 40 0 -0.234572 2.258213 -0.008590  
6 8 0 -2.174888 1.356814 0.327861  
7 40 0 -1.473036 0.000318 1.767036  
8 8 0 0.041382 1.388173 1.856912  
9 40 0 -0.231525 -2.259087 -0.008497  
10 8 0 1.691225 -1.693070 -0.349632  
11 40 0 -2.011353 -0.001311 -1.262614  
12 8 0 -0.609536 1.385329 -1.856900  
13 8 0 1.689129 1.694958 -0.349737  
14 8 0 -2.173335 -1.359235 0.327947  
15 6 0 4.180918 0.001950 -0.247298  
16 8 0 3.695732 0.001797 0.939042  
17 1 0 4.506875 0.949874 -0.697374  
18 1 0 4.506585 -0.945895 -0.697743  
19 1 0 2.987179 0.002099 -2.098367

\*\*\*\*\* 1 imaginary frequencies (negative Signs) \*\*\*\*\*

Diagonal vibrational polarizability:

130.6669269 27.1444745 21.7903263

Harmonic frequencies (cm<sup>-1</sup>), IR intensities (KM/Mole), Raman scattering activities (A<sup>4</sup>/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

1 2 3

A A A

Frequencies -- -507.6308 68.2551 147.3333

Red. masses -- 1.1240 2.6243 4.1862

Frc consts -- 0.1706 0.0072 0.0535

IR Inten -- 945.0892 2.7348 13.8859

Atom AN X Y Z X Y Z X Y Z

15 6 0.01 -0.00 -0.06 -0.00 0.36 0.00 0.22 -0.00 0.37  
16 8 0.01 0.00 -0.07 -0.00 0.10 0.00 0.01 -0.00 0.27  
17 1 0.14 -0.01 0.02 -0.40 0.52 0.04 0.29 0.00 0.42  
18 1 0.14 0.01 0.02 0.40 0.52 -0.04 0.29 -0.00 0.42  
19 1 0.42 0.00 0.88 0.00 -0.00 0.00 0.19 -0.00 0.42

ZCO-INT5

-----  
Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z  
-----

1	40	0	-0.650190	0.019670	-1.855106
2	8	0	1.117355	1.377007	-1.705897
3	40	0	-1.754486	0.030645	0.512824
4	8	0	-0.450138	1.393851	1.723024
5	40	0	0.228010	-2.258884	-0.023828
6	8	0	2.035478	-1.390402	0.794652
7	40	0	1.015374	-0.019756	2.015343
8	8	0	-0.495479	-1.382301	1.714317
9	40	0	0.301788	2.257501	-0.009448
10	8	0	-1.482090	1.724619	-0.827074
11	40	0	2.301842	-0.031562	-0.781072
12	8	0	1.072286	-1.394673	-1.714660
13	8	0	-1.537503	-1.662960	-0.837981
14	8	0	2.079815	1.325011	0.803306
15	6	0	-5.061854	-0.010039	0.223265
16	8	0	-3.710702	0.038229	0.538966
17	1	0	-5.682241	-0.055163	1.138078
18	1	0	-5.372353	0.885752	-0.347810
19	1	0	-5.299966	-0.901926	-0.387587

ZCO-INT6

-----  
Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z  
-----

1	40	0	0.579584	0.051325	-1.900567
2	8	0	-1.129885	-1.381610	-1.704551
3	40	0	1.775405	-0.004981	0.452904
4	8	0	0.544603	-1.431887	1.666825
5	40	0	-0.289706	2.244490	0.016129
6	8	0	-2.042363	1.304599	0.889727
7	40	0	-0.945437	-0.064631	2.043376
8	8	0	0.515862	1.353740	1.720321
9	40	0	-0.239220	-2.274337	-0.061627
10	8	0	1.502804	-1.673455	-0.923371
11	40	0	-2.324134	-0.025302	-0.709241
12	8	0	-1.163898	1.392484	-1.648140
13	8	0	1.467977	1.687225	-0.822678

```

14 8 0 -2.015287 -1.410227 0.831723
15 6 0 5.088226 0.004879 0.255495
16 1 0 5.386612 0.917041 -0.293373
17 1 0 5.665826 -0.028969 1.196996
18 1 0 5.376498 -0.872798 -0.352048
19 8 0 3.720401 0.004350 0.515750
20 1 0 -0.419722 4.131133 0.071641

```

ZCO-TS4

-----  
Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z  
-----

```

1 40 0 0.625620 -0.100692 -1.862652
2 8 0 -1.154678 -1.433071 -1.649033
3 40 0 1.751255 -0.037509 0.494842
4 8 0 0.442853 -1.341918 1.764966
5 40 0 -0.214039 2.250667 -0.109439
6 8 0 -2.022231 1.432478 0.756788
7 40 0 -1.004384 0.098162 2.019598
8 8 0 0.516123 1.429738 1.656125
9 40 0 -0.333892 -2.258968 0.070490
10 8 0 1.448841 -1.775949 -0.780453
11 40 0 -2.316345 0.020516 -0.766112
12 8 0 -1.080935 1.336025 -1.759172
13 8 0 1.538822 1.608184 -0.914746
14 8 0 -2.094234 -1.279936 0.864866
15 6 0 5.049841 -0.129551 0.177243
16 1 0 5.325789 0.737815 -0.451855
17 1 0 5.693672 -0.111616 1.076141
18 1 0 5.286689 -1.050696 -0.388143
19 8 0 3.705639 -0.087443 0.529066
20 1 0 2.664598 3.209825 1.084100

```

\*\*\*\*\* 1 imaginary frequencies (negative Signs) \*\*\*\*\*

Diagonal vibrational polarizability:

41.7031757 21.2591079 23.2166747

Harmonic frequencies (cm\*\*<sup>-1</sup>), IR intensities (KM/Mole), Raman scattering activities (A\*\*<sup>4</sup>/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

1 2 3

A A A

Frequencies -- -163.5297 30.9707 40.1291

Red. masses -- 1.0081 2.9634 3.1140

```

Frc consts -- 0.0159 0.0017 0.0030
IR Inten -- 5.8929 0.4539 1.2669
Atom AN X Y Z X Y Z X Y Z
15 6 -0.00 0.00 -0.00 0.01 0.40 -0.02 0.07 0.02 0.41
16 1 -0.00 0.00 0.00 -0.20 0.45 -0.05 0.19 0.02 0.46
17 1 0.00 -0.00 -0.00 0.01 0.58 -0.03 -0.12 0.03 0.54
18 1 -0.00 0.00 -0.01 0.22 0.44 0.01 0.20 0.02 0.46
19 8 0.00 -0.00 0.00 0.00 0.10 -0.01 -0.00 0.01 0.12
20 1 0.79 -0.51 0.35 0.01 0.02 -0.03 -0.00 0.00 0.03

```

ZCO-P

-----  
Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

-----  
1 40 0 -0.606480 0.321108 -1.833587  
2 8 0 1.423918 1.230700 -1.639174  
3 40 0 -1.674208 0.452449 0.547600  
4 8 0 -0.090344 1.415366 1.808829  
5 40 0 -0.265823 -2.194483 -0.138276  
6 8 0 1.693793 -1.805574 0.698098  
7 40 0 1.015638 -0.307483 2.004323  
8 8 0 -0.766563 -1.272940 1.654213  
9 40 0 0.834323 2.178912 0.113152  
10 8 0 -1.025927 2.111245 -0.704808  
11 40 0 2.258783 -0.458653 -0.807560  
12 8 0 0.748862 -1.453567 -1.793476  
13 8 0 -1.851208 -1.169411 -0.893647  
14 8 0 2.355262 0.824181 0.849358  
15 6 0 -5.204669 0.153548 0.503371  
16 1 0 -5.280080 1.050154 1.132446  
17 1 0 -5.896412 0.251758 -0.347370  
18 1 0 -5.470962 -0.731488 1.101817  
19 8 0 -3.857797 0.065503 0.042398  
20 1 0 -3.653831 -0.729752 -0.507602

ZMeOH-R

-----  
Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

-----  
1 40 0 -0.606480 0.321108 -1.833587  
2 8 0 1.423918 1.230700 -1.639174  
3 40 0 -1.674208 0.452449 0.547600



4 8 0 -0.090344 1.415366 1.808829  
 5 40 0 -0.265823 -2.194483 -0.138276  
 6 8 0 1.693793 -1.805574 0.698098  
 7 40 0 1.015638 -0.307483 2.004323  
 8 8 0 -0.766563 -1.272940 1.654213  
 9 40 0 0.834323 2.178912 0.113152  
 10 8 0 -1.025927 2.111245 -0.704808  
 11 40 0 2.258783 -0.458653 -0.807560  
 12 8 0 0.748862 -1.453567 -1.793476  
 13 8 0 -1.851208 -1.169411 -0.893647  
 14 8 0 2.355262 0.824181 0.849358  
 15 6 0 -5.204669 0.153548 0.503371  
 16 1 0 -5.280080 1.050154 1.132446  
 17 1 0 -5.896412 0.251758 -0.347370  
 18 1 0 -5.470962 -0.731488 1.101817  
 19 8 0 -3.857797 0.065503 0.042398  
 20 1 0 -3.653831 -0.729752 -0.507602

ZMeOH-TS1

-----  
 Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

-----  
 1 40 0 1.334507 -0.005356 -1.429960  
 2 8 0 -0.382170 -1.363405 -1.862843  
 3 40 0 1.474987 0.011448 1.238336  
 4 8 0 -0.195984 -1.347203 1.878318  
 5 40 0 -0.267186 2.215855 -0.008471  
 6 8 0 -2.192258 1.313186 0.085201  
 7 40 0 -1.693893 0.009814 1.643470  
 8 8 0 -0.210498 1.378870 1.873442  
 9 40 0 -0.262392 -2.221207 0.011844  
 10 8 0 1.633560 -1.711628 -0.107184  
 11 40 0 -1.857211 -0.012088 -1.492004  
 12 8 0 -0.386280 1.336423 -1.877477  
 13 8 0 1.627431 1.716859 -0.139345  
 14 8 0 -2.183986 -1.320931 0.101983  
 15 6 0 3.976219 0.015817 -0.746573  
 16 1 0 3.536505 -0.942231 -1.057544  
 17 1 0 3.509009 0.970842 -1.016169  
 18 1 0 5.060399 0.043257 -0.887756  
 19 8 0 3.624643 0.057660 0.984232  
 20 1 0 4.208601 -0.584041 1.421672

\*\*\*\*\* 1 imaginary frequencies (negative Signs) \*\*\*\*\*

Diagonal vibrational polarizability:  
344.6373663 7.3308900 45.9858238  
Harmonic frequencies (cm\*\*<sup>-1</sup>), IR intensities (KM/Mole), Raman scattering  
activities (A\*\*<sup>4</sup>/AMU), depolarization ratios for plane and unpolarized  
incident light, reduced masses (AMU), force constants (mDyne/A),  
and normal coordinates:  
1 2 3  
A A A  
Frequencies -- -803.0832 29.5901 63.4767  
Red. masses -- 11.4742 3.2282 3.6800  
Frc consts -- 4.3601 0.0017 0.0087  
IR Inten -- 7504.1672 1.6603 0.2603  
Atom AN X Y Z X Y Z X Y Z  
15 6 -0.45 -0.37 0.30 0.03 0.24 0.36 -0.14 0.31 -0.22  
16 1 -0.15 -0.03 0.12 0.27 0.29 0.41 -0.15 0.28 -0.20  
17 1 -0.14 -0.14 0.08 -0.02 0.16 0.25 -0.25 0.22 -0.22  
18 1 -0.20 -0.10 0.04 -0.14 0.31 0.49 -0.10 0.43 -0.29  
19 8 0.51 0.27 -0.25 0.01 0.05 0.10 0.03 0.23 -0.04  
20 1 0.18 0.09 -0.10 0.07 0.09 0.14 0.21 0.36 0.18

ZMeOH-INT1

-----  
Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z  
-----

1 40 0 0.408790 0.207584 -1.966946  
2 8 0 -1.180406 -1.337494 -1.693399  
3 40 0 1.846630 0.140982 0.213821  
4 8 0 0.870059 -1.439280 1.469048  
5 40 0 -0.402202 2.238708 0.162632  
6 8 0 -1.978349 1.124477 1.145026  
7 40 0 -0.663833 -0.216092 2.085956  
8 8 0 0.649704 1.318754 1.698931  
9 40 0 -0.043792 -2.248101 -0.211481  
10 8 0 1.541312 -1.469574 -1.219153  
11 40 0 -2.343926 -0.135269 -0.491989  
12 8 0 -1.400566 1.416337 -1.463754  
13 8 0 1.272427 1.896211 -0.938784  
14 8 0 -1.762765 -1.573482 0.920153  
15 6 0 3.576523 -1.280602 0.661848  
16 1 0 3.284696 -2.345467 0.714591  
17 1 0 4.355588 -1.153689 -0.109466  
18 1 0 4.013253 -0.975732 1.630644  
19 8 0 3.431542 1.362298 0.343910

20 1 0 3.276968 2.260001 0.017604

ZMeOH-TS2

-----  
Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z  
-----

1 40 0 -1.183392 0.384246 -1.631763  
2 8 0 0.913962 1.412739 -1.684658  
3 40 0 -1.656709 0.253986 0.939606  
4 8 0 0.167853 1.212949 1.922736  
5 40 0 -0.122884 -2.301786 -0.208678  
6 8 0 1.937490 -1.756190 0.251833  
7 40 0 1.388600 -0.372890 1.692671  
8 8 0 -0.330300 -1.430289 1.674913  
9 40 0 0.727721 2.248901 0.200072  
10 8 0 -1.155800 2.045517 -0.174122  
11 40 0 1.948255 -0.227720 -1.160796  
12 8 0 0.420636 -1.282765 -1.928290  
13 8 0 -1.806587 -1.419714 -0.500387  
14 8 0 2.441017 0.947537 0.489500  
15 6 0 -3.224798 0.702206 -0.912465  
16 1 0 -3.622975 1.732464 -0.971135  
17 1 0 -3.925030 -0.075249 -1.285635  
18 1 0 -3.839501 0.131360 0.481184  
19 8 0 -3.747273 -0.256642 1.509658  
20 1 0 -4.055327 -1.176415 1.516498

\*\*\*\*\* 1 imaginary frequencies (negative Signs) \*\*\*\*\*

Diagonal vibrational polarizability:

92.6416563 34.5273259 33.8860205

Harmonic frequencies (cm<sup>-1</sup>), IR intensities (KM/Mole), Raman scattering activities (A<sup>4</sup>/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

1 2 3

A A A

Frequencies -- -1247.8540 24.1511 94.7810

Red. masses -- 1.0410 3.1824 4.0299

Frc consts -- 0.9551 0.0011 0.0213

IR Inten -- 2105.8403 0.7137 6.6216

Atom AN X Y Z X Y Z X Y Z

15 6 -0.03 -0.02 0.01 0.07 0.18 0.37 0.01 0.02 0.16

16 1 0.06 0.01 0.01 0.25 0.10 0.52 0.28 0.21 0.11

17 1 0.08 -0.04 -0.01 -0.04 0.35 0.46 -0.22 -0.14 0.15

18 1 -0.04 0.94 -0.30 -0.01 0.11 0.13 -0.01 0.06 0.37  
19 8 0.03 -0.00 -0.00 -0.04 0.01 -0.13 0.04 0.11 0.41  
20 1 0.06 -0.05 0.06 -0.12 0.14 -0.26 -0.21 -0.00 0.62

ZMeOH-INT2

-----  
Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

-----  
1 40 0 -1.082828 0.593532 -1.619783  
2 8 0 1.121002 1.355525 -1.620462  
3 40 0 -1.657521 0.468026 0.929363  
4 8 0 0.264030 1.150169 1.960496  
5 40 0 -0.401855 -2.243455 -0.304434  
6 8 0 1.695637 -1.972016 0.222989  
7 40 0 1.273331 -0.575321 1.694581  
8 8 0 -0.560890 -1.414552 1.599032  
9 40 0 1.000202 2.154747 0.286682  
10 8 0 -0.880737 2.200789 -0.145231  
11 40 0 1.940591 -0.415538 -1.135818  
12 8 0 0.307456 -1.240160 -1.971752  
13 8 0 -1.962451 -1.162264 -0.615386  
14 8 0 2.523297 0.637646 0.567564  
15 6 0 -3.059079 1.153072 -0.850824  
16 1 0 -3.303872 2.230174 -0.790082  
17 1 0 -3.921999 0.509689 -1.127837  
18 1 0 -4.052383 0.042397 0.658479  
19 8 0 -3.710848 -0.503871 1.417814  
20 1 0 -3.616063 -1.390459 1.020278

ZMeOH-INT3

-----  
Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

-----  
1 40 0 -0.790471 1.755883 -0.003237  
2 8 0 0.946620 1.537619 1.383565  
3 40 0 -1.997927 -0.561273 0.001059  
4 8 0 -0.769413 -1.819746 1.391152  
5 40 0 0.044178 -0.124948 -2.257868  
6 8 0 1.799571 -1.016235 -1.355888  
7 40 0 0.704733 -2.183624 0.003341  
8 8 0 -0.768986 -1.824786 -1.385008  
9 40 0 0.043445 -0.116585 2.258433

```

10 8 0 -1.694060 0.775043 1.692385
11 40 0 2.112356 0.554025 -0.000625
12 8 0 0.947132 1.532613 -1.388620
13 8 0 -1.693174 0.769490 -1.696019
14 8 0 1.799075 -1.011655 1.359962
15 6 0 -1.526735 3.765723 -0.006342
16 1 0 -1.614672 4.389484 -0.913923
17 1 0 -1.613874 4.392246 0.899420
18 8 0 -3.922304 -0.821140 0.000930
19 1 0 -4.876629 -0.708008 0.000196
20 6 0 4.256922 1.229077 -0.001253
21 1 0 4.484762 1.839611 0.892485
22 1 0 4.483164 1.843699 -0.892587
23 1 0 4.947924 0.365414 -0.003834

```

ZMeOH-TS3

-----  
Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z  
-----

```

1 40 0 1.618161 -0.839597 -0.000751
2 8 0 0.184653 -1.845607 1.385531
3 40 0 0.951922 1.687205 0.000647
4 8 0 -0.805152 1.792775 1.388692
5 40 0 -0.262581 -0.011816 -2.257959
6 8 0 -2.161829 -0.532969 -1.357635
7 40 0 -2.138988 1.068639 0.000102
8 8 0 -0.805821 1.793556 -1.387505
9 40 0 -0.261453 -0.013171 2.258143
10 8 0 1.624512 0.495883 1.693759
11 40 0 -1.337810 -1.903872 0.000218
12 8 0 0.183887 -1.844649 -1.386505
13 8 0 1.623836 0.496177 -1.694567
14 8 0 -2.161421 -0.533339 1.358107
15 6 0 3.716866 -0.337707 -0.000957
16 1 0 4.345162 -0.327258 -0.908630
17 1 0 4.345454 -0.327659 0.906524
18 8 0 1.972288 3.327711 0.000758
19 1 0 2.608701 4.046392 0.000963
20 6 0 2.902555 -2.778932 -0.001535
21 1 0 3.995280 -2.866999 -0.001765
22 1 0 2.489439 -3.257968 -0.906953
23 1 0 2.489771 -3.258537 0.903734

```

\*\*\*\*\* 1 imaginary frequencies (negative Signs) \*\*\*\*\*

Diagonal vibrational polarizability:

73.4905217 63.6979976 37.2349265

Harmonic frequencies (cm\*\*<sup>-1</sup>), IR intensities (KM/Mole), Raman scattering activities (A\*\*<sup>4</sup>/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

1 2 3

A A A

Frequencies -- -234.9316 34.5449 90.6546

Red. masses -- 3.6767 1.2393 3.1663

Frc consts -- 0.1196 0.0009 0.0153

IR Inten -- 153.8471 0.0054 1.5456

Atom AN X Y Z X Y Z X Y Z

15 6 -0.08 0.40 0.00 -0.00 0.00 -0.02 -0.04 0.18 0.00

16 1 -0.08 0.52 -0.00 -0.03 0.02 -0.05 -0.05 0.25 -0.00

17 1 -0.08 0.52 0.00 0.03 -0.02 -0.05 -0.05 0.25 0.00

18 8 -0.05 0.02 0.00 0.00 -0.00 -0.00 0.23 -0.14 -0.00

19 1 -0.02 -0.01 0.00 0.00 -0.00 -0.00 0.52 -0.39 -0.00

20 6 -0.25 -0.12 -0.00 0.00 -0.00 0.14 0.22 0.14 -0.00

21 1 -0.23 0.12 0.00 -0.00 0.00 -0.26 0.22 0.25 0.00

22 1 -0.15 -0.22 0.01 -0.36 -0.31 0.47 0.27 0.09 -0.00

23 1 -0.15 -0.22 -0.01 0.36 0.31 0.47 0.27 0.09 -0.00

ZMeOH-INT4

-----  
Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z  
-----

1 40 0 1.667643 -0.357643 0.510165

2 8 0 0.208590 -1.149923 2.004077

3 40 0 0.563414 1.787828 -0.492163

4 8 0 -1.411672 1.932550 0.558410

5 40 0 0.123866 -0.807544 -2.084243

6 8 0 -1.782695 -1.431379 -1.268545

7 40 0 -2.307085 0.489688 -0.602514

8 8 0 -0.893068 1.001378 -2.004939

9 40 0 -0.719702 0.707314 2.085981

10 8 0 1.113266 1.429733 1.583405

11 40 0 -0.991270 -2.029630 0.579692

12 8 0 0.726430 -2.079871 -0.555616

13 8 0 1.746521 0.292593 -1.545061

14 8 0 -2.290265 -0.520176 1.239042

15 6 0 3.870019 -0.531381 0.945514

16 1 0 4.346693 0.455660 0.788090

```

17 1 0 4.003498 -0.779467 2.017290
18 8 0 1.554296 3.413591 -0.882578
19 1 0 2.229636 4.087950 -0.990001
20 6 0 4.495475 -1.601254 0.039662
21 1 0 5.575319 -1.751212 0.223430
22 1 0 4.389384 -1.337470 -1.027035
23 1 0 4.016660 -2.588096 0.174875

```

ZMeOH-TS4

-----  
Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z  
-----

```

1 40 0 -1.009586 -0.174051 -1.513635
2 8 0 0.462183 1.474599 -1.835665
3 40 0 -1.379241 -0.301731 1.069788
4 8 0 -0.042145 1.296470 1.896739
5 40 0 0.737311 -2.220211 -0.071755
6 8 0 2.522291 -1.030071 0.222788
7 40 0 1.669042 0.168538 1.720887
8 8 0 0.396996 -1.443718 1.824017
9 40 0 0.022705 2.237656 0.046496
10 8 0 -1.798553 1.381928 -0.244879
11 40 0 2.087764 0.317009 -1.325140
12 8 0 0.900807 -1.261691 -1.908355
13 8 0 -1.262376 -1.962609 -0.334340
14 8 0 2.092726 1.650652 0.294241
15 6 0 -4.733151 0.456259 0.244944
16 1 0 -5.639993 0.238721 0.813914
17 1 0 -4.314969 1.451327 0.402347
18 8 0 -3.492250 -0.445687 1.309866
19 1 0 -3.938406 -1.256767 1.594201
20 6 0 -4.588115 -0.117895 -1.113910
21 1 0 -4.753938 0.635506 -1.902811
22 1 0 -5.242768 -0.981993 -1.297593
23 1 0 -3.539560 -0.484408 -1.257174

```

\*\*\*\*\* 1 imaginary frequencies (negative Signs) \*\*\*\*\*

Diagonal vibrational polarizability:

429.2212605 11.2921217 86.7338438

Harmonic frequencies (cm<sup>-1</sup>), IR intensities (KM/Mole), Raman scattering activities (A<sup>4</sup>/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

1 2 3

A A A

Frequencies -- -879.3606 34.7099 43.6155

Red. masses -- 9.5906 2.3982 3.5665

Frc consts -- 4.3695 0.0017 0.0040

IR Inten -- 10531.4071 2.4085 1.2932

Atom AN X Y Z X Y Z X Y Z

15 6 -0.40 0.27 -0.33 0.07 -0.00 -0.13 0.04 0.25 0.14

16 1 -0.01 -0.20 0.06 0.01 -0.08 -0.26 0.05 0.27 0.16

17 1 -0.20 0.12 -0.02 0.00 0.01 -0.02 0.12 0.21 0.21

18 8 0.47 -0.20 0.26 -0.02 0.02 -0.04 0.00 0.09 0.04

19 1 0.19 -0.07 0.12 -0.03 0.03 -0.04 -0.06 0.13 0.06

20 6 -0.03 0.06 -0.03 0.26 0.09 -0.15 -0.04 0.35 0.09

21 1 0.14 -0.17 -0.29 0.65 0.20 -0.13 0.09 0.45 0.16

22 1 0.07 -0.02 -0.05 0.11 0.25 -0.39 -0.18 0.47 0.01

23 1 0.18 0.01 -0.11 0.21 -0.17 0.10 -0.09 0.20 0.07

ZMeOH-P

-----  
Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

-----  
1 40 0 0.951176 -0.000286 1.570610

2 8 0 -0.776869 1.386595 1.854909

3 40 0 1.447475 0.000314 -0.994360

4 8 0 -0.089804 1.387639 -1.852722

5 40 0 -0.384226 -2.258013 0.010573

6 8 0 -2.321376 -1.357865 -0.344606

7 40 0 -1.605724 -0.000848 -1.778413

8 8 0 -0.090068 -1.388534 -1.852227

9 40 0 -0.383674 2.258218 0.009937

10 8 0 1.536296 1.694020 0.370040

11 40 0 -2.173939 0.000839 1.246582

12 8 0 -0.777290 -1.385470 1.855591

13 8 0 1.535802 -1.694481 0.371233

14 8 0 -2.321059 1.358062 -0.345526

15 6 0 4.846257 -0.000240 -0.269342

16 1 0 5.458991 -0.896666 -0.455737

17 1 0 5.458741 0.896417 -0.455451

18 8 0 3.746000 -0.000254 -1.218367

19 1 0 4.085446 0.000129 -2.125408

20 6 0 4.300758 -0.000549 1.142580

21 1 0 5.135236 -0.000652 1.859596

22 1 0 3.701464 -0.909623 1.316714

23 1 0 3.701431 0.908441 1.317083



TGro.-R

-----  
Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z  
-----

1	7	0	1.411146	1.376306	0.020386
2	7	0	1.361917	-1.529487	-0.191562
3	7	0	-1.604509	-1.334109	-0.072884
4	7	0	-1.629624	1.715156	0.450817
5	6	0	1.265965	2.737010	0.103448
6	6	0	2.578392	3.357271	0.149435
7	6	0	3.498585	2.356007	0.044446
8	6	0	2.760542	1.113156	-0.065448
9	6	0	3.378001	-0.140966	-0.263790
10	6	0	2.699043	-1.371122	-0.378829
11	6	0	3.283222	-2.652398	-0.732904
12	6	0	2.264406	-3.564438	-0.726889
13	6	0	1.051462	-2.845211	-0.367658
14	6	0	-0.237433	-3.408330	-0.230910
15	6	0	-1.441034	-2.690360	-0.027678
16	6	0	-2.718596	-3.334164	0.263088
17	6	0	-3.641268	-2.337754	0.364952
18	6	0	-2.925816	-1.086446	0.134241
19	6	0	-3.570390	0.181734	0.061395
20	6	0	-2.922782	1.425698	-0.005101
21	6	0	-3.396279	2.612117	-0.647030
22	6	0	-2.381609	3.545011	-0.653773
23	6	0	-1.238539	2.972608	-0.015100
24	6	0	0.063330	3.493255	0.033886
25	1	0	2.766835	4.421749	0.253129
26	1	0	4.580960	2.445071	0.044891
27	1	0	4.329080	-2.822289	-0.974422
28	1	0	2.319159	-4.621642	-0.971467
29	1	0	-2.874931	-4.400686	0.398258
30	1	0	-4.698711	-2.431166	0.597211
31	1	0	-4.366556	2.693521	-1.129446
32	1	0	-2.382993	4.516231	-1.141031
33	29	0	0.235876	-0.185809	0.663624
34	6	0	-0.327942	-4.895373	-0.307954
35	6	0	0.354362	-5.703036	0.617787
36	6	0	-1.091589	-5.518633	-1.309532
37	6	0	0.271733	-7.094927	0.546921
38	1	0	0.942998	-5.228298	1.405516

39 6 0 -1.170129 -6.910525 -1.383823  
40 1 0 -1.617001 -4.899114 -2.039119  
41 6 0 -0.489877 -7.703305 -0.454943  
42 1 0 0.801254 -7.707016 1.280995  
43 1 0 -1.762529 -7.378378 -2.173885  
44 1 0 -0.553172 -8.792593 -0.511642  
45 6 0 -5.049276 0.215933 -0.099751  
46 6 0 -5.693761 -0.553076 -1.086371  
47 6 0 -5.834295 1.046897 0.720451  
48 6 0 -7.079615 -0.498902 -1.240228  
49 1 0 -5.093814 -1.183110 -1.745353  
50 6 0 -7.220604 1.097935 0.568993  
51 1 0 -5.345435 1.643989 1.492994  
52 6 0 -7.848296 0.324341 -0.411731  
53 1 0 -7.561731 -1.097106 -2.017158  
54 1 0 -7.814350 1.740427 1.223615  
55 1 0 -8.933508 0.364594 -0.531837  
56 6 0 4.865211 -0.181666 -0.380590  
57 6 0 5.627826 -0.838932 0.598850  
58 6 0 5.525684 0.413779 -1.467305  
59 6 0 7.019311 -0.894166 0.495164  
60 1 0 5.115285 -1.287070 1.452527  
61 6 0 6.917087 0.355086 -1.571956  
62 1 0 4.936941 0.916671 -2.237505  
63 6 0 7.667893 -0.298435 -0.590447  
64 1 0 7.600139 -1.401460 1.269329  
65 1 0 7.416613 0.817926 -2.426557  
66 1 0 8.756593 -0.343318 -0.671803  
67 6 0 0.160558 4.966021 -0.182539  
68 6 0 -0.506524 5.849923 0.683363  
69 6 0 0.872811 5.501861 -1.270225  
70 6 0 -0.448374 7.229848 0.480337  
71 1 0 -1.065467 5.443186 1.528858  
72 6 0 0.927525 6.881260 -1.476129  
73 1 0 1.372868 4.824015 -1.964550  
74 6 0 0.270300 7.750111 -0.599701  
75 1 0 -0.963957 7.901856 1.170569  
76 1 0 1.479977 7.279679 -2.330519  
77 1 0 0.315020 8.829826 -0.760689  
78 6 0 -0.986403 1.042725 1.491758  
79 1 0 -0.341875 1.685017 2.096939  
80 1 0 -1.630080 0.370789 2.057359  
81 6 0 3.168564 -0.031164 3.202835  
82 1 0 3.586010 0.868653 2.747756

83 1 0 3.767938 -0.571184 3.939476  
84 1 0 2.143389 -0.345846 2.975227  
85 8 0 0.132024 -1.008101 2.390198  
86 1 0 0.477657 -1.892269 2.200247

TGro.-TS1

-----  
Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z  
-----

1 7 0 0.094478 2.048137 0.002267  
2 7 0 2.001928 -0.174961 -0.361073  
3 7 0 -0.276571 -2.033401 -0.008382  
4 7 0 -2.309055 0.194438 0.424046  
5 6 0 -0.908662 2.958320 0.165515  
6 6 0 -0.340709 4.289312 0.319522  
7 6 0 1.011270 4.153110 0.201244  
8 6 0 1.276941 2.739754 -0.029889  
9 6 0 2.565048 2.213735 -0.291695  
10 6 0 2.881749 0.851040 -0.488429  
11 6 0 4.203296 0.311322 -0.793311  
12 6 0 4.082253 -1.048522 -0.784470  
13 6 0 2.685312 -1.342637 -0.476275  
14 6 0 2.131896 -2.627314 -0.276233  
15 6 0 0.768322 -2.921435 -0.026912  
16 6 0 0.260051 -4.265550 0.209862  
17 6 0 -1.096705 -4.163874 0.318937  
18 6 0 -1.423804 -2.756028 0.154230  
19 6 0 -2.746463 -2.243699 0.066185  
20 6 0 -3.080505 -0.880250 -0.036631  
21 6 0 -4.206676 -0.316925 -0.706298  
22 6 0 -4.078430 1.056825 -0.700147  
23 6 0 -2.866906 1.399337 -0.029079  
24 6 0 -2.298440 2.682397 0.080674  
25 1 0 -0.902551 5.199790 0.509056  
26 1 0 1.764333 4.933317 0.267211  
27 1 0 5.097322 0.898069 -0.987080  
28 1 0 4.858281 -1.785864 -0.972095  
29 1 0 0.864523 -5.165087 0.285907  
30 1 0 -1.808706 -4.962619 0.508351  
31 1 0 -4.970996 -0.904130 -1.208357  
32 1 0 -4.721631 1.779705 -1.194898  
33 29 0 0.133498 0.019078 0.317934  
34 6 0 3.087824 -3.774912 -0.302242

35 6 0 4.081719 -3.885196 0.684696  
36 6 0 3.020813 -4.755121 -1.305399  
37 6 0 4.983588 -4.951211 0.669832  
38 1 0 4.133200 -3.128967 1.471329  
39 6 0 3.925024 -5.819404 -1.322123  
40 1 0 2.256425 -4.670749 -2.080807  
41 6 0 4.908482 -5.921198 -0.333992  
42 1 0 5.746617 -5.026161 1.448465  
43 1 0 3.863784 -6.570438 -2.113551  
44 1 0 5.615217 -6.754411 -0.346627  
45 6 0 -3.875852 -3.198853 -0.099107  
46 6 0 -3.848423 -4.203081 -1.084425  
47 6 0 -5.019419 -3.090835 0.713294  
48 6 0 -4.924214 -5.078024 -1.241676  
49 1 0 -2.980210 -4.280086 -1.741175  
50 6 0 -6.093952 -3.967655 0.558157  
51 1 0 -5.052700 -2.315112 1.481188  
52 6 0 -6.049376 -4.965989 -0.419297  
53 1 0 -4.887654 -5.846389 -2.017717  
54 1 0 -6.968491 -3.873868 1.206474  
55 1 0 -6.890576 -5.652183 -0.542712  
56 6 0 3.706627 3.176250 -0.329420  
57 6 0 4.703530 3.120838 0.659011  
58 6 0 3.811081 4.142154 -1.342923  
59 6 0 5.777709 4.012773 0.633967  
60 1 0 4.618244 2.376345 1.454122  
61 6 0 4.887659 5.031595 -1.369326  
62 1 0 3.043009 4.184956 -2.118177  
63 6 0 5.873725 4.969896 -0.380490  
64 1 0 6.541716 3.962237 1.413651  
65 1 0 4.958561 5.773666 -2.168388  
66 1 0 6.715317 5.666523 -0.400523  
67 6 0 -3.245541 3.820501 -0.075937  
68 6 0 -4.379066 3.916824 0.751466  
69 6 0 -3.055108 4.801072 -1.066717  
70 6 0 -5.284906 4.968388 0.605477  
71 1 0 -4.537370 3.161092 1.523680  
72 6 0 -3.962854 5.850681 -1.215208  
73 1 0 -2.195096 4.722752 -1.734050  
74 6 0 -5.078983 5.940285 -0.377924  
75 1 0 -6.153435 5.031721 1.265451  
76 1 0 -3.802374 6.598493 -1.995578  
77 1 0 -5.788263 6.763156 -0.494246  
78 6 0 -1.511558 0.108493 1.626550

```

79 1 0 -1.541785 1.064501 2.147285
80 1 0 -1.889771 -0.735840 2.203973
81 6 0 3.477936 -0.043516 2.786534
82 1 0 3.884677 0.090853 3.790843
83 1 0 4.147502 -0.310614 1.968020
84 1 0 2.406938 0.074622 2.602815
85 8 0 0.182945 -0.209445 2.349628
86 1 0 0.253661 -1.178500 2.355596

```

\*\*\*\*\* 1 imaginary frequencies (negative Signs) \*\*\*\*\*

Diagonal vibrational polarizability:

25.6414801 35.2980561 77.9903941

Harmonic frequencies (cm<sup>-1</sup>), IR intensities (KM/Mole), Raman scattering activities (A<sup>4</sup>/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

1 2 3

A A A

Frequencies -- -324.1964 14.2630 25.7485

Red. masses -- 7.4943 6.0646 5.5471

Frc consts -- 0.4641 0.0007 0.0022

IR Inten -- 49.9674 0.0065 0.5122

Atom AN X Y Z X Y Z X Y Z

```

1 7 -0.01 -0.01 -0.02 0.00 -0.01 0.00 0.00 -0.01 0.06
2 7 -0.03 0.00 0.00 -0.00 -0.01 -0.00 0.01 -0.01 0.09
3 7 -0.01 0.00 -0.04 -0.00 -0.01 -0.01 0.01 -0.00 0.08
4 7 -0.12 0.03 -0.07 0.00 -0.00 -0.00 -0.00 -0.00 0.05
5 6 -0.01 -0.02 -0.01 0.01 -0.00 0.03 0.00 -0.00 0.05
6 6 -0.01 -0.01 0.00 0.01 -0.00 0.02 0.00 -0.00 0.03
7 6 -0.01 -0.01 -0.00 0.01 -0.01 -0.01 0.00 -0.00 0.03
8 6 -0.01 -0.00 -0.01 0.00 -0.01 -0.02 0.00 -0.00 0.05
9 6 -0.01 0.00 0.00 -0.00 -0.01 -0.04 0.00 -0.00 0.05
10 6 -0.02 0.00 0.00 -0.00 -0.01 -0.03 0.01 -0.01 0.07
11 6 -0.02 0.00 0.00 -0.00 -0.02 -0.02 0.00 -0.01 0.06
12 6 -0.02 0.00 0.00 -0.00 -0.02 0.01 0.00 -0.01 0.07
13 6 -0.02 0.00 0.00 -0.00 -0.01 0.02 0.01 -0.01 0.08
14 6 -0.01 -0.00 -0.00 -0.00 -0.01 0.04 0.00 -0.01 0.06
15 6 -0.01 0.00 -0.01 -0.00 -0.01 0.02 0.00 -0.01 0.06
16 6 -0.01 0.01 0.00 -0.01 -0.01 0.01 -0.00 -0.01 0.04
17 6 -0.01 0.01 0.00 -0.01 -0.00 -0.02 -0.00 -0.00 0.04
18 6 -0.01 0.02 -0.02 -0.01 -0.00 -0.03 0.00 -0.00 0.06
19 6 -0.02 0.01 -0.02 -0.00 0.00 -0.05 0.00 -0.00 0.04
20 6 -0.06 0.00 -0.06 0.00 0.01 -0.02 0.00 -0.00 0.04
21 6 -0.06 0.00 -0.05 0.00 0.02 -0.02 0.01 -0.00 0.02
22 6 -0.07 0.01 -0.05 0.00 0.02 0.02 0.01 -0.00 0.02

```

23 6 -0.07 0.02 -0.06 0.00 0.01 0.02 0.00 -0.00 0.04  
24 6 -0.02 -0.00 -0.02 0.00 0.00 0.04 0.00 -0.00 0.03  
25 1 -0.01 -0.02 0.00 0.02 -0.00 0.04 0.00 0.00 0.01  
26 1 -0.01 -0.01 0.01 0.01 -0.01 -0.03 0.00 0.00 0.01  
27 1 -0.03 0.00 0.00 -0.00 -0.02 -0.03 0.00 -0.01 0.05  
28 1 -0.03 -0.00 0.00 -0.00 -0.02 0.03 0.00 -0.01 0.06  
29 1 -0.01 0.01 0.02 -0.02 -0.01 0.02 -0.00 -0.01 0.04  
30 1 -0.01 0.02 0.01 -0.02 -0.00 -0.04 -0.01 -0.00 0.03  
31 1 -0.07 0.01 -0.04 0.00 0.03 -0.03 0.02 -0.00 0.01  
32 1 -0.08 0.00 -0.04 0.00 0.03 0.03 0.02 -0.00 0.01  
33 29 -0.01 -0.01 0.13 -0.00 -0.00 -0.00 0.00 -0.00 0.08  
34 6 -0.00 0.00 0.00 0.01 -0.00 0.08 -0.01 -0.02 -0.01  
35 6 -0.00 0.00 0.00 -0.01 0.03 0.11 0.03 -0.07 -0.05  
36 6 -0.00 0.00 0.00 0.03 -0.03 0.11 -0.06 0.02 -0.05  
37 6 -0.00 0.00 0.00 -0.01 0.03 0.16 0.01 -0.08 -0.13  
38 1 -0.00 0.00 0.00 -0.03 0.05 0.09 0.07 -0.10 -0.03  
39 6 -0.00 0.00 0.00 0.04 -0.03 0.16 -0.08 0.01 -0.13  
40 1 -0.00 -0.00 0.00 0.05 -0.06 0.09 -0.09 0.06 -0.01  
41 6 -0.00 0.00 0.00 0.02 0.00 0.18 -0.04 -0.04 -0.17  
42 1 -0.00 0.00 0.00 -0.02 0.06 0.18 0.04 -0.12 -0.17  
43 1 -0.00 0.00 0.00 0.06 -0.05 0.18 -0.12 0.04 -0.15  
44 1 -0.00 0.00 0.00 0.02 0.01 0.22 -0.05 -0.05 -0.23  
45 6 -0.00 -0.00 -0.01 -0.00 0.01 -0.08 0.01 -0.00 -0.02  
46 6 -0.00 -0.00 -0.00 0.02 0.02 -0.10 0.05 0.03 -0.05  
47 6 -0.00 -0.00 -0.00 -0.02 -0.01 -0.11 -0.01 -0.03 -0.05  
48 6 -0.00 -0.00 -0.00 0.02 0.03 -0.14 0.05 0.03 -0.11  
49 1 -0.00 -0.00 -0.00 0.04 0.03 -0.08 0.07 0.05 -0.02  
50 6 -0.00 -0.00 0.00 -0.02 -0.00 -0.15 -0.01 -0.03 -0.11  
51 1 -0.00 0.00 -0.00 -0.04 -0.02 -0.10 -0.04 -0.05 -0.03  
52 6 -0.00 -0.00 0.00 0.01 0.01 -0.17 0.03 0.00 -0.14  
53 1 -0.00 -0.00 0.00 0.04 0.04 -0.15 0.08 0.05 -0.13  
54 1 0.00 -0.00 0.00 -0.03 -0.01 -0.17 -0.03 -0.05 -0.14  
55 1 -0.00 -0.00 0.00 0.01 0.02 -0.20 0.03 0.01 -0.19  
56 6 -0.00 0.00 0.00 -0.01 -0.01 -0.08 -0.01 0.00 -0.01  
57 6 -0.00 -0.00 0.00 0.02 0.02 -0.10 0.02 0.05 -0.04  
58 6 -0.00 -0.00 0.00 -0.03 -0.03 -0.10 -0.04 -0.03 -0.05  
59 6 -0.00 -0.00 0.00 0.01 0.02 -0.15 0.02 0.05 -0.11  
60 1 -0.00 -0.00 0.00 0.04 0.03 -0.09 0.05 0.08 -0.01  
61 6 -0.00 -0.00 0.00 -0.04 -0.02 -0.15 -0.05 -0.03 -0.12  
62 1 -0.00 0.00 0.00 -0.05 -0.04 -0.09 -0.07 -0.07 -0.03  
63 6 -0.00 -0.00 0.00 -0.02 0.00 -0.17 -0.02 0.02 -0.15  
64 1 -0.00 -0.00 0.00 0.03 0.04 -0.16 0.04 0.09 -0.13  
65 1 -0.00 -0.00 -0.00 -0.06 -0.04 -0.16 -0.08 -0.06 -0.15  
66 1 -0.00 -0.00 0.00 -0.02 0.01 -0.20 -0.03 0.02 -0.20

67 6 -0.00 0.01 -0.01 0.00 0.01 0.09 0.01 -0.00 -0.01  
 68 6 -0.00 0.00 -0.00 0.02 -0.01 0.11 -0.00 0.02 -0.03  
 69 6 -0.00 0.01 -0.00 -0.02 0.03 0.10 0.03 -0.03 -0.03  
 70 6 -0.00 0.00 0.00 0.02 -0.01 0.16 0.00 0.02 -0.08  
 71 1 0.00 0.00 -0.00 0.04 -0.03 0.10 -0.02 0.05 -0.01  
 72 6 -0.00 0.01 -0.00 -0.02 0.03 0.15 0.03 -0.03 -0.08  
 73 1 -0.00 0.01 -0.01 -0.03 0.04 0.08 0.04 -0.05 -0.02  
 74 6 -0.00 0.00 0.00 -0.00 0.01 0.17 0.02 -0.01 -0.10  
 75 1 -0.00 0.00 0.00 0.03 -0.02 0.18 -0.01 0.04 -0.09  
 76 1 -0.01 0.01 -0.00 -0.04 0.05 0.16 0.05 -0.06 -0.10  
 77 1 -0.00 0.00 0.00 -0.01 0.02 0.21 0.02 -0.01 -0.14  
 78 6 0.02 0.02 -0.32 -0.00 -0.02 -0.00 -0.02 0.00 0.06  
 79 1 0.23 -0.06 -0.18 -0.01 -0.03 0.01 -0.03 0.00 0.06  
 80 1 0.41 -0.11 -0.28 0.00 -0.03 -0.02 -0.02 0.00 0.06  
 81 6 0.02 0.00 0.00 -0.00 0.03 -0.01 -0.03 0.19 0.07  
 82 1 0.04 0.02 -0.00 -0.00 0.05 -0.01 -0.00 0.34 0.04  
 83 1 0.04 0.01 0.01 0.00 0.05 -0.01 -0.04 0.09 0.09  
 84 1 0.00 -0.11 0.03 -0.00 0.01 -0.01 -0.04 0.13 0.09  
 85 8 0.48 -0.03 0.08 -0.00 -0.02 -0.00 -0.03 0.01 0.08  
 86 1 0.43 -0.03 0.13 0.00 -0.02 -0.01 -0.02 0.01 0.09

TGro.-INT1

-----  
 Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

-----

1	7	0	-1.331934	-1.456400	-0.118974
2	7	0	-1.516941	1.491060	-0.424192
3	7	0	1.412144	1.495666	0.032027
4	7	0	1.665624	-1.498750	0.474748
5	6	0	-1.104722	-2.792632	0.097309
6	6	0	-2.370480	-3.479709	0.280243
7	6	0	-3.351246	-2.541304	0.143692
8	6	0	-2.692937	-1.273784	-0.126409
9	6	0	-3.407541	-0.064162	-0.322043
10	6	0	-2.849948	1.224805	-0.425111
11	6	0	-3.589085	2.485063	-0.451975
12	6	0	-2.660808	3.484217	-0.405951
13	6	0	-1.352362	2.835521	-0.350223
14	6	0	-0.110968	3.482016	-0.173860
15	6	0	1.141135	2.850407	0.015886
16	6	0	2.375553	3.586609	0.213450
17	6	0	3.384113	2.670018	0.296964
18	6	0	2.779722	1.360667	0.160835

19 6 0 3.512856 0.150627 0.099407  
20 6 0 2.945301 -1.134166 0.009120  
21 6 0 3.488756 -2.243966 -0.697939  
22 6 0 2.549388 -3.255100 -0.707325  
23 6 0 1.395229 -2.797982 -0.010168  
24 6 0 0.151473 -3.449634 0.055056  
25 1 0 -2.486739 -4.532651 0.522302  
26 1 0 -4.424613 -2.686616 0.227548  
27 1 0 -4.670663 2.585087 -0.488882  
28 1 0 -2.838241 4.556474 -0.389337  
29 1 0 2.457486 4.668241 0.274441  
30 1 0 4.440139 2.861125 0.466982  
31 1 0 4.441376 -2.225824 -1.221071  
32 1 0 2.602859 -4.199209 -1.243117  
33 29 0 -0.074525 0.104571 -0.253562  
34 6 0 -0.128439 4.978813 -0.148328  
35 6 0 -0.644675 5.670173 0.958574  
36 6 0 0.364777 5.717656 -1.234960  
37 6 0 -0.667006 7.066867 0.979131  
38 1 0 -1.027113 5.101331 1.808975  
39 6 0 0.343492 7.114180 -1.215447  
40 1 0 0.764317 5.185333 -2.101040  
41 6 0 -0.172742 7.793035 -0.107980  
42 1 0 -1.069584 7.589971 1.850054  
43 1 0 0.728619 7.674523 -2.070970  
44 1 0 -0.189995 8.885432 -0.092342  
45 6 0 4.990449 0.215780 -0.074420  
46 6 0 5.577277 0.992247 -1.090235  
47 6 0 5.832722 -0.542558 0.758336  
48 6 0 6.962634 1.019425 -1.257110  
49 1 0 4.933795 1.562816 -1.762227  
50 6 0 7.218401 -0.512487 0.594512  
51 1 0 5.387790 -1.151971 1.547804  
52 6 0 7.788537 0.270443 -0.413393  
53 1 0 7.399588 1.622308 -2.056854  
54 1 0 7.856226 -1.100499 1.258851  
55 1 0 8.873020 0.293551 -0.544137  
56 6 0 -4.900063 -0.158006 -0.323559  
57 6 0 -5.647127 0.329965 0.760465  
58 6 0 -5.578818 -0.740938 -1.404947  
59 6 0 -7.040966 0.239378 0.760658  
60 1 0 -5.118781 0.768068 1.609614  
61 6 0 -6.972786 -0.829999 -1.405678  
62 1 0 -5.002385 -1.122437 -2.250667



```

63 6 0 -7.708094 -0.339636 -0.322715
64 1 0 -7.608379 0.618797 1.614105
65 1 0 -7.486967 -1.282364 -2.257279
66 1 0 -8.798510 -0.410083 -0.322478
67 6 0 0.184031 -4.928418 -0.102340
68 6 0 1.021023 -5.708238 0.716756
69 6 0 -0.581825 -5.579335 -1.087416
70 6 0 1.079383 -7.094579 0.568534
71 1 0 1.620158 -5.214317 1.484543
72 6 0 -0.520591 -6.965183 -1.238320
73 1 0 -1.214245 -4.984355 -1.748399
74 6 0 0.307178 -7.728419 -0.409187
75 1 0 1.727347 -7.683357 1.222294
76 1 0 -1.116436 -7.451677 -2.014372
77 1 0 0.352869 -8.813636 -0.527388
78 6 0 1.342129 -1.228166 1.918387
79 1 0 0.778812 -2.099792 2.274210
80 1 0 2.316392 -1.185359 2.437862
81 6 0 -2.745928 -0.191823 3.055108
82 1 0 -3.386199 -1.042848 2.821015
83 1 0 -3.080988 0.550165 3.782198
84 1 0 -1.765937 -0.101570 2.584820
85 8 0 0.571370 -0.113469 2.190253
86 1 0 0.974587 0.673388 1.776650

```

TGro.-TS2

-----  
Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

-----  
1 7 0 -1.201053 -1.536701 -0.364553  
2 7 0 -1.664020 1.288666 -0.195410  
3 7 0 1.172592 1.744776 -0.210700  
4 7 0 1.635860 -1.079310 -0.293267  
5 6 0 -0.787757 -2.846479 -0.271299  
6 6 0 -1.937877 -3.717938 -0.182088  
7 6 0 -3.043931 -2.921958 -0.245364  
8 6 0 -2.574916 -1.557474 -0.352984  
9 6 0 -3.424789 -0.441868 -0.378536  
10 6 0 -2.971969 0.882745 -0.320944  
11 6 0 -3.839841 2.039744 -0.368160  
12 6 0 -3.042412 3.139008 -0.245939  
13 6 0 -1.680939 2.661253 -0.133308  
14 6 0 -0.564629 3.500280 -0.005521

15 6 0 0.761230 3.043095 -0.020869  
16 6 0 1.913137 3.902087 0.149650  
17 6 0 3.017759 3.111228 0.036235  
18 6 0 2.548023 1.762513 -0.194344  
19 6 0 3.398814 0.658069 -0.350683  
20 6 0 2.947607 -0.665274 -0.437287  
21 6 0 3.799001 -1.812480 -0.630227  
22 6 0 2.999841 -2.920103 -0.572082  
23 6 0 1.650926 -2.458100 -0.367696  
24 6 0 0.536688 -3.300660 -0.272366  
25 1 0 -1.893757 -4.797914 -0.075039  
26 1 0 -4.087180 -3.220506 -0.197790  
27 1 0 -4.918449 2.005974 -0.491775  
28 1 0 -3.338115 4.184193 -0.250872  
29 1 0 1.872313 4.969614 0.345378  
30 1 0 4.060815 3.401710 0.122313  
31 1 0 4.872139 -1.770968 -0.793119  
32 1 0 3.289022 -3.962071 -0.677169  
33 29 0 -0.025533 0.111615 -0.278047  
34 6 0 -0.804754 4.966804 0.139523  
35 6 0 -1.443008 5.475791 1.282220  
36 6 0 -0.402479 5.863546 -0.863612  
37 6 0 -1.671078 6.846679 1.419686  
38 1 0 -1.753862 4.785214 2.069081  
39 6 0 -0.632198 7.234288 -0.727707  
40 1 0 0.087289 5.474728 -1.758935  
41 6 0 -1.266623 7.730118 0.414867  
42 1 0 -2.163540 7.226795 2.318010  
43 1 0 -0.317928 7.917796 -1.520224  
44 1 0 -1.445664 8.802626 0.521813  
45 6 0 4.870431 0.902095 -0.394447  
46 6 0 5.448725 1.616860 -1.455691  
47 6 0 5.702326 0.423703 0.631133  
48 6 0 6.826010 1.845112 -1.492682  
49 1 0 4.807943 1.988170 -2.258368  
50 6 0 7.079076 0.654202 0.595672  
51 1 0 5.256128 -0.123343 1.464477  
52 6 0 7.645044 1.364628 -0.466955  
53 1 0 7.261806 2.397920 -2.328445  
54 1 0 7.712014 0.281245 1.404521  
55 1 0 8.722419 1.544222 -0.495180  
56 6 0 -4.896731 -0.685185 -0.428584  
57 6 0 -5.715213 -0.346633 0.661238  
58 6 0 -5.487897 -1.266702 -1.561700

```

59 6 0 -7.091090 -0.581627 0.618012
60 1 0 -5.259791 0.094822 1.550246
61 6 0 -6.864124 -1.500007 -1.606211
62 1 0 -4.857588 -1.530285 -2.413786
63 6 0 -7.669804 -1.158048 -0.516376
64 1 0 -7.713290 -0.317881 1.476682
65 1 0 -7.309585 -1.948045 -2.497751
66 1 0 -8.746354 -1.341473 -0.550531
67 6 0 0.789670 -4.766003 -0.145297
68 6 0 1.355881 -5.264415 1.039551
69 6 0 0.475787 -5.658046 -1.181604
70 6 0 1.602690 -6.631647 1.181308
71 1 0 1.577720 -4.562909 1.848240
72 6 0 0.726702 -7.024986 -1.038767
73 1 0 0.039484 -5.271285 -2.105348
74 6 0 1.290612 -7.514611 0.142959
75 1 0 2.037342 -7.010196 2.109738
76 1 0 0.483757 -7.709783 -1.854957
77 1 0 1.485777 -8.583964 0.254588
78 6 0 0.823542 -1.906177 3.025269
79 1 0 0.776112 -1.855077 4.126202
80 1 0 -0.247373 -2.295344 2.591097
81 6 0 -1.428543 -1.593441 2.977556
82 1 0 -2.081418 -2.230718 2.366017
83 1 0 -1.674758 -1.650704 4.043521
84 1 0 -1.381594 -0.565318 2.601830
85 8 0 1.338102 -0.766867 2.557709
86 1 0 1.478657 -0.855077 1.591444
***** 1 imaginary frequencies (negative Signs) *****
Diagonal vibrational polarizability:
29.7103966 27.7549862 45.9427634
Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman scattering
activities (A**4/AMU), depolarization ratios for plane and unpolarized
incident light, reduced masses (AMU), force constants (mDyne/A),
and normal coordinates:
1 2 3
A A A
Frequencies -- -1267.0519 9.1127 22.4692
Red. masses -- 1.1220 6.0903 4.4095
Frc consts -- 1.0613 0.0003 0.0013
IR Inten -- 133.6966 0.0048 0.0801
Atom AN X Y Z X Y Z X Y Z
1 7 -0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.01 0.00 0.04
2 7 -0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.01 0.01 0.01

```

3 7 0.00 0.00 -0.00 -0.00 0.01 -0.00 -0.01 0.00 0.03  
4 7 0.00 -0.00 -0.00 -0.00 0.01 -0.01 -0.01 0.00 -0.00  
5 6 -0.00 0.00 0.00 0.00 0.00 -0.02 -0.01 0.01 0.06  
6 6 -0.00 -0.00 0.00 0.00 -0.00 -0.01 -0.01 0.01 0.10  
7 6 0.00 -0.00 0.00 0.00 -0.00 0.02 -0.01 0.01 0.11  
8 6 0.00 0.00 0.00 -0.00 0.00 0.03 -0.01 0.01 0.06  
9 6 0.00 -0.00 -0.00 -0.00 -0.00 0.05 -0.01 0.01 0.02  
10 6 0.00 0.00 0.00 -0.01 0.00 0.02 -0.01 0.01 -0.02  
11 6 -0.00 0.00 0.00 -0.01 -0.00 0.01 -0.00 0.01 -0.07  
12 6 -0.00 -0.00 -0.00 -0.01 0.00 -0.03 -0.00 0.01 -0.07  
13 6 -0.00 -0.00 -0.00 -0.01 0.01 -0.03 -0.01 0.01 -0.02  
14 6 0.00 -0.00 -0.00 -0.01 0.01 -0.05 -0.01 0.00 0.01  
15 6 0.00 -0.00 -0.00 -0.01 0.01 -0.03 -0.01 -0.00 0.04  
16 6 0.00 0.00 -0.00 -0.01 0.01 -0.02 -0.01 -0.01 0.08  
17 6 0.00 0.00 0.00 -0.01 0.01 0.02 -0.01 -0.01 0.07  
18 6 -0.00 -0.00 0.00 -0.00 0.01 0.03 -0.01 -0.00 0.04  
19 6 0.00 -0.00 -0.00 -0.00 0.01 0.04 -0.01 0.00 0.00  
20 6 -0.00 0.00 -0.00 0.00 0.01 0.02 -0.02 0.00 -0.03  
21 6 0.00 0.00 0.00 0.00 0.01 0.01 -0.02 0.01 -0.07  
22 6 0.00 -0.00 0.00 0.00 0.01 -0.03 -0.02 0.01 -0.07  
23 6 0.00 0.00 -0.00 0.00 0.01 -0.03 -0.02 0.00 -0.02  
24 6 -0.00 0.00 -0.00 0.00 0.00 -0.05 -0.01 0.00 0.02  
25 1 -0.00 -0.00 0.00 0.01 -0.00 -0.03 -0.01 0.01 0.13  
26 1 0.00 0.00 0.00 0.00 -0.00 0.04 -0.01 0.01 0.13  
27 1 -0.00 -0.00 0.00 -0.01 -0.01 0.03 0.00 0.01 -0.11  
28 1 -0.00 -0.00 0.00 -0.01 0.00 -0.05 0.00 0.01 -0.10  
29 1 -0.00 -0.00 0.00 -0.01 0.02 -0.04 -0.01 -0.01 0.10  
30 1 -0.00 0.00 0.00 -0.01 0.01 0.04 -0.01 -0.01 0.09  
31 1 0.00 0.00 -0.00 0.01 0.02 0.03 -0.03 0.01 -0.10  
32 1 0.00 0.00 -0.00 0.00 0.01 -0.05 -0.03 0.01 -0.09  
33 29 -0.00 0.00 0.00 -0.00 0.01 -0.00 -0.01 0.00 0.02  
34 6 -0.00 0.00 0.00 -0.01 0.01 -0.09 -0.01 0.01 -0.00  
35 6 -0.00 -0.00 0.00 -0.01 0.05 -0.11 -0.07 0.01 -0.04  
36 6 0.00 -0.00 -0.00 0.00 -0.02 -0.11 0.05 0.00 0.02  
37 6 0.00 -0.00 -0.00 -0.01 0.05 -0.15 -0.07 0.01 -0.05  
38 1 0.00 -0.00 0.00 -0.02 0.07 -0.09 -0.12 0.01 -0.05  
39 6 -0.00 -0.00 -0.00 0.01 -0.01 -0.16 0.05 0.00 0.01  
40 1 0.00 0.00 -0.00 0.01 -0.04 -0.10 0.10 0.00 0.05  
41 6 0.00 -0.00 -0.00 0.00 0.02 -0.17 -0.01 0.01 -0.03  
42 1 0.00 -0.00 0.00 -0.01 0.08 -0.16 -0.12 0.01 -0.08  
43 1 0.00 -0.00 -0.00 0.01 -0.03 -0.17 0.10 0.00 0.03  
44 1 0.00 -0.00 -0.00 0.00 0.03 -0.20 -0.01 0.01 -0.04  
45 6 0.00 -0.00 -0.00 0.00 0.00 0.09 -0.01 -0.00 -0.00  
46 6 -0.00 0.00 -0.00 0.04 0.00 0.11 -0.02 0.05 0.02

47 6 -0.00 -0.00 0.00 -0.03 -0.01 0.11 -0.00 -0.05 -0.04  
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49 1 0.00 0.00 0.00 0.07 0.01 0.09 -0.03 0.09 0.05  
50 6 -0.00 -0.00 -0.00 -0.03 -0.01 0.16 -0.00 -0.06 -0.04  
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53 1 -0.00 0.00 0.00 0.07 -0.00 0.17 -0.03 0.08 0.04  
54 1 -0.00 0.00 0.00 -0.06 -0.02 0.17 0.01 -0.10 -0.07  
55 1 -0.00 0.00 0.00 0.01 -0.02 0.21 -0.01 -0.01 -0.02  
56 6 -0.00 -0.00 -0.00 -0.01 -0.00 0.09 -0.01 0.01 -0.02  
57 6 0.00 0.00 0.00 0.02 0.00 0.11 -0.05 0.09 -0.08  
58 6 0.00 -0.00 -0.00 -0.04 -0.00 0.10 0.03 -0.07 0.00  
59 6 0.00 0.00 -0.00 0.02 0.00 0.15 -0.05 0.10 -0.12  
60 1 0.00 -0.00 0.00 0.05 0.01 0.09 -0.09 0.15 -0.09  
61 6 -0.00 -0.00 -0.00 -0.04 -0.00 0.14 0.03 -0.07 -0.04  
62 1 -0.00 -0.00 -0.00 -0.06 -0.01 0.09 0.06 -0.14 0.05  
63 6 0.00 0.00 -0.00 -0.01 0.00 0.16 -0.01 0.02 -0.10  
64 1 0.00 -0.00 0.00 0.05 0.01 0.16 -0.09 0.16 -0.16  
65 1 -0.00 -0.00 -0.00 -0.06 -0.01 0.16 0.07 -0.13 -0.03  
66 1 0.00 -0.00 -0.00 -0.01 0.00 0.19 -0.01 0.02 -0.13  
67 6 -0.00 0.00 -0.00 0.00 0.00 -0.08 -0.01 0.00 0.01  
68 6 -0.00 -0.00 -0.00 0.01 -0.03 -0.10 0.08 0.00 -0.03  
69 6 0.00 -0.00 0.00 -0.01 0.03 -0.10 -0.09 0.00 0.03  
70 6 0.00 -0.00 0.00 0.01 -0.03 -0.13 0.08 0.00 -0.05  
71 1 0.01 -0.01 0.00 0.02 -0.05 -0.08 0.14 0.01 -0.05  
72 6 0.00 0.00 0.00 -0.01 0.02 -0.13 -0.08 0.00 0.02  
73 1 0.00 0.00 0.00 -0.01 0.05 -0.09 -0.15 -0.00 0.06  
74 6 0.00 0.00 0.00 0.00 -0.01 -0.15 0.00 0.00 -0.02  
75 1 0.00 -0.00 0.00 0.02 -0.05 -0.14 0.15 0.01 -0.08  
76 1 0.00 0.00 0.00 -0.01 0.04 -0.15 -0.14 -0.00 0.04  
77 1 0.00 0.00 0.00 0.00 -0.01 -0.18 0.01 0.00 -0.03  
78 6 -0.09 0.03 0.01 0.03 -0.07 -0.02 0.17 -0.05 0.00  
79 1 0.04 -0.17 -0.01 0.05 -0.09 -0.02 0.21 -0.08 0.01  
80 1 0.78 -0.47 -0.30 0.03 -0.06 -0.01 0.16 -0.07 0.03  
81 6 -0.00 0.03 0.03 0.03 -0.07 0.02 0.16 -0.10 0.09  
82 1 0.16 -0.08 -0.03 0.02 -0.06 0.01 0.15 -0.08 0.08  
83 1 -0.05 0.02 0.02 0.05 -0.09 0.02 0.19 -0.14 0.09  
84 1 -0.00 0.02 -0.00 0.03 -0.06 0.03 0.13 -0.08 0.13  
85 8 0.01 -0.00 -0.01 0.02 -0.05 0.00 0.12 -0.03 0.01  
86 1 -0.02 0.02 -0.01 0.01 -0.03 -0.00 0.07 -0.01 -0.00

TGro.-P

-----  
Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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1 7 0 0.450530 2.025625 -0.233837  
2 7 0 2.089731 -0.333033 -0.213382  
3 7 0 -0.262586 -1.967565 -0.371766  
4 7 0 -1.898316 0.391838 -0.376752  
5 6 0 -0.493756 3.025432 -0.194681  
6 6 0 0.150334 4.297630 0.048344  
7 6 0 1.489060 4.053982 0.138465  
8 6 0 1.671689 2.631733 -0.052668  
9 6 0 2.921543 1.995448 -0.057002  
10 6 0 3.090401 0.608787 -0.179210  
11 6 0 4.378375 -0.041171 -0.292486  
12 6 0 4.140255 -1.380990 -0.377796  
13 6 0 2.705575 -1.558589 -0.309665  
14 6 0 2.068062 -2.807388 -0.318878  
15 6 0 0.674746 -2.969750 -0.296258  
16 6 0 0.013824 -4.249533 -0.153559  
17 6 0 -1.327689 -4.004759 -0.143508  
18 6 0 -1.494921 -2.576769 -0.297774  
19 6 0 -2.737918 -1.937460 -0.361870  
20 6 0 -2.896619 -0.551190 -0.488014  
21 6 0 -4.165495 0.101456 -0.699530  
22 6 0 -3.925348 1.445868 -0.709995  
23 6 0 -2.509576 1.623737 -0.486255  
24 6 0 -1.877980 2.868289 -0.356904  
25 1 0 -0.365301 5.247758 0.153919  
26 1 0 2.286625 4.765506 0.331711  
27 1 0 5.335618 0.471390 -0.320815  
28 1 0 4.864166 -2.182977 -0.489513  
29 1 0 0.520295 -5.204974 -0.051365  
30 1 0 -2.139383 -4.718190 -0.033827  
31 1 0 -5.113233 -0.412596 -0.832731  
32 1 0 -4.638794 2.251230 -0.858725  
33 29 0 0.099597 0.027193 -0.307777  
34 6 0 2.916544 -4.035416 -0.331784  
35 6 0 3.758138 -4.339911 0.750711  
36 6 0 2.884282 -4.913788 -1.427307  
37 6 0 4.547246 -5.491937 0.738002  
38 1 0 3.782452 -3.667150 1.610580  
39 6 0 3.674723 -6.064889 -1.441651  
40 1 0 2.235957 -4.681916 -2.274994  
41 6 0 4.508580 -6.357676 -0.358746  
42 1 0 5.191820 -5.716889 1.591198

43 1 0 3.641751 -6.734365 -2.304622  
44 1 0 5.126329 -7.258803 -0.369136  
45 6 0 -3.974247 -2.757265 -0.204408  
46 6 0 -4.403386 -3.655147 -1.192361  
47 6 0 -4.722290 -2.626042 0.978215  
48 6 0 -5.565927 -4.407626 -1.005561  
49 1 0 -3.823844 -3.754650 -2.112984  
50 6 0 -5.881606 -3.382011 1.163043  
51 1 0 -4.366613 -1.934759 1.747015  
52 6 0 -6.306869 -4.272569 0.172077  
53 1 0 -5.895909 -5.099673 -1.784249  
54 1 0 -6.454052 -3.277723 2.088033  
55 1 0 -7.215431 -4.862019 0.317598  
56 6 0 4.144317 2.843014 0.067451  
57 6 0 4.976463 2.736692 1.193817  
58 6 0 4.487127 3.760600 -0.939020  
59 6 0 6.120847 3.528277 1.311785  
60 1 0 4.713418 2.029905 1.983701  
61 6 0 5.632556 4.550929 -0.822761  
62 1 0 3.849226 3.844240 -1.821467  
63 6 0 6.452686 4.437615 0.303453  
64 1 0 6.754094 3.437116 2.197622  
65 1 0 5.887881 5.255644 -1.617879  
66 1 0 7.348429 5.056497 0.395043  
67 6 0 -2.730214 4.093455 -0.373223  
68 6 0 -3.667643 4.324065 0.647111  
69 6 0 -2.609807 5.038253 -1.405196  
70 6 0 -4.463859 5.471151 0.635929  
71 1 0 -3.761309 3.597410 1.457076  
72 6 0 -3.407762 6.184268 -1.417953  
73 1 0 -1.887291 4.862616 -2.205080  
74 6 0 -4.336802 6.404344 -0.397046  
75 1 0 -5.183959 5.638626 1.440508  
76 1 0 -3.306044 6.906709 -2.231438  
77 1 0 -4.960477 7.301411 -0.406328  
78 6 0 -1.229577 -1.039996 2.996271  
79 1 0 -1.421582 -1.539906 3.959814  
80 1 0 -0.953246 -1.831612 2.274425  
81 8 0 -2.443772 -0.412638 2.626297  
82 1 0 -2.305185 -0.006321 1.757609  
83 6 0 -0.078098 -0.053160 3.143031  
84 1 0 0.139586 0.450205 2.186166  
85 1 0 0.845077 -0.564413 3.460731  
86 1 0 -0.324630 0.727166 3.879908

CO--Zr<sub>6</sub>O<sub>8</sub> (TCPP-Cu)<sub>6</sub>

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Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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1 8 0 2.898920 2.633727 -0.964588  
2 6 0 4.644338 4.746561 -1.024762  
3 1 0 4.715858 4.070924 -1.690628  
4 6 0 5.492056 5.816240 -1.037992  
5 1 0 6.149081 5.891902 -1.717699  
6 6 0 7.310252 8.028274 0.926033  
7 6 0 7.503079 7.009486 1.928193  
8 1 0 7.004060 6.206421 2.022062  
9 6 0 13.692099 15.412250 -0.363849  
10 1 0 14.609714 15.304088 -0.590257  
11 6 0 12.854237 14.334761 -0.359509  
12 1 0 13.188521 13.473577 -0.574039  
13 6 0 9.638350 13.230266 -1.062712  
14 6 0 9.524239 14.186680 -2.135881  
15 1 0 10.066392 14.955565 -2.268659  
16 8 0 -3.732450 1.194853 -0.965264  
17 6 0 -6.434916 1.650009 -1.025907  
18 1 0 -5.885448 2.049731 -1.691703  
19 6 0 -7.785142 1.849314 -1.039370  
20 1 0 -8.179068 2.380449 -1.719169  
21 6 0 -10.610242 2.318000 0.924165  
22 6 0 -9.824524 2.994438 1.926421  
23 1 0 -8.879555 2.963812 2.020447  
24 6 0 -20.195663 4.152789 -0.367391  
25 1 0 -20.560762 5.001536 -0.593903  
26 6 0 -18.843600 3.965923 -0.362819  
27 1 0 -18.264899 4.686004 -0.577290  
28 6 0 -16.279020 1.733096 -1.065486  
29 6 0 -17.050066 1.156012 -2.138752  
30 1 0 -17.986995 1.241080 -2.271690  
31 8 0 0.829337 -3.828644 -0.964933  
32 6 0 1.786404 -6.396630 -1.025288  
33 1 0 1.165610 -6.120672 -1.691200  
34 6 0 2.288915 -7.665613 -1.038604  
35 1 0 2.026015 -8.272366 -1.718415  
36 6 0 3.295247 -10.346465 0.925233  
37 6 0 2.316410 -10.004182 1.927310  
38 1 0 1.870433 -9.170498 2.021221



39 6 0 6.499197 -19.565144 -0.365328  
40 1 0 5.946748 -20.305714 -0.591892  
41 6 0 5.984996 -18.300790 -0.360904  
42 1 0 5.072073 -18.159671 -0.575533  
43 6 0 6.636507 -14.963421 -1.063632  
44 6 0 7.521977 -15.342677 -2.136734  
45 1 0 7.916792 -16.196623 -2.269563  
46 6 0 14.571340 2.863901 5.012819  
47 1 0 14.970558 3.725935 4.962821  
48 6 0 14.468071 2.089002 3.893945  
49 1 0 14.802935 2.406097 3.065256  
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52 1 0 11.234155 1.016994 3.452454  
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57 6 0 14.426001 -3.699876 -2.322750  
58 6 0 15.633439 -4.223365 -2.912234  
59 1 0 15.695728 -4.752910 -3.698649  
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61 1 0 -10.188235 -8.413871 -7.245655  
62 6 0 -10.001268 -8.891641 -5.293395  
63 1 0 -9.117242 -9.228712 -5.358904  
64 6 0 -10.419094 -10.644428 -2.325317  
65 6 0 -11.476093 -11.428286 -2.915027  
66 1 0 -11.965737 -11.217365 -3.701479  
67 6 0 -4.808292 -14.053047 5.010560  
68 1 0 -4.261352 -14.829790 4.960540  
69 6 0 -5.427598 -13.576031 3.891664  
70 1 0 -5.320313 -14.024483 3.062935  
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72 6 0 -5.271748 -9.994221 2.703110  
73 1 0 -4.738969 -10.239322 3.450651  
74 6 0 -1.966692 13.409027 -6.402074  
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76 6 0 -2.701285 13.106439 -5.292196  
77 1 0 -3.435201 12.509393 -5.357868  
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79 6 0 -4.160971 15.651717 -2.913713  
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81 6 0 -9.768982 11.188681 5.010641  
82 1 0 -10.715126 11.103395 4.960491

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84 1 0 -9.487988 11.618051 3.063102  
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86 6 0 -6.021917 9.560905 2.703473  
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90 6 0 11.975409 8.383691 3.893843  
91 1 0 12.436591 8.381799 3.065159  
92 6 0 8.967032 8.684371 2.186333  
93 6 0 8.524050 7.413798 2.704838  
94 1 0 8.884315 6.951015 3.452358  
95 6 0 5.755248 12.269203 -6.401349  
96 1 0 5.863221 11.840418 -7.243645  
97 6 0 6.370883 11.767309 -5.291345  
98 1 0 6.901012 10.983680 -5.356898  
99 6 0 7.981569 12.574171 -2.323013  
100 6 0 8.503268 13.782368 -2.912525  
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102 6 0 -13.126295 6.952306 5.010221  
103 1 0 -13.259418 7.892918 4.960172  
104 6 0 -13.251110 6.180587 3.891344  
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106 6 0 -12.007037 3.424830 2.184179  
107 6 0 -10.685281 3.676509 2.702889  
108 1 0 -10.464757 4.219937 3.450418  
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110 1 0 -13.186792 -0.841650 -7.245777  
111 6 0 -13.377632 -0.365350 -5.293533  
112 1 0 -12.964042 0.485567 -5.359061  
113 6 0 -14.882226 0.626265 -2.325499  
114 6 0 -16.189309 0.473941 -2.915220  
115 1 0 -16.401793 -0.015044 -3.701660  
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117 1 0 -0.208851 -15.427973 4.960920  
118 6 0 1.270094 -14.564667 3.892292  
119 1 0 1.037969 -14.963019 3.063532  
120 6 0 3.034894 -12.109476 2.185293  
121 6 0 2.155971 -11.090615 2.703807  
122 1 0 1.574962 -11.171312 3.451244  
123 6 0 7.746427 -11.119396 -6.401677  
124 1 0 7.321208 -10.998412 -7.244012  
125 6 0 7.003817 -11.401736 -5.291800  
126 1 0 6.060118 -11.469018 -5.357480

127 6 0 6.896860 -13.200410 -2.323693  
128 6 0 7.682416 -14.256243 -2.913230  
129 1 0 8.212262 -14.195808 -3.699586  
130 8 0 3.915761 0.065913 -0.964546  
131 6 0 6.634489 -0.279146 -1.024681  
132 1 0 6.224066 0.262265 -1.690566  
133 6 0 7.984718 -0.478450 -1.037891  
134 1 0 8.515426 -0.083799 -1.717602  
135 6 0 10.824388 -0.845932 0.926176  
136 6 0 10.267433 0.028696 1.928306  
137 1 0 9.353899 0.272400 2.022158  
138 6 0 16.082782 -3.043780 -1.062449  
139 6 0 16.654409 -3.819054 -2.135590  
140 1 0 17.575984 -4.008316 -2.268353  
141 6 0 -11.877659 -16.852564 -0.367052  
142 1 0 -11.562696 -17.721172 -0.593535  
143 6 0 -11.020088 -15.790696 -0.362499  
144 1 0 -10.105287 -15.919365 -0.576957  
145 6 0 -10.679447 -12.407439 -1.065257  
146 6 0 -11.636532 -12.514719 -2.138531  
147 1 0 -12.261208 -13.218180 -2.271456  
148 8 0 -1.902876 -3.425347 -0.965189  
149 6 0 -3.561062 -5.607299 -1.025789  
150 1 0 -2.886890 -5.522489 -1.691580  
151 6 0 -4.408778 -6.676977 -1.039232  
152 1 0 -4.332267 -7.333830 -1.719012  
153 6 0 -6.147109 -8.952694 0.924347  
154 6 0 -5.111308 -8.907788 1.926613  
155 1 0 -4.443499 -8.238507 2.020628  
156 6 0 -8.658072 18.711324 -0.365946  
157 1 0 -9.567762 18.872888 -0.592526  
158 6 0 -8.167253 17.437711 -0.361482  
159 1 0 -8.736057 16.709830 -0.576096  
160 6 0 -5.407499 15.451161 -1.064124  
161 6 0 -5.021728 16.333788 -2.137246  
162 1 0 -5.318587 17.226518 -2.270103  
163 8 0 -2.017076 3.359370 -0.965049  
164 6 0 -3.077602 5.886384 -1.025486  
165 1 0 -3.341156 5.260208 -1.691384  
166 6 0 -3.580111 7.155368 -1.038844  
167 1 0 -4.187132 7.417615 -1.718669  
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169 6 0 -5.161160 8.878835 1.927005  
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171 6 0 -12.584163 -7.889691 -5.093803  
172 1 0 -13.465325 -7.534679 -5.043824  
173 6 0 -11.978383 -8.383776 -3.974908  
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 Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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Center Atomic Atomic Coordinates (Angstroms)

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CH<sub>3</sub>--Zr<sub>6</sub>O<sub>8</sub> (TCPP-Cu)<sub>6</sub>

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 Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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Center Atomic Atomic Coordinates (Angstroms)

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Zr<sub>6</sub>O<sub>8</sub>(TCPP-Cu)<sub>6</sub>--CH<sub>2</sub>

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 Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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