Supporting Information

XPS and IR Spectroscopic Studies of Titanyl and Vanadyl Complexes with Etioporphyrin II

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VO-EP II

Energy = -2478.5328197484
Atomic Coordinates:

7	0.92597383	1.70789776	-0.59014438
6	0.86389374	-2.46482676	-3.43169126
6	1.54541897	-1.32655825	-3.80319089
6	0.78505745	-3.77866932	-4.15025396
6	0.21735832	-2.16737367	-2.16576024
6	1.30640336	-0.34389979	-2.75744625
7	0.49664527	-0.87393130	-1.77527273
6	1.82769170	0.94861231	-2.74566165
6	1.66448402	1.89862017	-1.73913846
6	1.05800067	2.86688291	0.14610982
6	0.48075752	3.08985240	1.39436738
6	-0.29591304	2.18777342	2.11853614
6	-0.84525204	2.44497799	3.43824649
6	-1.52966618	1.30820517	3.80857547
6	-0.66759199	3.71867436	4.20962367
7	-0.64062807	0.92244083	1.69192331
6	-1.38970207	0.36678211	2.70817537
6	-1.90934207	-0.92624457	2.69655853
6	-1.74767376	-1.87612804	1.68962966
6	-2.26006692	-3.23654447	1.74049494
6	-1.87816617	-3.84147205	0.56292845
7	-1.07146408	-1.66097051	0.50706718
6	-3.00992535	-3.84426662	2.89299584
6	-2.08400736	-4.41542038	3.98897811
6	-2.30758555	1.06417365	5.07168998
6	-3.81563425	1.36164311	4.92232589
6	-2.13947788	-5.24740826	0.11149077
6	-1.13716124	-2.84748856	-0.19326209
6	-0.55502842	-3.07134950	-1.43935529
1	1.26593798	-4.58645681	-3.57150764
1	-0.26161855	-4.07949632	-4.32725169
1	1.28759484	-3.72711979	-5.12752880
1	-1.09424970	4.58048413	3.66800098
1	-1.16567761	3.66304897	5.18881287
1	0.39923275	3.93833470	4.38777465

1	-3.66405957	-4.64843705	2.51456784
1	-3.68432867	-3.09120718	3.33694832
1	-2.67525085	-4.84445478	4.81485650
1	-1.43715182	-5.20747066	3.57941250
1	-2.16958590	0.01820952	5.39761253
1	-1.89200165	1.68921921	5.88050863
1	-2.80464041	-5.77209071	0.81331597
1	-2.61691721	-5.26949018	-0.88287717
1	-1.20471458	-5.83049416	0.04050068
1	-0.69691066	-4.06100472	-1.87805875
6	2.41484618	-1.12079512	-5.01218041
6	3.90805371	-1.41033529	-4.74512379
1	2.05858915	-1.77257704	-5.82828873
1	4.50726481	-1.24139182	-5.65513558
1	4.29977816	-0.76048676	-3.94671293
6	2.27715676	3.21836525	-1.73601526
1	2.44222266	1.23817808	-3.59969891
6	1.89735627	3.82123825	-0.55705550
1	-2.48326091	-1.23271227	3.57274090
23	-0.50679826	0.20216728	-0.27701515
8	-1.82050731	0.74546806	-0.99127587
6	3.12335102	3.78981081	-2.83942390
6	2.29138356	4.42511657	-3.97483142
1	3.77334896	3.00074681	-3.25678395
1	3.80381858	4.54969569	-2.41850898
1	2.94932189	4.82319359	-4.76501382
1	1.61162002	3.68661119	-4.42829374
1	1.67386747	5.25196365	-3.58956539
1	-4.26531781	0.73985628	4.13221026
1	-4.34817533	1.16218480	5.86696012
1	-3.97958851	2.41597437	4.64853599
1	-1.43018059	-3.63107022	4.40189110
1	0.66752443	4.06101258	1.85691710
6	2.25614042	5.18646569	-0.05081958
1	1.35948577	5.81713544	0.07766168
1	2.76393585	5.13452230	0.92764371
1	2.92883321	5.70530825	-0.74962190
1	2.30097164	-0.08643702	-5.38106100
1	4.05190138	-2.45476772	-4.42576229

Harmonic Frequencies (cm^-1), Reduced Masses (amu),
IR Intensities (km/mol),
Raman Scattering Activities (A^4/amu),
Raman Depolarization Ratios,
Raman Optical Activities (10^-4)

Mode	Freq.	Mass.	IR Int.	Raman A.	Raman D.	ROA (90)	ROA (180)
1	22.01	4.03	0.001	0.082	0.7499	0.00000	0.00000
2	29.18	3.77	0.138	0.089	0.7439	0.00000	0.00000
3	45.62	3.71	2.563	0.382	0.7217	0.00000	0.00000
4	46.88	3.53	0.037	2.001	0.6769	0.00000	0.00000
5	50.66	2.68	0.010	0.057	0.7172	0.00000	0.00000
6	51.55	2.70	0.021	2.977	0.6743	0.00000	0.00000
7	53.65	2.58	0.002	2.346	0.7482	0.00000	0.00000
8	58.26	2.95	1.568	0.147	0.7410	0.00000	0.00000
9	72.21	2.74	0.000	0.834	0.7499	0.00000	0.00000
10	74.95	3.01	0.004	0.022	0.7467	0.00000	0.00000
11	77.56	3.62	0.140	0.595	0.7499	0.00000	0.00000
12	91.73	1.08	0.046	0.194	0.7469	0.00000	0.00000
13	92.54	1.07	0.065	1.152	0.7500	0.00000	0.00000
14	94.93	1.07	0.592	0.305	0.7116	0.00000	0.00000
15	96.34	1.13	0.084	0.450	0.7499	0.00000	0.00000
16	110.93	4.09	0.287	0.633	0.6286	0.00000	0.00000
17	131.57	4.27	0.023	0.411	0.6210	0.00000	0.00000

18	139.79	3.78	0.095	1.310	0.7500	0.00000	0.00000
19	146.50	2.58	0.017	3.071	0.6497	0.00000	0.00000
20	149.38	5.56	1.071	3.428	0.7498	0.00000	0.00000
21	158.40	2.76	0.971	1.607	0.1362	0.00000	0.00000
22	162.89	2.13	0.560	1.482	0.7496	0.00000	0.00000
23	166.71	2.82	0.234	3.079	0.1332	0.00000	0.00000
24	180.33	3.43	0.033	7.812	0.7500	0.00000	0.00000
25	181.63	4.90	0.113	2.510	0.6404	0.00000	0.00000
26	188.97	4.43	1.356	1.434	0.4715	0.00000	0.00000
27	196.05	1.24	0.001	0.271	0.7496	0.00000	0.00000
28	203.18	1.38	0.069	4.472	0.5567	0.00000	0.00000
29	205.33	1.33	0.089	0.577	0.3640	0.00000	0.00000
30	214.59	1.40	0.557	0.215	0.7480	0.00000	0.00000
31	227.16	4.89	0.004	14.175	0.6214	0.00000	0.00000
32	233.12	3.96	0.035	0.455	0.7498	0.00000	0.00000
33	241.06	3.97	0.053	4.145	0.2869	0.00000	0.00000
34	247.36	4.45	0.002	1.897	0.7500	0.00000	0.00000
35	257.12	4.41	0.015	0.589	0.7360	0.00000	0.00000
36	259.32	2.63	0.100	20.642	0.0814	0.00000	0.00000
37	272.08	3.80	0.014	0.059	0.7492	0.00000	0.00000
38	274.55	2.64	0.078	0.022	0.7428	0.00000	0.00000
39	288.44	4.14	0.009	1.700	0.4187	0.00000	0.00000
40	290.90	2.67	0.109	0.146	0.0629	0.00000	0.00000
41	304.33	2.12	0.002	2.094	0.7500	0.00000	0.00000
42	314.47	3.74	0.033	6.763	0.1161	0.00000	0.00000
43	325.61	4.08	0.025	0.026	0.7343	0.00000	0.00000
44	328.43	4.06	2.934	6.627	0.1118	0.00000	0.00000
45	345.51	4.44	4.701	22.946	0.0693	0.00000	0.00000
46	345.76	6.99	2.089	1.504	0.2229	0.00000	0.00000
47	352.82	9.96	4.798	0.355	0.2961	0.00000	0.00000
48	358.92	6.61	3.027	0.230	0.7379	0.00000	0.00000
49	371.99	4.21	0.028	0.958	0.7495	0.00000	0.00000
50	397.68	4.13	1.124	11.133	0.1244	0.00000	0.00000
51	405.63	4.28	2.987	0.462	0.1293	0.00000	0.00000
52	450.33	6.09	2.930	0.074	0.7499	0.00000	0.00000
53	476.21	4.06	0.033	0.811	0.1848	0.00000	0.00000
54	496.01	3.93	2.772	0.015	0.6016	0.00000	0.00000
55	504.91	3.88	3.982	0.024	0.7499	0.00000	0.00000
56	513.61	4.27	0.064	1.027	0.2352	0.00000	0.00000
57	521.01	5.58	0.001	0.268	0.7500	0.00000	0.00000
58	538.44	3.61	0.000	0.733	0.7498	0.00000	0.00000
59	568.87	4.83	0.979	0.028	0.6445	0.00000	0.00000
60	585.57	4.16	0.007	1.531	0.7500	0.00000	0.00000
61	596.84	3.57	1.010	0.055	0.7499	0.00000	0.00000
62	603.02	3.85	0.136	0.024	0.6596	0.00000	0.00000
63	656.00	2.88	0.020	2.716	0.5993	0.00000	0.00000
64	669.80	4.06	0.062	7.514	0.1948	0.00000	0.00000
65	682.17	4.94	0.004	5.122	0.7500	0.00000	0.00000
66	688.40	6.70	0.191	0.491	0.7500	0.00000	0.00000
67	693.44	3.69	10.952	0.075	0.6277	0.00000	0.00000
68	697.11	5.32	2.103	0.985	0.7499	0.00000	0.00000
69	706.41	3.76	3.968	1.867	0.3981	0.00000	0.00000
70	707.41	4.09	23.077	0.285	0.7500	0.00000	0.00000
71	710.68	3.84	17.343	2.900	0.1539	0.00000	0.00000
72	725.02	4.06	0.203	0.275	0.7491	0.00000	0.00000
73	725.76	7.59	0.126	8.410	0.1225	0.00000	0.00000
74	728.65	4.18	3.699	1.697	0.0510	0.00000	0.00000
75	729.13	4.97	12.842	0.086	0.7358	0.00000	0.00000
76	742.37	1.91	16.729	0.040	0.7492	0.00000	0.00000
77	746.64	1.87	26.241	0.118	0.6530	0.00000	0.00000
78	750.31	3.00	0.055	2.943	0.7499	0.00000	0.00000
79	764.22	1.47	0.003	0.657	0.4521	0.00000	0.00000
80	766.23	1.83	0.620	41.539	0.0768	0.00000	0.00000
81	784.13	1.90	10.185	0.089	0.7190	0.00000	0.00000
82	799.61	2.41	1.110	52.503	0.0742	0.00000	0.00000

83	804.88	2.03	4.570	0.120	0.7484	0.00000	0.00000
84	832.20	1.47	46.066	0.029	0.0237	0.00000	0.00000
85	835.11	1.44	0.290	0.068	0.7224	0.00000	0.00000
86	836.85	1.51	0.041	0.217	0.7482	0.00000	0.00000
87	840.31	1.47	0.425	0.004	0.7462	0.00000	0.00000
88	903.71	2.49	0.001	14.642	0.7500	0.00000	0.00000
89	913.89	2.86	2.824	0.032	0.7458	0.00000	0.00000
90	918.47	3.67	50.752	0.051	0.6612	0.00000	0.00000
91	932.46	2.69	0.258	18.878	0.4835	0.00000	0.00000
92	948.33	2.04	0.003	13.130	0.7500	0.00000	0.00000
93	954.45	2.24	14.684	0.037	0.7078	0.00000	0.00000
94	955.50	1.93	5.646	0.043	0.7500	0.00000	0.00000
95	964.10	2.54	96.422	0.020	0.7282	0.00000	0.00000
96	972.01	1.72	0.198	1.640	0.5438	0.00000	0.00000
97	982.06	1.73	0.019	27.171	0.7500	0.00000	0.00000
98	984.01	1.77	26.513	0.103	0.2880	0.00000	0.00000
99	985.71	4.46	0.449	8.638	0.1633	0.00000	0.00000
100	1015.19	1.50	2.180	0.212	0.5770	0.00000	0.00000
101	1015.32	1.50	2.142	1.527	0.2105	0.00000	0.00000
102	1015.57	1.50	1.331	0.257	0.6370	0.00000	0.00000
103	1015.68	1.50	2.507	1.355	0.2292	0.00000	0.00000
104	1031.63	18.74	93.682	21.880	0.0251	0.00000	0.00000
105	1045.00	2.01	11.420	0.573	0.1221	0.00000	0.00000
106	1045.68	2.00	11.314	5.195	0.7006	0.00000	0.00000
107	1046.32	1.99	50.092	3.609	0.2038	0.00000	0.00000
108	1046.55	1.99	3.805	51.922	0.0915	0.00000	0.00000
109	1081.03	1.85	0.013	1.117	0.0806	0.00000	0.00000
110	1086.70	1.99	12.419	0.024	0.5975	0.00000	0.00000
111	1094.29	1.86	6.093	0.002	0.7430	0.00000	0.00000
112	1109.73	2.12	0.032	1.453	0.7493	0.00000	0.00000
113	1118.67	2.53	0.008	4.639	0.7499	0.00000	0.00000
114	1119.11	2.43	0.010	30.474	0.7500	0.00000	0.00000
115	1121.96	2.58	3.096	0.046	0.6565	0.00000	0.00000
116	1122.16	2.76	5.289	0.151	0.3390	0.00000	0.00000
117	1126.57	3.55	0.131	58.609	0.1158	0.00000	0.00000
118	1137.83	4.30	55.280	0.023	0.7500	0.00000	0.00000
119	1139.89	3.80	65.248	0.045	0.7333	0.00000	0.00000
120	1151.09	5.67	0.005	8.471	0.6709	0.00000	0.00000
121	1206.67	2.54	0.000	134.082	0.7500	0.00000	0.00000
122	1218.28	2.17	5.815	0.352	0.6889	0.00000	0.00000
123	1230.01	2.66	23.377	0.396	0.7470	0.00000	0.00000
124	1248.95	1.25	0.052	17.924	0.2919	0.00000	0.00000
125	1251.91	1.30	14.867	0.078	0.6759	0.00000	0.00000
126	1258.03	1.44	0.009	50.486	0.7500	0.00000	0.00000
127	1266.00	1.45	27.950	0.181	0.7057	0.00000	0.00000
128	1292.15	1.48	0.752	8.698	0.7500	0.00000	0.00000
129	1292.35	1.47	2.525	2.316	0.7241	0.00000	0.00000
130	1296.15	1.49	16.417	1.792	0.2944	0.00000	0.00000
131	1297.20	1.47	0.371	77.697	0.2750	0.00000	0.00000
132	1299.79	1.78	0.006	4.929	0.7443	0.00000	0.00000
133	1342.39	1.78	0.030	0.215	0.7464	0.00000	0.00000
134	1343.08	1.84	4.921	0.313	0.7303	0.00000	0.00000
135	1343.72	1.66	0.014	60.144	0.7499	0.00000	0.00000
136	1349.89	1.42	0.029	168.565	0.2375	0.00000	0.00000
137	1354.58	8.47	0.719	167.379	0.1319	0.00000	0.00000
138	1357.74	1.28	0.201	1.416	0.3744	0.00000	0.00000
139	1358.24	1.45	5.659	3.701	0.2772	0.00000	0.00000
140	1358.59	1.23	0.076	8.561	0.7151	0.00000	0.00000
141	1359.02	1.22	0.499	67.592	0.3266	0.00000	0.00000
142	1360.83	1.99	9.577	1.132	0.4558	0.00000	0.00000
143	1363.46	2.44	5.203	0.315	0.5637	0.00000	0.00000
144	1372.50	2.23	0.052	274.609	0.7500	0.00000	0.00000
145	1373.78	2.50	22.251	0.177	0.7378	0.00000	0.00000
146	1373.82	2.56	14.936	1.133	0.7356	0.00000	0.00000
147	1376.62	2.54	0.003	11.883	0.7500	0.00000	0.00000

148	1385.20	4.03	0.047	230.914	0.7466	0.00000	0.00000
149	1434.53	1.31	0.102	32.605	0.4145	0.00000	0.00000
150	1436.32	1.11	0.070	0.687	0.7500	0.00000	0.00000
151	1437.12	1.07	0.062	45.503	0.7500	0.00000	0.00000
152	1438.12	1.07	22.064	2.261	0.7428	0.00000	0.00000
153	1438.26	1.05	0.873	0.059	0.3757	0.00000	0.00000
154	1438.48	1.05	1.228	3.543	0.7498	0.00000	0.00000
155	1438.97	1.05	0.525	49.324	0.7219	0.00000	0.00000
156	1439.49	1.06	12.106	0.200	0.4359	0.00000	0.00000
157	1447.27	1.48	1.052	5.531	0.6178	0.00000	0.00000
158	1447.92	1.29	1.618	2.402	0.7443	0.00000	0.00000
159	1448.43	1.05	1.340	42.275	0.7496	0.00000	0.00000
160	1448.85	1.09	28.056	9.853	0.4771	0.00000	0.00000
161	1448.99	1.06	3.116	26.408	0.7461	0.00000	0.00000
162	1449.44	1.10	7.964	31.636	0.4452	0.00000	0.00000
163	1451.53	1.16	10.110	11.653	0.7494	0.00000	0.00000
164	1451.98	1.08	1.739	30.127	0.7499	0.00000	0.00000
165	1457.59	1.82	2.237	0.600	0.5324	0.00000	0.00000
166	1458.09	1.42	0.025	43.444	0.4728	0.00000	0.00000
167	1463.42	1.40	7.679	0.369	0.6762	0.00000	0.00000
168	1464.24	1.10	0.255	0.205	0.7484	0.00000	0.00000
169	1464.54	1.23	0.163	10.909	0.7412	0.00000	0.00000
170	1466.06	1.92	9.073	0.686	0.7222	0.00000	0.00000
171	1466.88	1.53	33.547	0.331	0.7499	0.00000	0.00000
172	1492.69	9.28	0.953	14.083	0.1144	0.00000	0.00000
173	1549.10	7.31	0.056	1.834	0.7432	0.00000	0.00000
174	1549.21	7.22	1.158	0.755	0.7006	0.00000	0.00000
175	1561.89	7.35	0.003	1109.831	0.7500	0.00000	0.00000
176	1568.03	6.30	0.000	5.458	0.7499	0.00000	0.00000
177	1584.31	7.60	0.005	992.179	0.1121	0.00000	0.00000
178	1592.21	7.00	1.857	3.069	0.2364	0.00000	0.00000
179	1592.52	7.06	0.909	0.959	0.7252	0.00000	0.00000
180	1630.50	7.94	0.004	112.285	0.7500	0.00000	0.00000
181	2965.03	1.04	1.939	41.731	0.7066	0.00000	0.00000
182	2965.26	1.04	1.345	47.549	0.7317	0.00000	0.00000
183	2965.58	1.04	96.802	191.386	0.1276	0.00000	0.00000
184	2965.87	1.04	20.119	868.001	0.1244	0.00000	0.00000
185	2972.05	1.05	12.818	108.963	0.6365	0.00000	0.00000
186	2972.08	1.05	17.570	48.805	0.4763	0.00000	0.00000
187	2972.36	1.04	124.730	12.272	0.7474	0.00000	0.00000
188	2972.46	1.05	3.176	66.947	0.5177	0.00000	0.00000
189	2972.49	1.04	38.284	28.638	0.6707	0.00000	0.00000
190	2972.66	1.04	34.794	887.450	0.0492	0.00000	0.00000
191	2972.88	1.06	19.750	269.739	0.1242	0.00000	0.00000
192	2973.06	1.06	35.061	417.930	0.0436	0.00000	0.00000
193	3007.51	1.10	9.668	78.134	0.6723	0.00000	0.00000
194	3007.69	1.10	17.619	64.388	0.6889	0.00000	0.00000
195	3007.82	1.10	2.097	82.630	0.5751	0.00000	0.00000
196	3007.94	1.10	6.325	103.967	0.5812	0.00000	0.00000
197	3020.40	1.10	0.296	4.025	0.7488	0.00000	0.00000
198	3020.74	1.10	0.312	11.110	0.7497	0.00000	0.00000
199	3020.80	1.10	15.082	169.403	0.7492	0.00000	0.00000
200	3021.16	1.10	17.207	148.974	0.7474	0.00000	0.00000
201	3049.15	1.10	45.119	89.966	0.6585	0.00000	0.00000
202	3049.20	1.10	16.428	174.735	0.4713	0.00000	0.00000
203	3049.56	1.10	79.695	53.631	0.6342	0.00000	0.00000
204	3049.60	1.10	7.685	551.221	0.4699	0.00000	0.00000
205	3056.49	1.10	8.606	4.761	0.7121	0.00000	0.00000
206	3056.58	1.10	38.240	13.915	0.6714	0.00000	0.00000
207	3056.98	1.10	10.146	26.671	0.6725	0.00000	0.00000
208	3057.02	1.10	7.885	19.275	0.6922	0.00000	0.00000
209	3058.51	1.10	26.742	76.829	0.7494	0.00000	0.00000
210	3058.72	1.10	15.501	82.163	0.5139	0.00000	0.00000
211	3059.43	1.10	25.628	82.980	0.7174	0.00000	0.00000
212	3059.70	1.10	14.666	93.900	0.5229	0.00000	0.00000

213	3135.98	1.09	2.228	89.091	0.3229	0.00000	0.00000
214	3136.17	1.09	1.894	101.310	0.3270	0.00000	0.00000
215	3138.02	1.09	4.454	95.862	0.2261	0.00000	0.00000
216	3138.60	1.09	3.257	124.982	0.2388	0.00000	0.00000

TiO-Ep II

Energy = -2384.0078186479
Atomic Coordinates:

7	0.91107218	1.73477229	-0.61246515
6	0.86084678	-2.47265620	-3.44913426
6	1.54324775	-1.33379544	-3.82065951
6	0.79744376	-3.79152528	-4.15940895
6	0.19869128	-2.17176586	-2.18997440
6	1.29218389	-0.34270673	-2.78327132
7	0.47504696	-0.87608282	-1.81112900
6	1.81545773	0.95345370	-2.76086283
6	1.65547398	1.91365062	-1.75768071
6	1.04314499	2.88650073	0.13208608
6	0.46197146	3.09989007	1.38501337
6	-0.31897195	2.20214615	2.11804213
6	-0.85570089	2.45135668	3.44645712
6	-1.53880507	1.31316949	3.81850197
6	-0.66560746	3.71852855	4.22501547
7	-0.67415268	0.93950053	1.69642793
6	-1.41397913	0.37424040	2.71176929
6	-1.92923843	-0.92503154	2.69266905
6	-1.77629856	-1.88177569	1.68488303
6	-2.27356900	-3.24962056	1.74062187
6	-1.89085085	-3.85494193	0.56252760
7	-1.11059915	-1.67144199	0.49748643
6	-3.00701632	-3.86354890	2.90019333
6	-2.06607851	-4.41967386	3.99098325
6	-2.30280857	1.06516315	5.08912024
6	-3.81120671	1.36864010	4.95794754
6	-2.13629334	-5.26642392	0.12049482
6	-1.16324217	-2.85622292	-0.20400700
6	-0.57394237	-3.07305224	-1.45254017
1	1.27300852	-4.59347593	-3.56805284
1	-0.24569708	-4.09752524	-4.34914746
1	1.31332467	-3.74534086	-5.13000747
1	-1.10355490	4.58434114	3.69855032
1	-1.14530942	3.65458554	5.21288865
1	0.40413650	3.93836826	4.38517198
1	-3.65438177	-4.67682471	2.52947876
1	-3.68772416	-3.11736692	3.34649172
1	-2.64560482	-4.84790623	4.82552111
1	-1.41633582	-5.20900285	3.58056545
1	-2.16452726	0.01690166	5.40781100
1	-1.87622333	1.68406356	5.89706708
1	-2.78667735	-5.79784402	0.83109545
1	-2.62387286	-5.30000203	-0.86885591
1	-1.19387402	-5.83630719	0.04218628
1	-0.70652551	-4.06677327	-1.88597555
6	2.42799374	-1.13530559	-5.01955226
6	3.91853768	-1.41649907	-4.73025727
1	2.08538248	-1.79467273	-5.83548685
1	4.53027498	-1.24632214	-5.63164818
1	4.29523248	-0.76326657	-3.92716030
6	2.28037013	3.22948187	-1.74447216
1	2.44062958	1.23824202	-3.60930153
6	1.89770719	3.83380160	-0.56597227
1	-2.49314488	-1.23594287	3.57422110
22	-0.57718277	0.23015967	-0.31669678

8	-1.92126545	0.78956106	-1.04708477
6	3.14075787	3.79604674	-2.83916430
6	2.32354227	4.44578007	-3.97695505
1	3.78437698	3.00116886	-3.25564688
1	3.82773811	4.54603045	-2.41089753
1	2.99044929	4.83593629	-4.76352866
1	1.63463631	3.71812918	-4.43466674
1	1.71572432	5.28033593	-3.59268815
1	-4.27067381	0.75594847	4.16607386
1	-4.33523771	1.16213361	5.90580429
1	-3.97457307	2.42586348	4.69492319
1	-1.41433839	-3.62724769	4.39207352
1	0.65723413	4.06754746	1.85242380
6	2.26941901	5.19315503	-0.05414952
1	1.37977375	5.83564728	0.06589916
1	2.76624432	5.13304171	0.92959614
1	2.95625459	5.70443400	-0.74478747
1	2.31454490	-0.10437234	-5.39853256
1	4.06321100	-2.45945331	-4.40626164

Harmonic Frequencies (cm^-1), Reduced Masses (amu),
IR Intensities (km/mol),
Raman Scattering Activities (A^4/amu),
Raman Depolarization Ratios,
Raman Optical Activities (10^-4)

Mode	Freq.	Mass.	IR Int.	Raman A.	Raman D.	ROA (90)	ROA (180)
1	23.31	3.99	0.001	0.097	0.7500	0.00000	0.00000
2	29.61	3.79	0.210	0.150	0.6671	0.00000	0.00000
3	44.03	3.84	2.806	0.320	0.7487	0.00000	0.00000
4	47.13	3.54	0.036	1.947	0.6690	0.00000	0.00000
5	50.46	2.69	0.009	0.022	0.6421	0.00000	0.00000
6	51.19	2.75	0.029	2.776	0.6704	0.00000	0.00000
7	53.42	2.58	0.007	2.421	0.7494	0.00000	0.00000
8	57.94	2.94	1.285	0.254	0.7118	0.00000	0.00000
9	74.14	3.44	0.188	0.276	0.7500	0.00000	0.00000
10	74.92	3.68	0.098	0.923	0.7500	0.00000	0.00000
11	76.53	3.15	0.000	0.041	0.7495	0.00000	0.00000
12	99.61	1.41	0.106	2.090	0.7485	0.00000	0.00000
13	100.14	1.10	0.055	0.310	0.7445	0.00000	0.00000
14	103.03	1.18	0.885	0.196	0.7500	0.00000	0.00000
15	104.07	1.18	0.121	0.243	0.7340	0.00000	0.00000
16	106.91	1.52	0.305	0.029	0.6715	0.00000	0.00000
17	130.65	4.18	0.010	0.509	0.5705	0.00000	0.00000
18	139.91	4.29	0.750	3.165	0.7500	0.00000	0.00000
19	140.60	2.67	0.014	4.074	0.7199	0.00000	0.00000
20	142.84	4.89	0.719	2.622	0.7494	0.00000	0.00000
21	156.89	2.93	1.243	1.778	0.1552	0.00000	0.00000
22	161.03	2.06	0.707	1.029	0.7481	0.00000	0.00000
23	166.40	2.72	0.122	2.553	0.1344	0.00000	0.00000
24	176.25	4.89	0.291	3.248	0.4686	0.00000	0.00000
25	178.73	3.52	0.047	7.840	0.7500	0.00000	0.00000
26	187.01	4.44	1.697	1.673	0.5587	0.00000	0.00000
27	195.60	1.25	0.000	0.248	0.7374	0.00000	0.00000
28	200.88	1.46	0.108	6.522	0.5973	0.00000	0.00000
29	204.71	1.33	0.053	0.131	0.2016	0.00000	0.00000
30	214.48	1.38	0.491	0.175	0.7479	0.00000	0.00000
31	221.74	3.79	0.005	10.893	0.6004	0.00000	0.00000
32	230.46	3.90	0.076	0.420	0.7498	0.00000	0.00000
33	237.22	3.82	0.052	3.378	0.2467	0.00000	0.00000
34	244.60	4.54	0.023	2.223	0.7500	0.00000	0.00000
35	257.73	4.48	0.006	0.597	0.7483	0.00000	0.00000
36	259.26	2.64	0.202	21.010	0.0780	0.00000	0.00000
37	267.11	3.50	0.484	0.081	0.7451	0.00000	0.00000

38	270.00	3.70	0.019	0.007	0.4543	0.00000	0.00000
39	283.94	5.66	0.263	1.466	0.2927	0.00000	0.00000
40	287.91	2.88	0.311	0.377	0.6483	0.00000	0.00000
41	297.18	3.74	2.922	0.441	0.1372	0.00000	0.00000
42	301.51	3.55	3.055	0.080	0.7442	0.00000	0.00000
43	304.02	2.14	0.066	2.055	0.7500	0.00000	0.00000
44	319.08	3.54	2.502	8.659	0.1002	0.00000	0.00000
45	344.00	4.48	3.337	29.079	0.0770	0.00000	0.00000
46	344.41	5.70	1.935	1.665	0.2389	0.00000	0.00000
47	346.92	5.64	7.729	1.013	0.1038	0.00000	0.00000
48	355.37	5.58	4.129	0.123	0.7500	0.00000	0.00000
49	371.67	4.23	0.069	1.007	0.7489	0.00000	0.00000
50	397.69	4.09	1.379	12.061	0.1228	0.00000	0.00000
51	406.07	4.27	3.046	0.620	0.1422	0.00000	0.00000
52	448.52	5.88	3.477	0.095	0.7494	0.00000	0.00000
53	476.72	3.97	0.062	0.663	0.2066	0.00000	0.00000
54	490.02	3.76	3.342	0.030	0.4089	0.00000	0.00000
55	499.13	3.80	4.185	0.038	0.7482	0.00000	0.00000
56	515.06	4.35	0.093	1.020	0.2056	0.00000	0.00000
57	522.44	5.53	0.002	0.199	0.7492	0.00000	0.00000
58	533.77	3.65	0.000	0.822	0.7500	0.00000	0.00000
59	568.19	4.75	0.951	0.073	0.1898	0.00000	0.00000
60	585.57	4.16	0.007	1.516	0.7499	0.00000	0.00000
61	596.08	3.60	0.881	0.081	0.7182	0.00000	0.00000
62	602.23	3.89	0.111	0.025	0.6399	0.00000	0.00000
63	655.29	2.87	0.025	3.035	0.5496	0.00000	0.00000
64	669.40	4.15	0.090	9.229	0.1756	0.00000	0.00000
65	680.93	5.31	0.009	4.688	0.7499	0.00000	0.00000
66	686.76	6.17	0.197	0.881	0.7500	0.00000	0.00000
67	691.75	3.54	7.496	0.125	0.6469	0.00000	0.00000
68	695.92	5.48	2.510	0.836	0.7498	0.00000	0.00000
69	702.92	3.72	2.986	1.789	0.4226	0.00000	0.00000
70	708.92	3.98	20.300	0.405	0.7428	0.00000	0.00000
71	710.58	4.00	20.625	3.817	0.1324	0.00000	0.00000
72	722.65	3.96	0.012	0.293	0.7462	0.00000	0.00000
73	724.55	6.36	0.353	4.541	0.1639	0.00000	0.00000
74	726.34	4.22	7.176	7.028	0.0661	0.00000	0.00000
75	729.28	4.91	18.061	0.066	0.6838	0.00000	0.00000
76	741.51	1.93	17.669	0.035	0.6122	0.00000	0.00000
77	745.72	1.90	26.271	0.130	0.5241	0.00000	0.00000
78	750.69	2.68	0.038	2.242	0.7497	0.00000	0.00000
79	764.20	1.56	0.001	0.600	0.6780	0.00000	0.00000
80	766.51	1.75	0.959	37.049	0.0743	0.00000	0.00000
81	782.68	1.88	9.778	0.085	0.5636	0.00000	0.00000
82	801.20	2.54	2.625	52.955	0.0697	0.00000	0.00000
83	804.26	2.03	3.821	0.119	0.7482	0.00000	0.00000
84	825.56	1.48	43.602	0.022	0.7093	0.00000	0.00000
85	828.16	1.46	1.034	0.105	0.7470	0.00000	0.00000
86	831.00	1.53	0.007	0.264	0.7446	0.00000	0.00000
87	833.89	1.50	1.176	0.004	0.2656	0.00000	0.00000
88	900.55	2.51	0.001	14.013	0.7500	0.00000	0.00000
89	909.08	2.98	0.744	0.056	0.7489	0.00000	0.00000
90	916.77	3.92	56.153	0.115	0.4464	0.00000	0.00000
91	931.85	2.79	0.493	19.618	0.4995	0.00000	0.00000
92	948.04	2.06	0.002	13.830	0.7500	0.00000	0.00000
93	952.61	2.26	9.706	0.109	0.3941	0.00000	0.00000
94	954.06	2.07	15.863	0.077	0.7094	0.00000	0.00000
95	964.08	2.28	97.781	0.093	0.1667	0.00000	0.00000
96	971.87	1.87	0.367	1.919	0.7169	0.00000	0.00000
97	980.15	3.63	0.806	10.010	0.1320	0.00000	0.00000
98	981.19	1.72	0.028	31.125	0.7500	0.00000	0.00000
99	982.01	1.71	34.884	0.096	0.7407	0.00000	0.00000
100	1002.34	19.12	116.215	19.046	0.0565	0.00000	0.00000
101	1016.26	1.50	2.205	0.590	0.4607	0.00000	0.00000
102	1016.37	1.50	2.322	0.427	0.5096	0.00000	0.00000

103	1016.83	1.50	1.429	1.436	0.2138	0.00000	0.00000
104	1016.94	1.50	2.296	0.503	0.2877	0.00000	0.00000
105	1045.27	2.01	10.935	1.167	0.0310	0.00000	0.00000
106	1045.97	1.99	14.993	4.318	0.7274	0.00000	0.00000
107	1046.71	1.99	51.223	1.288	0.6311	0.00000	0.00000
108	1046.82	1.99	0.780	54.891	0.0901	0.00000	0.00000
109	1079.88	1.85	0.038	0.647	0.1193	0.00000	0.00000
110	1085.34	1.97	14.208	0.028	0.2961	0.00000	0.00000
111	1092.93	1.85	6.439	0.007	0.5023	0.00000	0.00000
112	1109.03	2.02	0.037	1.469	0.7499	0.00000	0.00000
113	1122.87	2.70	0.018	0.144	0.7490	0.00000	0.00000
114	1123.23	2.82	4.899	0.332	0.6510	0.00000	0.00000
115	1123.54	2.65	3.155	0.376	0.0746	0.00000	0.00000
116	1123.84	2.37	0.106	29.746	0.7496	0.00000	0.00000
117	1126.77	3.57	0.480	54.771	0.1139	0.00000	0.00000
118	1138.35	4.14	66.075	0.046	0.2526	0.00000	0.00000
119	1140.86	3.72	80.428	0.047	0.6203	0.00000	0.00000
120	1152.79	5.53	0.002	10.668	0.6907	0.00000	0.00000
121	1203.97	2.59	0.001	142.943	0.7500	0.00000	0.00000
122	1216.22	2.24	3.973	0.968	0.1566	0.00000	0.00000
123	1226.91	2.73	19.086	0.774	0.4773	0.00000	0.00000
124	1249.08	1.25	0.104	18.438	0.2833	0.00000	0.00000
125	1251.53	1.28	12.241	0.160	0.4489	0.00000	0.00000
126	1257.49	1.42	0.003	47.416	0.7500	0.00000	0.00000
127	1264.85	1.42	24.892	0.299	0.3379	0.00000	0.00000
128	1291.42	1.49	0.095	9.365	0.7498	0.00000	0.00000
129	1291.81	1.47	3.514	0.452	0.2798	0.00000	0.00000
130	1295.93	1.50	15.351	0.509	0.3442	0.00000	0.00000
131	1297.27	1.47	0.057	73.080	0.2713	0.00000	0.00000
132	1300.10	1.80	0.021	5.308	0.7452	0.00000	0.00000
133	1340.44	1.96	0.038	0.370	0.5987	0.00000	0.00000
134	1341.28	2.01	4.741	0.260	0.6749	0.00000	0.00000
135	1342.77	1.75	0.004	57.021	0.7500	0.00000	0.00000
136	1349.48	1.47	0.031	169.843	0.2553	0.00000	0.00000
137	1352.38	8.44	1.627	184.465	0.1353	0.00000	0.00000
138	1357.84	1.27	0.167	1.333	0.5442	0.00000	0.00000
139	1358.28	1.43	6.032	7.104	0.2657	0.00000	0.00000
140	1359.01	1.23	0.042	6.104	0.7487	0.00000	0.00000
141	1359.42	1.26	0.489	61.315	0.2993	0.00000	0.00000
142	1361.14	1.96	10.349	0.833	0.7181	0.00000	0.00000
143	1363.43	2.47	5.664	0.304	0.7473	0.00000	0.00000
144	1372.16	2.35	5.567	0.414	0.5154	0.00000	0.00000
145	1372.19	2.19	24.325	0.339	0.5897	0.00000	0.00000
146	1373.40	2.30	0.016	237.687	0.7500	0.00000	0.00000
147	1375.55	2.33	0.014	47.529	0.7500	0.00000	0.00000
148	1383.05	3.70	0.081	238.981	0.7403	0.00000	0.00000
149	1428.78	2.37	0.124	16.859	0.3985	0.00000	0.00000
150	1435.04	1.24	0.183	0.506	0.7437	0.00000	0.00000
151	1436.63	1.08	0.013	40.329	0.7499	0.00000	0.00000
152	1437.61	1.11	18.641	0.360	0.7366	0.00000	0.00000
153	1438.12	1.06	0.155	2.109	0.7495	0.00000	0.00000
154	1438.39	1.05	0.120	7.290	0.7463	0.00000	0.00000
155	1438.69	1.10	1.348	51.199	0.7486	0.00000	0.00000
156	1439.22	1.06	16.356	0.788	0.1276	0.00000	0.00000
157	1441.51	1.52	9.005	9.140	0.4332	0.00000	0.00000
158	1441.95	1.73	10.623	5.379	0.4212	0.00000	0.00000
159	1444.52	2.34	4.099	1.631	0.7246	0.00000	0.00000
160	1448.50	1.04	1.599	61.064	0.7491	0.00000	0.00000
161	1448.58	1.04	22.763	8.972	0.5090	0.00000	0.00000
162	1449.03	1.05	6.567	21.982	0.4372	0.00000	0.00000
163	1449.19	1.07	4.198	6.727	0.6562	0.00000	0.00000
164	1451.25	1.06	0.120	39.819	0.7500	0.00000	0.00000
165	1452.76	1.13	17.994	0.101	0.4512	0.00000	0.00000
166	1455.15	1.15	0.013	59.974	0.4966	0.00000	0.00000
167	1457.01	1.52	2.207	1.007	0.6079	0.00000	0.00000

168	1462.89	1.16	0.484	9.545	0.7454	0.00000	0.00000
169	1463.26	1.10	2.055	0.246	0.7484	0.00000	0.00000
170	1463.77	1.12	9.898	0.661	0.7204	0.00000	0.00000
171	1464.11	1.17	26.655	0.290	0.7419	0.00000	0.00000
172	1480.78	7.73	1.499	16.044	0.0940	0.00000	0.00000
173	1537.20	6.83	1.086	1.424	0.2243	0.00000	0.00000
174	1537.41	6.98	0.009	1.585	0.4918	0.00000	0.00000
175	1552.86	6.00	0.000	52.327	0.7500	0.00000	0.00000
176	1556.26	7.25	0.005	1079.184	0.7500	0.00000	0.00000
177	1580.27	7.49	0.007	931.684	0.1167	0.00000	0.00000
178	1584.83	6.94	1.668	1.835	0.4854	0.00000	0.00000
179	1585.07	6.98	0.554	1.372	0.6797	0.00000	0.00000
180	1615.22	7.65	0.004	64.395	0.7499	0.00000	0.00000
181	2964.08	1.04	1.124	67.374	0.6983	0.00000	0.00000
182	2964.20	1.04	2.343	41.425	0.4012	0.00000	0.00000
183	2964.43	1.04	114.121	35.205	0.1392	0.00000	0.00000
184	2964.68	1.04	3.258	1036.145	0.1194	0.00000	0.00000
185	2971.15	1.04	10.295	95.974	0.7398	0.00000	0.00000
186	2971.20	1.05	17.009	58.691	0.5736	0.00000	0.00000
187	2971.38	1.04	130.118	69.768	0.0818	0.00000	0.00000
188	2971.60	1.04	12.871	362.189	0.1182	0.00000	0.00000
189	2971.63	1.05	2.874	121.356	0.2185	0.00000	0.00000
190	2971.72	1.05	41.167	798.990	0.0247	0.00000	0.00000
191	2972.10	1.06	23.826	101.834	0.2805	0.00000	0.00000
192	2972.23	1.06	40.075	139.243	0.0994	0.00000	0.00000
193	3006.64	1.10	9.907	77.452	0.6667	0.00000	0.00000
194	3006.85	1.10	16.635	66.887	0.7134	0.00000	0.00000
195	3007.03	1.10	1.414	69.747	0.5892	0.00000	0.00000
196	3007.12	1.10	6.727	117.119	0.5655	0.00000	0.00000
197	3019.25	1.10	0.075	1.227	0.7490	0.00000	0.00000
198	3019.54	1.10	0.452	5.583	0.7494	0.00000	0.00000
199	3019.66	1.10	14.702	175.814	0.7497	0.00000	0.00000
200	3019.98	1.10	17.072	148.602	0.7479	0.00000	0.00000
201	3048.90	1.10	42.805	86.910	0.6871	0.00000	0.00000
202	3048.95	1.10	15.838	165.577	0.4595	0.00000	0.00000
203	3049.25	1.10	88.522	35.146	0.7252	0.00000	0.00000
204	3049.33	1.10	5.399	597.331	0.4586	0.00000	0.00000
205	3055.17	1.10	11.563	4.642	0.7267	0.00000	0.00000
206	3055.27	1.10	44.468	7.734	0.6974	0.00000	0.00000
207	3055.47	1.10	6.354	13.054	0.6956	0.00000	0.00000
208	3055.56	1.10	6.613	41.364	0.6753	0.00000	0.00000
209	3058.06	1.10	23.903	81.007	0.7435	0.00000	0.00000
210	3058.28	1.10	13.737	78.324	0.5194	0.00000	0.00000
211	3058.92	1.10	24.450	80.495	0.7070	0.00000	0.00000
212	3059.20	1.10	13.018	95.215	0.5289	0.00000	0.00000
213	3131.13	1.09	2.206	77.218	0.3236	0.00000	0.00000
214	3131.27	1.09	1.521	115.632	0.3213	0.00000	0.00000
215	3134.09	1.09	7.004	0.472	0.3357	0.00000	0.00000
216	3134.16	1.09	0.033	220.237	0.2394	0.00000	0.00000
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