

Energies in a.u., Coordinates in Angstrom, Frequencies in cm^{-1}

Figure 1 e)

Educts

Zr_2O_5^-

E= -470.713832336

Coordinates:

	x	y	z
O	0.123722	-0.642546	1.260911
Zr	-0.891001	-0.516318	-0.264597
O	-0.263807	1.023908	-1.545813
Zr	-1.772522	2.250999	-1.227550
O	-2.778064	2.647115	-2.692742
O	-2.497237	0.825352	-0.078411
O	-1.195162	-2.382801	-1.025569

Frequencies:

70.9633 133.2396 136.9198 156.6728 160.6999
246.5391 268.5700 296.0695 411.4133 432.3444
560.8409 603.7443 688.6257 781.1931 850.2256

CO

E=-113.356524437

Coordinates:

	x	y	z
C	0.000000	0.000000	0.005636
O	0.000000	0.000000	1.132364

Frequency:

2218.6470

Minimum I

E=-584.141725467

Coordinates:

	x	y	z
C	0.179274	0.319181	0.125203
O	-0.121213	-0.288407	1.117374
O	0.825243	-0.006751	-0.926838
Zr	1.358141	0.024721	-3.002472
O	2.741268	-1.332972	-3.744123
Zr	4.008960	-0.021007	-4.498364
O	5.683730	-0.080425	-3.802602
O	-0.067675	0.096264	-4.109984
O	2.814409	1.327678	-3.687283

Frequencies:

31.1297 38.0814 72.1943 75.3304 112.5355
136.1272 165.0487 171.9365 247.5174 256.6480

304.8956 361.4801 424.8555 584.4705 599.4547
685.9464 734.9988 855.7188 871.0434 1268.6499
1785.9207

Transition state I

E=-584.139578020

Coordinates:

	x	y	z
O	-0.362471	-0.190562	0.061567
Zr	-0.259443	-0.105928	1.862097
O	1.733410	-0.177587	2.435923
Zr	1.776293	-2.067498	2.992223
O	2.204617	-2.334476	4.734877
O	-0.162248	-2.031361	2.607324
O	-1.998094	3.461519	3.069729
C	-1.465741	2.449045	2.707024
O	-1.790471	1.214043	2.739232

Frequencies:

-72.6883 29.7357 66.1727 75.8499 128.7872
161.2936 168.4511 194.1985 254.9857 257.7066
302.7314 373.3157 420.3344 582.5880 600.6274
687.2665 742.0998 855.6667 872.7993 1226.2793
1797.5061

Minimum II

E=-584.140505048

Coordinates:

	x	y	z
C	0.559753	0.173293	-0.327837
O	0.266180	0.614686	0.747447
O	0.672086	-0.967677	-0.866962
Zr	1.257215	-0.106063	-2.871048
O	2.661910	-1.285425	-3.835754
Zr	3.900196	0.158635	-4.369477
O	5.585101	0.024334	-3.703332
O	-0.172557	0.096756	-3.954399
O	2.692257	1.329742	-3.347725

Frequencies:

37.1409 67.4252 72.8169 100.9375 127.4595
161.1419 170.1890 254.4021 262.0217 295.3656
310.4491 370.2417 413.6022 576.3431 600.2405
687.1115 731.1416 852.2451 872.0790 1227.8820
1826.4105

Transition state II

E=-584.103736938

Coordinates:

	x	y	z
C	-0.054427	-0.020460	0.308032
O	-0.345455	-0.063806	1.446810
O	0.641656	0.019145	-0.667670
Zr	2.772259	0.117245	-2.741131
O	2.420054	-1.061214	-4.327783
Zr	4.103368	-2.184808	-4.215394
O	3.810764	-3.919061	-3.794359
O	3.129410	1.819649	-3.223667
O	4.440191	-0.989527	-2.611077

Minimum III

E=-584.106169745

Coordinates:

	x	y	z
C	0.128339	-0.102874	0.334814
O	-0.525144	-0.187524	1.289022
O	0.803164	-0.026337	-0.611939
Zr	2.847266	0.190299	-2.826639
O	2.413306	-1.016138	-4.351450
Zr	4.042622	-2.258699	-4.181398
O	3.621662	-3.907306	-3.561690
O	3.091567	1.945314	-3.229143
O	4.495038	-0.919574	-2.687816

Products

Zr₂O₄-

E=-395.444159686

Coordinates:

	x	y	z
O	0.211468	-0.589778	1.395848
Zr	-0.788171	-0.464880	-0.111889
O	-2.404284	0.736801	0.030246
Zr	-1.797818	2.157547	-1.272896
O	-0.184598	0.953386	-1.419827
O	-2.797808	2.300901	-2.779247

Frequencies:

83.7794 136.0028 156.9226 237.1218 274.4197
278.2396 447.1676 509.3868 567.8116 625.2095
846.2549 861.4423

CO₂

E=-188.658402383

Coordinates:

x	y	z
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C	0.439936	0.000000	0.311086
O	-0.230012	0.000000	1.258664
O	1.110009	0.000000	-0.636417

Frequencies:

807.3729 999.9757 1693.2629

Figure 5

Educts

Zr₂O₅⁻

E= -470.713832336

Coordinates:

	x	y	z
O	0.123722	-0.642546	1.260911
Zr	-0.891001	-0.516318	-0.264597
O	-0.263807	1.023908	-1.545813
Zr	-1.772522	2.250999	-1.227550
O	-2.778064	2.647115	-2.692742
O	-2.497237	0.825352	-0.078411
O	-1.195162	-2.382801	-1.025569

Frequencies:

70.9633 133.2396 136.9198 156.6728 160.6999
 246.5391 268.5700 296.0695 411.4133 432.3444
 560.8409 603.7443 688.6257 781.1931 850.2256

C₂H₂

E=-77.3623447917

Coordinates:

	x	y	z
H	0.000000	0.000000	0.012024
C	0.000000	0.000000	1.074964
C	0.000000	0.000000	2.273049
H	0.000000	0.000000	3.335963

Frequencies:

641.4028 641.4044 767.7949 767.7964 2076.2626
 3421.8046 3521.2184

Minimum I

E=-548.151646221

Coordinates:

	x	y	z
C	-1.853386	2.210357	0.894494
Zr	-0.371360	0.749909	0.139469
O	1.068485	-0.075259	1.154109
Zr	0.784052	-2.066730	0.490383
O	-0.744981	-1.031166	-0.547852

C	-1.345838	3.002901	-0.084333
O	-0.331320	2.562768	-0.910960
O	0.235095	-3.280753	1.762424
H	-2.648215	2.592752	1.520260
H	-1.664778	4.023244	-0.317138
O	2.241334	-2.892600	-0.598632

Frequencies:

50.8131	80.0177	96.1553	119.6261	149.7884
150.8071	205.9962	245.0405	253.2016	287.3415
346.8325	398.6128	419.8397	478.2696	551.9746
628.3021	703.9041	746.3114	750.9928	761.8848
926.0592	953.5861	1139.1521	1289.7044	1452.1009
3033.3427	3197.7141			

Transition state I

E=-548.112154576

Coordinates:

	x	y	z
C	0.007596	0.192835	-0.374318
Zr	0.174661	0.315121	1.961722
O	1.601547	-0.000796	3.302555
Zr	1.059182	1.876325	4.052042
O	-0.806652	1.128298	3.485853
C	-0.540383	-1.041212	-0.182759
O	-0.720712	-1.463501	1.080423
O	1.136584	2.348731	2.196062
H	0.091572	0.592433	-1.379092
H	-0.830440	-1.770771	-0.952260
O	1.655792	2.933687	5.617599

Frequencies:

-498.0873	61.4965	78.6756	85.8479	111.2711
128.2844	175.1805	199.3796	269.4561	285.6103
345.8219	371.1476	393.2677	425.6566	547.7133
617.2229	648.2722	684.2933	705.3260	717.9438
882.7658	969.5542	1161.6233	1247.3261	1446.3033
2973.3385	3162.9176			

Minimum II

E=-548.131885310

Coordinates:

	x	y	z
C	0.063628	-0.946770	-1.454794
C	-0.691577	-0.972375	-0.369321
O	-0.484670	-0.387449	0.797378
Zr	-0.157770	0.538552	2.643340
O	-0.706410	-0.117390	4.428458
Zr	0.160007	1.733606	5.044826

O	1.523777	1.085982	3.550219
O	-0.856385	2.286458	3.256323
H	0.000211	-1.388663	-2.435280
H	-1.627170	-1.553356	-0.432229
O	0.375504	2.549486	6.673341

Frequencies:

4.3165	28.9423	45.6702	85.7867	97.9969
116.4370	134.1641	251.1025	269.4487	273.2907
360.8024	362.3953	388.3032	484.8564	516.6981
546.7182	616.1059	617.8082	694.7203	830.4270
843.6424	857.8635	1235.8032	1318.8357	1631.5407
2932.7623	3257.9891			

Transition state II

E=-548.071011580

Coordinates:

	x	y	z
C	-0.243211	0.300876	0.089972
C	0.015942	0.076640	1.406997
O	1.095992	0.008566	2.098958
Zr	2.709724	0.058904	3.488402
O	2.641923	-0.431318	5.399953
Zr	4.717011	0.058529	5.297599
O	4.400621	-0.964041	3.457020
O	3.825000	1.573769	4.086068
H	-1.312363	0.364175	-0.135766
H	-0.417993	-0.918186	0.754042
O	6.083526	0.053854	6.515954

Frequencies:

-1238.504	6.4759	29.5548	39.2923	75.5396
96.8319	108.9352	122.0570	241.0554	268.0193
273.8982	360.7414	364.2987	376.2899	535.9038
587.7505	618.7633	623.7188	693.7580	706.7650
837.2824	966.7385	1144.9389	1244.6400	1576.0405
2085.9266	3056.0085			

Minimum III

E=-548.157155997

Coordinates:

	x	y	z
C	-0.020920	0.549052	1.070478
C	1.193287	0.007795	1.055849
O	1.986960	-0.483591	1.926688
Zr	3.532355	-1.408215	3.067439
O	4.127753	-3.288305	3.062478
Zr	5.467421	-2.561902	4.560617
O	3.656854	-1.547912	5.035925

O	5.457030	-0.969451	3.142006
H	-0.581927	0.650033	2.000827
H	-0.481567	0.899748	0.157793
O	6.776134	-3.339943	5.578044

Frequencies:

15.1393	35.5255	44.8046	85.4483	90.1455
115.7921	119.0527	238.4973	272.8706	274.5849
362.4890	363.6181	369.4800	496.5378	541.9859
622.9651	623.5862	635.2915	703.4829	722.9326
837.4214	1020.9802	1207.4988	1433.4427	1704.8317
3059.1668	3206.7485			

Products

Zr₂O₄-

E=-395.444159686

Coordinates:

	x	y	z
O	0.211468	-0.589778	1.395848
Zr	-0.788171	-0.464880	-0.111889
O	-2.404284	0.736801	0.030246
Zr	-1.797818	2.157547	-1.272896
O	-0.184598	0.953386	-1.419827
O	-2.797808	2.300901	-2.779247

Frequencies:

83.7794	136.0028	156.9226	237.1218	274.4197
278.2396	447.1676	509.3868	567.8116	625.2095
846.2549	861.4423			

C₂H₂O

E=-152.661468334

Coordinates:

	x	y	z
C	0.000651	0.000000	0.049852
O	-0.000445	0.000000	1.210996
C	0.002320	0.000000	-1.257882
H	-0.932530	0.000000	-1.797312
H	0.938711	0.000000	-1.794646

Frequencies:

442.7948	553.5956	613.8890	993.9192	1176.6416
1415.2971	2225.1629	3186.1190	3276.2115	

Figure 6 a)

Educts

Zr₂O₅-

E= -470.713832336

Coordinates:

	x	y	z
O	0.123722	-0.642546	1.260911
Zr	-0.891001	-0.516318	-0.264597
O	-0.263807	1.023908	-1.545813
Zr	-1.772522	2.250999	-1.227550
O	-2.778064	2.647115	-2.692742
O	-2.497237	0.825352	-0.078411
O	-1.195162	-2.382801	-1.025569

Frequencies:

70.9633 133.2396 136.9198 156.6728 160.6999
246.5391 268.5700 296.0695 411.4133 432.3444
560.8409 603.7443 688.6257 781.1931 850.2256

C₂H₄

E=-78.6215440748

Coordinates:

	x	y	z
H	-0.029073	0.000000	0.008174
C	0.003935	0.000000	1.091280
C	1.152209	0.000000	1.754220
H	-0.950568	0.000000	1.604234
H	1.185217	0.000000	2.837326
H	2.106712	0.000000	1.241266

Frequencies:

838.5752 978.1798 980.9715 1062.1192 1244.9367
1384.5453 1478.4882 1692.1683 3133.3101 3146.3445
3204.1514 3232.2022

Minimum I

E=-549.373090593

Coordinates:

	x	y	z
O	1.920843	1.157985	2.405553
Zr	1.191137	-0.201446	1.405124
O	1.146320	0.117111	-0.688612
Zr	-0.790655	0.238390	-0.885743
O	-1.887865	-0.735094	-2.279990
O	-0.890555	-0.054348	1.041099
O	1.913335	-1.951245	2.076657
C	-2.471286	0.498543	-2.842553
C	-1.963930	1.775044	-2.116662
H	-1.404993	2.442713	-2.772280
H	-3.557801	0.402775	-2.756098
H	-2.762385	2.328779	-1.622865

H -2.207283 0.518056 -3.904216

Frequencies:

51.9875 67.0719 97.4674 109.3582 150.5989
155.6657 163.2207 213.6531 239.1675 258.5153
360.7851 381.3421 396.6451 502.9864 511.1886
549.4837 635.3880 663.2545 710.0931 768.4014
793.3858 840.4528 913.7908 982.8071 1160.5718
1248.7533 1326.9565 1448.3103 1495.4237 2992.6551
3030.8604 3062.3829 3116.6546

Transition state I

E=-549.333901834

Coordinates:

	x	y	z
C	1.270856	0.090102	0.331251
C	0.160633	-0.124639	1.363130
O	0.670889	-0.284767	2.706801
Zr	2.665811	-0.077108	2.322679
O	3.718911	1.241215	3.283194
Zr	5.448604	0.072823	2.742606
O	7.244652	0.126794	3.262901
O	4.866497	0.291747	0.907212
O	3.924145	-1.439369	2.901179
H	1.477746	-0.722678	-0.359744
H	-0.523029	0.733515	1.358738
H	1.341288	1.068500	-0.135656
H	-0.414797	-1.024278	1.110485

Frequencies:

-332.2987 55.9991 58.0588 84.2083 111.6863
148.1286 149.7590 178.0202 232.2562 255.7783
294.2143 340.5906 361.3055 425.9095 432.6153
476.7030 601.0035 644.4410 663.8746 731.8403
743.8429 817.3461 897.2821 943.1118 1133.2141
1250.2369 1324.9076 1454.8985 1494.6290 2962.5772
2996.1147 3097.4946 3174.1755

Minimum II

E=-549.371455171

Coordinates:

	x	y	z
C	0.017670	0.382314	-0.077976
C	0.127202	-0.399142	1.190828
O	1.430980	-0.334148	1.702372
Zr	3.387389	-0.109680	2.294094
O	4.432542	1.553645	2.609166
Zr	5.947254	0.140294	3.112348
O	7.690851	0.296487	3.671051

O	5.045655	-0.779750	1.419403
O	4.227943	-0.751588	3.982932
H	0.354556	-0.053167	-1.011731
H	-0.583148	-0.006695	1.933354
H	-0.078241	1.461390	-0.039395
H	-0.148450	-1.448104	1.008333

Frequencies:

16.9268	33.2807	42.6315	81.8158	90.5270
105.6651	128.3936	136.3770	258.2057	271.1610
275.1527	355.0944	358.5856	360.5779	446.1356
543.2072	611.8404	614.4007	671.6743	684.7086
794.5997	828.1002	1038.8398	1098.4302	1165.9591
1287.2781	1373.3697	1464.0027	1508.6783	2948.2327
2967.2533	3122.5657	3222.8304		

Transition state II

E=-549.315581605

Coordinates:

	x	y	z
C	-2.563685	0.843862	-2.960311
C	-1.165118	1.336476	-2.796398
H	-2.141916	1.645529	-1.979051
H	-0.900921	2.227941	-3.367292
H	-3.204091	1.284175	-3.716014
H	-2.788894	-0.143238	-2.581353
O	-0.171732	0.512776	-2.456799
Zr	1.329548	-0.789592	-1.834506
O	3.231001	-0.853526	-2.403632
Zr	3.298612	-2.420952	-0.965869
O	1.420816	-2.773228	-1.904587
O	2.050146	-0.992891	0.003240
O	4.644243	-3.522591	-0.378572

Frequencies:

-1884.294	13.0143	35.2753	47.5818	90.5638
100.6901	122.1715	130.4614	250.1151	269.1200
272.1852	340.3043	359.3263	360.1298	386.6840
501.9556	543.6765	614.6818	616.9975	677.0538
690.4974	779.1461	830.4493	960.1716	1120.0925
1253.8348	1281.0204	1386.4202	1418.9663	2044.8204
3055.7351	3112.2764	3244.1615		

Minimum III

E=-549.393629723

Coordinates:

	x	y	z
C	-2.328221	0.746537	-3.651073
C	-1.101888	1.346173	-3.048457

O	-1.212382	2.013580	-1.905389
Zr	-1.371900	2.978790	-0.066360
O	-2.889249	2.979520	1.212964
Zr	-1.583783	4.272623	2.294549
O	-1.289534	4.930507	0.291776
O	-0.228589	2.811621	1.551852
H	-0.258975	1.606108	-3.689899
H	-2.079031	0.168484	-4.545209
H	-2.833920	0.080854	-2.942186
H	-3.069445	1.511468	-3.942853
O	-1.715242	5.160049	3.896178

Frequencies:

19.6228	34.7450	51.3029	89.9678	102.3934
121.3934	131.6230	210.4564	251.4248	269.5021
271.9679	359.3918	360.3117	371.8144	442.4792
519.4713	546.3940	612.3107	615.6361	688.6114
829.5303	938.9322	1008.2187	1118.0339	1306.4184
1384.6982	1415.9405	1461.9313	1491.7166	2904.2580
3007.6420	3060.8428	3080.9263		

Products

Zr₂O₄⁻

E=-395.444159686

Coordinates:

	x	y	z
O	0.211468	-0.589778	1.395848
Zr	-0.788171	-0.464880	-0.111889
O	-2.404284	0.736801	0.030246
Zr	-1.797818	2.157547	-1.272896
O	-0.184598	0.953386	-1.419827
O	-2.797808	2.300901	-2.779247

Frequencies:

83.7794	136.0028	156.9226	237.1218	274.4197
278.2396	447.1676	509.3868	567.8116	625.2095
846.2549	861.4423			

C₂H₄O

E=-153.892225538

Coordinates:

	x	y	z
C	-0.096088	0.000000	0.449945
H	-0.789720	0.000000	1.318266
O	1.095808	0.000000	0.628598
C	-0.761775	0.000000	-0.896821
H	-0.021990	0.000000	-1.695687
H	-1.409587	-0.877619	-0.984686

H -1.409587 0.877619 -0.984686
 Frequencies:
 152.3917 513.6913 780.1019 885.9302 1131.4483
 1139.9046 1384.0341 1433.2529 1464.7756 1473.1812
 1811.8414 2872.7024 3026.9755 3080.6838 3140.8311

Figure SI1

a)
 I

E= -272.916314956
 Coordinates:

	x	y	z
Zr	0.266435	-0.389243	0.190336
O	-0.014457	0.159093	1.946295
O	1.829607	0.155542	-0.659082
O	-1.101062	-1.623705	-0.784215

 Frequencies:
 25.2520 163.0365 233.6609 460.0927 737.5412
 779.4225

II

E= -272.861618672
 Coordinates:

	x	y	z
Zr	0.068940	-0.555694	-0.194125
O	-0.298489	0.423625	1.281047
O	0.096883	0.488151	-1.931393
O	-1.191267	-0.256082	-1.752506

 Frequencies:
 63.1825 212.6859 526.3175 552.2678 838.2850
 862.7029

III

E= -272.803620029
 Coordinates:

	x	y	z
Zr	0.255719	0.000110	0.394873
O	-0.049422	-0.000180	2.267706
O	2.008634	-0.000033	-0.009741
O	0.348507	0.000103	3.587163

 Frequencies:
 131.0956 229.3087 304.3874 528.4358 867.8116
 1004.7433

b)

I

E= -470.713832336

Coordinates:

	x	y	z
O	0.123722	-0.642546	1.260911
Zr	-0.891001	-0.516318	-0.264597
O	-0.263807	1.023908	-1.545813
Zr	-1.772522	2.250999	-1.227550
O	-2.778064	2.647115	-2.692742
O	-2.497237	0.825352	-0.078411
O	-1.195162	-2.382801	-1.025569

Frequencies:

70.9633	133.2396	136.9198	156.6728	160.6999
246.5391	268.5700	296.0695	411.4133	432.3444
560.8409	603.7443	688.6257	781.1931	850.2256

II

E= -470.706198246

Coordinates:

	x	y	z
O	0.163358	-1.232139	1.488613
Zr	-0.570033	0.007104	0.358908
O	-2.525856	0.197605	-0.251193
Zr	-1.876581	1.791639	-1.377925
O	-0.103111	0.616940	-1.641593
O	-2.837696	2.882019	-2.490078
O	-0.557049	2.156304	0.277098

Frequencies:

59.9451	118.1266	124.5670	160.5530	200.1836
244.0223	251.5137	331.8174	337.3111	422.2757
522.7984	551.1361	615.2558	814.9169	852.4550

III

E= -470.646614437

Coordinates:

	x	y	z
O	-0.988469	-1.936281	1.392767
Zr	-0.736951	-0.854427	-0.100307
O	-1.664516	0.772919	-0.084972
O	-0.216940	-1.737573	-1.844366
Zr	0.367077	-2.642861	-3.556281
O	2.108503	-2.356758	-4.149596
O	-0.877062	-3.061709	-4.890427

Frequencies:

22.3649	44.3193	52.0252	69.3620	76.0046
---------	---------	---------	---------	---------

162.1237 209.0191 225.8872 230.3412 308.6589
372.9109 491.4239 535.6104 789.5817 802.3740

IV

E= -470.622474886

Coordinates:

	x	y	z
O	-1.163676	-1.918031	-0.190176
Zr	-0.888415	-0.140066	-0.427875
O	-1.742437	1.392342	0.907396
Zr	-1.643100	2.711382	-0.860474
O	-0.297491	1.745002	0.722941
O	-2.761282	4.119793	-1.106449
O	-1.735987	0.969672	-1.897465

Frequencies:

45.0941 79.1514 118.7455 141.3281 167.0198
215.3897 249.3850 299.6683 383.0696 429.8479
464.2541 614.4986 839.1692 840.2137 865.9235

V

E= -470.620837817

Coordinates:

	x	y	z
O	-0.724370	-1.838318	0.850832
Zr	-1.217382	-0.094266	0.884022
O	-2.681042	0.582751	-0.329450
Zr	-1.865435	2.284004	-1.062756
O	-0.093865	1.511294	-0.035764
O	-2.719151	3.763931	-0.497499
O	0.119848	1.429248	1.437171

Frequencies:

79.2320 106.3216 123.4244 186.6733 205.0865
218.9758 252.9093 300.4247 441.6104 522.6100
555.7153 591.7324 849.6251 859.1885 871.8633

VI

E= -470.601289891

Coordinates:

	x	y	z
O	-0.973835	-0.286977	0.760636
Zr	-0.559839	-0.143850	-1.140071
O	0.732085	1.204791	-0.579219
Zr	-0.993522	1.864038	0.549654
O	-2.508594	0.956596	-0.933901
O	-1.074041	3.117664	1.860155
O	-1.545188	1.800411	-1.688130

Frequencies:

101.6663 116.7199 190.3285 216.2346 217.5608
277.9547 292.6331 328.3719 364.4429 436.4408
463.0140 614.8034 685.1562 845.2857 890.2033

VII

E= -470.600017288

Coordinates:

	x	y	z
Zr	-1.406320	0.362300	0.620428
O	0.149475	0.409742	1.708640
Zr	1.952907	0.339220	2.813949
O	-0.957151	-0.167198	-1.025659
O	3.527490	1.606117	2.555202
O	2.651023	2.016679	3.718757
O	2.248801	-1.239240	3.672928

Frequencies:

41.2497 48.7993 53.1900 108.5939 159.7252
173.8209 207.1933 264.7616 294.1029 552.3094
557.2879 801.9082 820.7223 860.7276 908.9341

VIII

E= -470.573660475

Coordinates:

	x	y	z
Zr	-0.854586	1.003549	0.113252
O	0.531796	0.952062	1.778987
Zr	1.615377	0.858482	3.309326
O	-1.088264	-0.492576	-0.927514
O	3.581072	1.059634	3.041793
O	2.956272	2.311723	3.559461
O	-2.363764	2.045079	0.230268

Frequencies:

38.3470 52.4615 55.0834 82.9560 121.4354
169.0422 203.7185 223.9770 309.6698 555.1149
576.9930 800.6998 808.7681 862.2486 870.9312

c)

I

E= -668.544917938

Coordinates:

	x	y	z
Zr	0.868177	-0.591288	-0.915865
O	0.443260	-1.861025	0.614602
O	2.564487	-0.378099	-1.524511
O	-0.859832	-0.128114	-2.058865

O	-2.634555	-0.311855	0.607846
Zr	-1.895930	0.875565	-0.749622
Zr	-0.882538	-0.774726	1.712453
O	-0.184092	0.851642	0.386973
O	-0.809710	-0.734621	3.525258
O	-2.895282	2.610081	-1.297090

Frequencies:

94.6529	100.8296	111.0046	115.1525	132.0934
167.9065	174.2984	180.2956	236.5629	241.8657
262.8806	282.9536	375.8128	409.2825	440.3996
517.2001	536.3929	545.8126	582.0336	584.6788
662.6375	703.1595	846.2013	870.1950	

II

E= -668.503979317

Coordinates:

	x	y	z
Zr	1.511712	-0.472429	-0.985038
O	0.884115	-1.067734	0.881088
O	1.821772	-1.865452	-2.161487
O	-0.175028	0.734227	-1.583380
O	-2.231015	-0.645941	0.098214
Zr	-1.747372	1.072989	-0.569326
Zr	-0.830204	-0.590818	1.765416
O	-1.068778	1.490510	1.163444
O	-1.235915	-1.187320	3.437364
O	3.208089	0.550844	-0.996528

Frequencies:

51.4511	104.3272	122.9118	125.9032	134.6454
147.7203	154.6275	160.7099	178.5003	228.0437
268.3666	284.5114	310.3773	324.3311	358.4805
400.3230	458.4563	505.6011	642.3003	661.2394
721.2302	770.5078	808.6498	851.2268	

III

E= -668.501720869

Coordinates:

	x	y	z
O	0.107155	-0.785759	1.324867
Zr	-0.871203	-0.546289	-0.211159
O	-0.170616	0.957028	-1.519281
Zr	-1.658978	2.208867	-1.301284
O	-2.823638	3.014960	-2.805087
O	-2.428200	0.901205	-0.089308
O	-1.311432	-2.339978	-0.997349
O	-1.564311	4.212696	-0.783726
Zr	-2.715179	4.914377	-2.236549

O -1.830352 5.963773 -3.408840

Frequencies:

39.3711 43.5171 93.7770 99.9427 114.2162
146.9448 152.0669 195.6154 203.4405 236.1671
265.7107 280.2724 333.9180 378.1563 396.9330
436.0568 549.6378 586.2450 589.0975 632.8727
670.5186 719.8235 771.8742 871.6246

IV

E= -668.481951441

Coordinates:

	x	y	z
Zr	0.840070	-0.810695	-1.079636
O	1.103968	-0.975083	0.935244
O	1.525959	-2.058921	-2.214848
O	0.029562	1.042815	-1.768585
O	-1.220563	-0.909095	-0.492559
Zr	-1.580106	1.058314	-0.632313
Zr	-0.701104	-0.546212	1.785323
O	-0.651687	1.543271	0.994003
O	-0.906753	-1.225816	3.451598
O	-2.695826	0.536051	1.120096

Frequencies:

57.2036 94.8719 122.5171 145.7504 164.7899
176.9791 188.8680 205.3392 230.8742 247.1889
276.8236 330.2886 354.2894 367.2536 400.3905
432.6593 516.1166 554.5274 563.0809 586.3050
651.5754 708.7331 841.2719 866.5613

V

E= -668.470612301

Coordinates:

	x	y	z
Zr	0.884621	-0.688251	-0.950911
O	0.195259	-2.037590	0.429799
O	2.575181	-0.730750	-1.602171
O	-0.730058	0.251777	-1.943555
O	-2.418852	-0.016400	0.785681
Zr	-1.495897	1.205148	-0.434267
Zr	-0.847846	-0.965425	1.750073
O	0.174219	0.731381	0.561801
O	-1.141829	-1.729628	3.578930
O	-0.211460	-0.547223	3.609182

Frequencies:

87.4226 100.8473 115.0959 146.0240 158.7698
168.9674 176.7764 217.2002 235.4523 258.8937
277.0432 358.9974 402.4993 449.8918 534.0230

544.5987 569.2253 575.0161 581.3126 600.4846
663.1523 706.9987 844.6475 864.3484

VI

E= -668.459541422

Coordinates:

	x	y	z
Zr	0.909521	-1.047785	-1.340090
O	0.641563	-1.501922	0.541748
O	1.694811	-2.357068	-2.633695
O	-0.393666	0.369450	-1.886201
O	-2.374686	-0.385006	0.396289
Zr	-1.659635	1.160657	-0.533167
Zr	-0.760460	-0.531980	1.754518
O	-0.531970	1.440434	1.019796
O	-0.994357	-0.906521	3.515172
O	2.684641	-1.290809	-2.232667

Frequencies:

20.3433 81.0408 118.1631 127.4344 128.6157
143.3874 151.9204 156.9787 212.0830 252.4393
254.9924 321.9616 393.9967 463.0570 480.0678
513.9496 577.6444 579.2002 609.3370 614.5576
724.3289 731.3937 831.3956 856.7440

VII

E= -668.457544398

Coordinates:

	x	y	z
Zr	0.805628	-0.971185	-0.923948
O	0.851677	-1.876938	1.080066
O	1.557452	-1.990813	-2.203968
O	0.236304	0.949135	-1.533566
O	-1.353129	-0.814094	-0.230571
Zr	-1.471280	1.144281	-0.619871
Zr	-0.636555	-0.488951	1.908179
O	-1.209661	1.427648	1.287771
O	-1.327774	-1.021647	3.483072
O	1.491927	-0.515389	1.172768

Frequencies:

94.2518 98.5134 122.0651 144.3250 151.8187
177.5494 189.5899 219.6515 260.2369 267.1429
308.5947 356.1756 367.2772 381.8015 410.4261
449.1458 514.5674 528.6035 562.8888 630.4902
709.3889 848.4298 868.3678 887.1717

VIII

E= -668.443908857

Coordinates:

	x	y	z
Zr	1.013010	-0.571825	-0.886223
O	0.576648	-1.948488	0.574669
O	2.719323	-0.156414	-1.336103
O	-0.627780	-0.131271	-2.139374
O	-2.766962	-0.445147	0.887640
Zr	-1.881129	0.601213	-0.858316
Zr	-0.780065	-0.968239	1.695348
O	-0.235420	0.675833	0.417231
O	-0.480501	-0.840004	3.471534
O	-3.327530	-0.784620	-0.447078

Frequencies:

97.4148	104.1459	115.9751	126.8225	138.0549
158.3153	179.1211	207.1396	239.7601	249.4066
258.6019	286.4524	383.1468	402.3128	455.5301
501.2224	531.4035	556.6258	573.6124	606.9794
677.8636	853.5669	874.4494	879.4818	

d)

I

E= -866.346533110

Coordinates:

	x	y	z
Zr	-0.932637	1.704100	-0.843403
O	-0.808004	1.384045	1.233959
O	0.974768	1.422504	-1.441134
O	-1.791737	3.184355	-1.449659
O	-1.758270	-0.232471	-1.338974
Zr	2.135754	-0.130673	-0.877641
Zr	0.103812	-0.106364	2.059194
Zr	-0.989712	-1.874067	-0.799459
O	0.128676	-0.106646	4.121670
O	-0.855852	-1.692542	1.123784
O	1.834374	-0.203568	1.205711
O	0.808529	-1.762572	-1.377227
O	3.835271	-0.182901	-1.514541

Frequencies:

102.9788	108.2708	110.1036	110.9904	138.1476
143.2993	145.3247	149.6976	151.8304	156.8324
159.8297	188.0706	189.6721	201.0301	235.0832
277.2219	293.0356	297.0078	394.5767	413.9392
438.2405	446.7340	467.7055	502.3712	515.8117
583.1166	624.6308	650.9025	761.8700	776.6868
828.6968	849.5579	863.5703		

II

E= -866.286744720

Coordinates:

	x	y	z
O	0.122858	-1.207019	1.289970
Zr	-0.859309	-0.538479	-0.243839
O	-1.074325	-2.390197	-0.783280
O	-0.141580	0.947993	-1.500702
Zr	-1.661126	2.207118	-1.323498
Zr	-2.758650	4.899105	-2.221028
O	-1.821702	5.928805	-3.355248
O	-2.420896	0.859090	-0.127337
O	-2.814547	2.998830	-2.814339
O	-1.621655	4.172281	-0.755444
Zr	-0.054870	-3.282955	0.858325
O	-1.114490	-4.231321	2.012264
O	1.623859	-4.320456	0.492671

Frequencies:

20.4504	22.0498	52.5477	65.2236	75.2151
92.5993	112.0830	133.2587	136.1497	161.2335
174.6123	211.0177	237.2369	262.7447	264.6069
265.4296	292.4248	359.6174	389.0557	390.0011
425.0575	443.9325	540.1183	572.4469	584.7259
609.8751	614.2953	642.7211	661.6159	700.5053
733.3892	780.5030	885.6177		

III

E= -866.275194052

Coordinates:

	x	y	z
Zr	-1.077030	1.682782	-0.945256
O	-0.827776	1.536108	1.017094
O	0.965993	1.225029	-1.485448
O	-2.488061	2.999029	-1.490336
O	-1.682105	-0.274485	-1.452860
Zr	1.979414	-0.235920	-0.838122
Zr	0.056837	0.025454	2.062873
Zr	-0.853361	-1.855187	-0.747985
O	0.042997	0.126363	3.872595
O	-0.831295	-1.681600	1.159241
O	1.932858	-0.126233	1.072359
O	1.034802	-1.916485	-1.398271
O	-1.125570	3.435852	-1.965887

Frequencies:

75.7303	100.3012	110.6781	117.6890	121.7162
134.9746	144.4899	147.4070	150.4179	156.7191
177.5158	191.8479	195.6038	199.1459	271.1103
275.9733	286.8515	380.0690	422.2625	438.7043

440.1283 483.1229 521.6839 525.8649 556.5049
578.7391 605.8568 648.1530 690.4165 773.5586
800.8805 849.4834 861.9604

IV

E= -866.254068120

Coordinates:

	x	y	z
Zr	-0.968941	1.886624	-0.764624
O	-0.888200	1.503851	1.198246
O	0.989163	1.437794	-1.388415
O	-1.621227	3.513317	-1.204611
O	-1.729169	-0.019002	-1.547369
Zr	1.917526	-0.147821	-0.806589
Zr	-0.000934	-0.087043	2.108713
Zr	-0.890143	-1.765266	-0.833058
O	0.001468	-0.119386	3.920943
O	-0.923064	-1.718374	1.070458
O	1.870222	-0.182126	1.109198
O	0.982338	-1.791772	-1.521422
O	-2.621402	-1.155725	-1.859793

Frequencies:

85.4133 103.2059 104.1325 119.9004 125.3203
130.6414 140.3166 146.2701 146.6229 153.7846
170.3553 177.7652 189.0882 197.5243 246.1096
264.9931 272.4944 281.4642 421.0474 434.9114
440.5857 472.3070 490.8845 509.3402 530.6748
569.1731 601.4237 676.7554 734.4596 779.9350
857.6644 869.4076 902.9943

V

E= -866.253277964

Coordinates:

	x	y	z
Zr	-0.956503	1.593447	-0.848430
O	-0.818828	1.395540	1.162903
O	1.334042	1.718982	-1.061862
O	-1.936969	2.994360	-1.434693
O	-1.794518	-0.358054	-1.231959
Zr	1.899331	-0.312764	-0.784694
Zr	0.038051	-0.113085	2.184418
Zr	-0.990101	-1.953485	-0.600004
O	0.075863	0.011547	3.996510
O	-0.922617	-1.809718	1.297062
O	1.876473	-0.323651	1.122019
O	0.885457	-1.996549	-1.241847
O	0.760867	0.872102	-2.175273

Frequencies:

103.4047 113.3194 124.6508 133.7669 144.2577
145.8257 147.9726 149.6686 152.9919 165.7287
189.3032 197.9991 203.6905 251.5096 284.5960
289.8305 296.9693 341.6313 372.5145 399.3703
427.1849 436.7745 464.6954 489.4850 507.5792
579.0170 617.5454 675.1913 755.7452 786.2448
852.4802 859.0681 866.1428

VI

E= -866.250182432

Coordinates:

	x	y	z
Zr	-0.843631	1.775766	-0.760487
O	-0.586672	1.635944	1.189764
O	1.077065	1.267155	-1.565412
O	-1.644298	3.286145	-1.388459
O	-1.737017	-0.143114	-1.220679
Zr	2.043531	-0.286711	-1.032914
Zr	-0.008226	0.093421	2.424743
Zr	-1.012221	-1.807789	-0.688455
O	-1.232609	-0.128402	3.784897
O	-0.653801	-1.627284	1.117100
O	1.958932	-0.279767	0.780690
O	0.794340	-1.803931	-1.518037
O	1.546502	0.354789	3.659777

Frequencies:

42.9734 80.4801 96.4345 116.3850 124.9133
133.3221 136.1261 141.1344 147.2470 159.4492
167.2319 176.7837 191.8950 201.2438 222.6659
245.2135 287.6402 298.1764 311.4585 331.3751
403.2358 408.5026 419.8244 462.2400 490.4007
609.7598 657.9872 712.3310 758.5460 798.7418
848.2317 852.0090 875.0895

VII

E= -866.247787098

Coordinates:

	x	y	z
Zr	-1.121592	1.927510	-0.759538
O	-0.768516	1.333199	1.571049
O	0.935167	1.540058	-1.144028
O	-1.826800	3.145288	-1.895300
O	-1.802663	-0.052337	-1.147135
Zr	1.908781	-0.038779	-0.706916
Zr	0.165915	-0.286554	2.327679
Zr	-0.917035	-1.679913	-0.704320

O	0.328757	-0.584453	4.104929
O	-0.786366	-1.800629	1.204871
O	1.955138	-0.214935	1.201803
O	0.934626	-1.621461	-1.457846
O	-1.485736	2.543618	1.201974

Frequencies:

74.0309	99.4272	115.8886	123.6617	124.4799
132.5231	140.4336	144.5714	151.4526	157.4381
168.7632	187.4384	190.7015	193.4951	249.0351
272.2132	277.5132	290.7577	388.0336	410.9199
417.0509	440.9401	446.5755	524.9164	529.4965
554.1908	645.7458	696.0656	726.6403	802.9832
856.7541	870.9955	993.2532		