SUPPORTING INFORMATION for:

Direct observation of the gas phase reaction of cyclohexyl radical with dioxygen using a distonic ion approach

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Figure S1 – Collision induced dissociation mass spectra of *m/z* 158 ions formed from addition of dioxygen to (a) the 4-carboxylatocyclohexyl radical **E** and (b) the 3-carboxylatocyclohexyl radical **F**. Both spectra are measured with a collision energy 20 (arbitrary units).

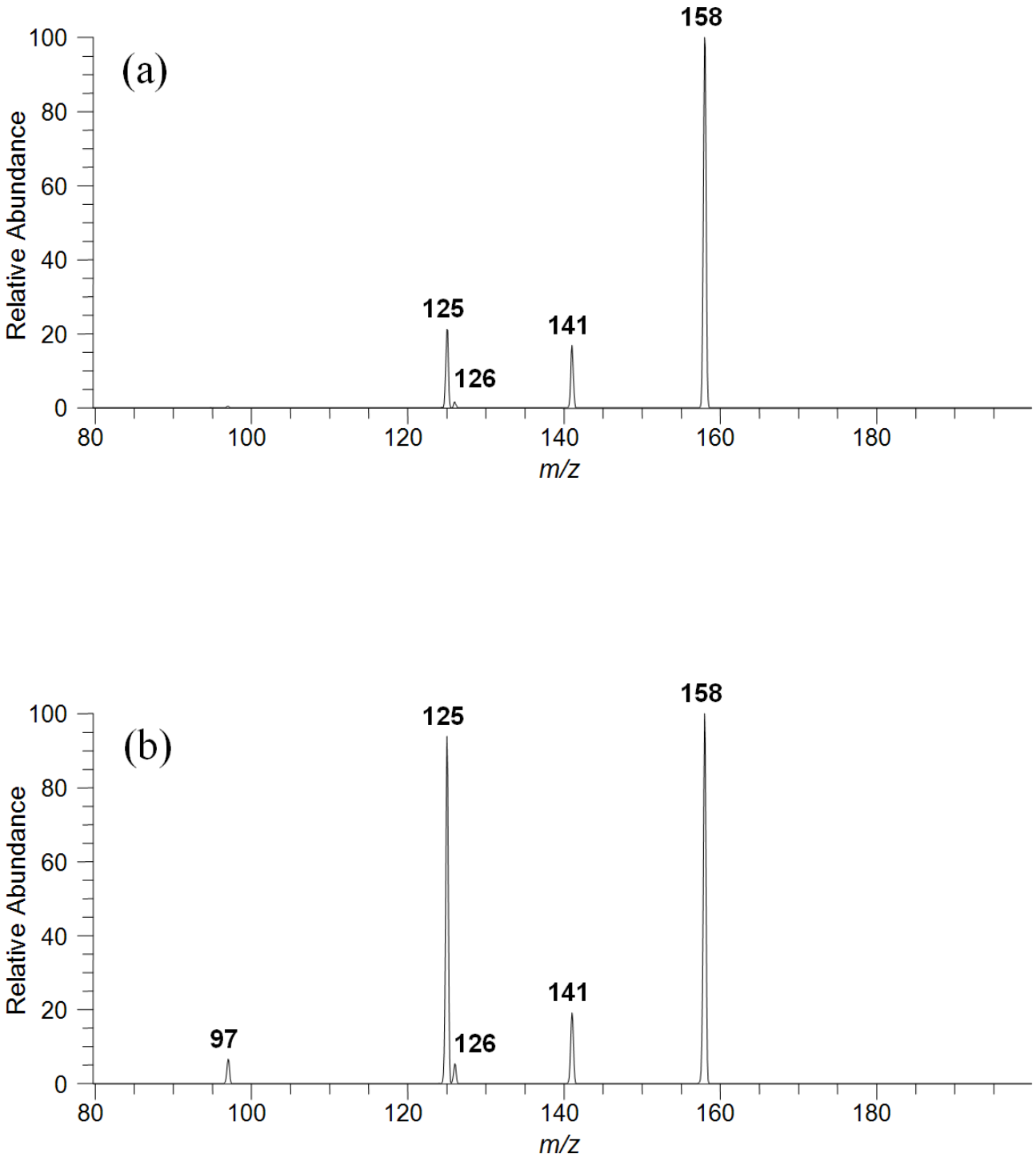
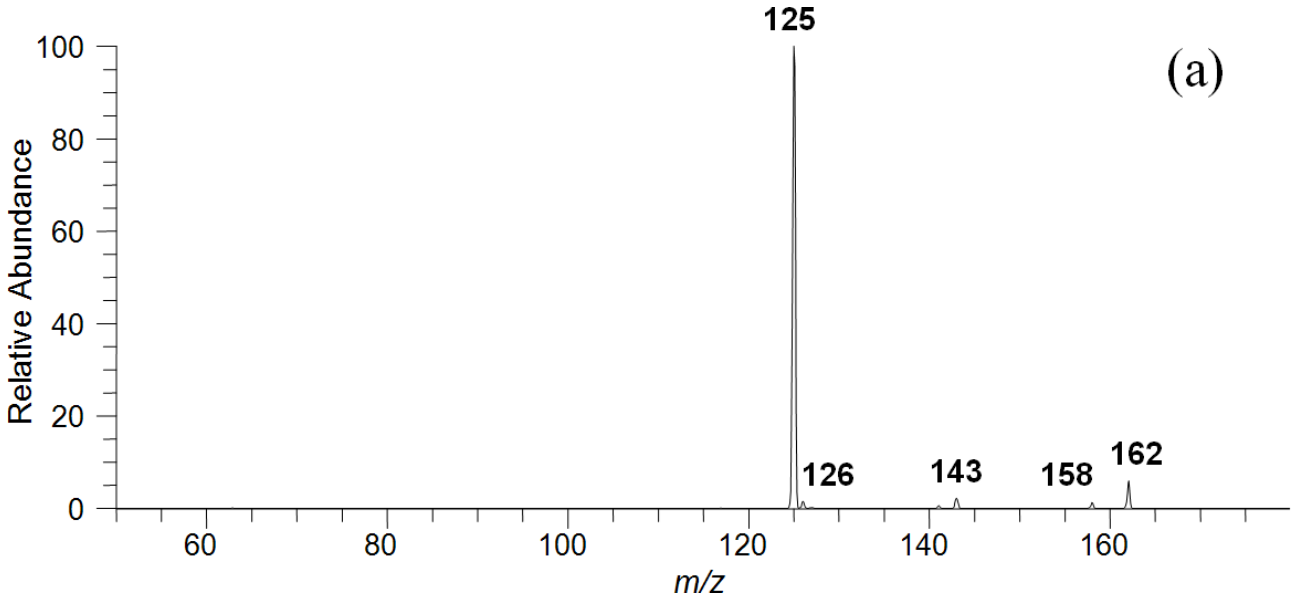


Figure S2. The mass spectrum obtained following isolation of (a) the 4-carboxylatocyclohexyl radical anion (**E**) and (b) the 1-carboxylatocyclohexyl radical anion (**H**) both at *m/z* 126, in the presence of $^{18}O_2$ for 1000 ms. It should be noted that adventitious $^{16}O_2$ is always present in the ion trap so the reactions of both isotopologues are observed in these spectra.



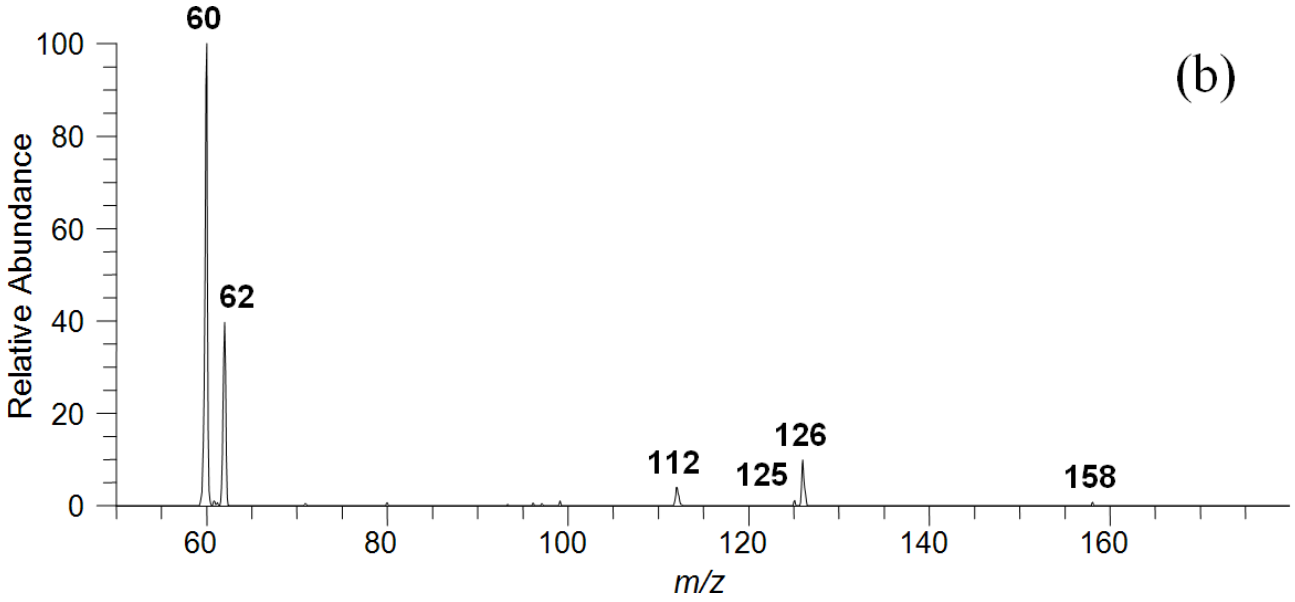


Table S1. Geometry and electronic and zero-point energies (Hartrees) for stationary points on the carboxylatocyclohexyl radical anion potential energy surface. Negative frequencies for all transitions states are reported in cm^{-1} and are presented in parentheses. The relative energies derived from this data are presented in Scheme 3.

chxl001

HF = -423.2588087
ZeroPoint = 0.1578238
Energy+ZP = -423.1009849
Thermal = 0.1662805
Free Energy Correction = 0.122922

C -0.334686 1.274106 0.437339
C 0.429694 0.000112 0.238845
C -0.334687 -1.273863 0.437807
C -1.678258 -1.269590 -0.327458
C -2.493203 -0.000015 -0.030463
C -1.678281 1.269470 -0.327886
H 0.298082 -2.115585 0.139550
H -0.565655 1.412654 1.515452
H 0.297988 2.115815 0.138821
H -1.472725 -1.319679 -1.407601
H -2.265397 -2.166543 -0.073666
H -3.430335 -0.000088 -0.608946
H -2.781729 0.000157 1.034200
H -1.472766 1.319190 -1.408050
H -2.265439 2.166504 -0.074410
H -0.565728 -1.411925 1.515964
C 1.909770 -0.000066 -0.070057
O 2.456520 1.139973 -0.182070
O 2.456181 -1.140151 -0.182940

45.3094 50.5490 174.7568
257.1478 258.4274 346.6597
377.6313 432.3235 506.8882
508.3358 624.7336 738.8026
778.2005 796.0920 830.0752
862.0475 889.3646 934.6879
954.4205 1025.9744 1039.3670
1072.6236 1088.1638 1144.4044
1153.9988 1255.8008 1257.3850
1282.0481 1289.6097 1334.8833
1337.5727 1350.2799 1365.9646
1377.8933 1385.0938 1491.5676
1494.8441 1502.9005 1506.8556
1520.9167 1601.1007 2878.5696
2887.2601 2981.4009 2995.2205
2997.0401 3017.0608 3029.9376
3039.8563 3101.8306 3102.7662

chxl102

HF = -423.2466736
ZeroPoint = 0.1566232
Energy+ZP = -423.0900504
Thermal = 0.1651718
Free Energy Correction = 0.121827

C -0.337839 -1.275383 0.031832
C 0.424868 0.015619 0.393199
C -0.277438 1.230399 -0.118597
C -1.770040 1.338021 -0.029022
C -2.479939 0.019193 -0.399800
C -1.842540 -1.171309 0.333529
H 0.324188 2.121500 -0.278703
H -0.190698 -1.479389 -1.037436
H 0.109450 -2.123285 0.562934
H -2.070515 1.595735 1.011923
H -2.145007 2.162715 -0.654481
H -3.555237 0.089781 -0.171755
H -2.391456 -0.142573 -1.484911
H -1.995508 -1.046984 1.419220
H -2.356050 -2.104385 0.051981
H 0.451981 0.079937 1.505078
C 1.958786 -0.001835 -0.011692
O 2.411583 -1.102892 -0.418646
O 2.558880 1.092730 0.153577

30.4017 101.5878 195.2559
199.4508 293.9501 316.0609
383.2158 441.6314 471.0772
486.9932 577.1268 654.8239
759.1835 796.4148 841.4206
851.4752 903.1090 908.7158
918.6941 1023.4844 1048.9753
1064.9864 1082.5123 1100.6083
1152.8635 1188.9480 1203.6937
1257.2151 1287.3153 1305.6410
1335.0462 1342.5933 1355.3946
1369.4348 1381.5255 1391.7700
1486.6873 1498.6496 1504.1075
1515.8377 1677.3173 2839.8932
2849.9844 2979.6102 2993.5910
3009.0987 3014.9593 3032.9791
3046.3556 3085.4974 3192.4939

chxl1101

HF = -423.1922569
ZeroPoint = 0.1524371
Energy+ZP = -423.0398198
Thermal = 0.1607098
Free Energy Correction = 0.117364

C 0.293292 0.000050 0.126818
C -0.393128 1.265843 0.635624
C -1.815779 1.271018 -0.029189
C -1.865807 -0.000065 -0.866568
C -1.815676 -1.271109 -0.029160
C -0.393158 -1.265618 0.635922
H -2.625421 1.293187 0.721015
H -0.455240 1.267104 1.735783
H 0.202110 2.134243 0.339842
H -2.480419 -0.000089 -1.770580
H -2.625474 -1.293471 0.720870
H -1.947559 -2.160218 -0.661291
H -0.455503 -1.266464 1.736070
H 0.202186 -2.134095 0.340583
H -1.948025 2.160103 -0.661276
H -0.435550 -0.000049 -1.026622
C 1.811727 -0.000025 -0.124732
O 2.352434 -1.138541 -0.223001
O 2.352575 1.138440 -0.222834

-1865.2101 24.9252 72.1204
143.5049 227.7970 299.7293
343.7997 417.9214 468.8791
557.2164 639.1791 737.9194
767.5457 787.9096 788.1140
813.1462 882.4569 904.1875
932.8117 955.6166 973.8859
1031.6873 1059.1425 1079.9092
1140.7345 1185.8287 1220.9939
1232.6164 1236.7679 1247.0177
1305.9253 1309.6380 1336.7689
1338.1214 1340.0726 1453.2187
1492.6754 1502.1915 1513.2440
1525.8639 1633.6183 1656.6055
2961.9865 2964.5937 2995.3762
3003.5512 3035.7409 3037.2080
3106.9225 3112.2119 3113.2391

chxl1201

HF = -423.1797723
ZeroPoint = 0.1524414
Energy+ZP = -423.0273309
Thermal = 0.1605149
Free Energy Correction = 0.118556

C -0.348845 -0.020878 0.112756
C 0.309248 -1.312033 0.604717
C 1.388807 -1.238465 -0.471348
C 2.467522 -0.209745 -0.175483
C 1.849138 1.211217 -0.144939
C 0.445334 1.215427 0.508510
H 1.670493 -2.139931 -1.024694
H 0.673990 -1.293700 1.645399
H -0.378309 -2.150162 0.466829
H 3.272986 -0.248538 -0.923247
H 2.524476 1.922950 0.353797
H 1.736636 1.550965 -1.184650
H 0.549926 1.239714 1.608676
H -0.117339 2.106773 0.215312
H 0.347096 -0.407089 -1.055800
C -1.877003 0.065153 -0.099382
O -2.328333 1.229697 -0.289523
O -2.499246 -1.031843 -0.074655
H 2.935466 -0.427871 0.802815

-2044.2199 50.5833 128.0658
176.2395 248.5696 309.8260
356.8276 423.5608 473.9190
529.5643 550.7875 675.5141
765.6781 776.2346 804.7548
841.5544 879.7344 891.4501
923.0763 952.8578 1012.0265
1017.3588 1051.6726 1081.2663
1156.6197 1180.7864 1205.1075
1216.8378 1262.6651 1277.0703
1301.2328 1325.5142 1337.2747
1343.3614 1366.9211 1378.0531
1496.4814 1502.3478 1507.7066
1520.4311 1648.7805 1685.6043
2940.3229 2953.8645 2989.4771
3005.6978 3027.0092 3045.5269
3085.3059 3106.4229 3126.4804

chxl1301

HF = -423.1856176
ZeroPoint = 0.1528984
Energy+ZP = -423.0327192
Thermal = 0.1612591
Free Energy Correction = 0.118832

C -0.445338 -0.011313 0.161007
C 0.317967 1.275257 0.034875
C 1.831094 1.306510 0.023627
C 2.455740 -0.028232 -0.424370
C 1.813882 -1.198390 0.335749
C 0.312763 -1.305830 0.013612
H 2.171106 2.123632 -0.628916
H -0.269417 2.146694 -0.236709
H 3.545245 -0.006938 -0.266214
H 2.316508 -2.143605 0.081770
H 1.960334 -1.046078 1.418837
H 0.215174 -1.627773 -1.041317
H -0.170022 -2.095358 0.599801
H -0.146582 0.785956 1.146275
C -1.962596 0.011239 -0.018516
O -2.492897 -1.120821 -0.214084
O -2.518759 1.145427 0.045046
H 2.285927 -0.171003 -1.502882
H 2.243907 1.542174 1.025754

-1806.9490 74.3821 100.4131
174.7356 201.7515 288.4156
327.0408 363.4652 465.7411
490.1889 520.7449 657.7326
678.7441 762.6174 788.6463
827.6145 847.5192 907.7120
919.3492 944.8177 1045.0771
1064.4894 1073.1843 1098.0031
1144.1770 1163.1323 1231.5092
1257.8471 1263.9470 1287.5789
1325.7360 1346.6390 1359.9896
1364.2547 1374.5250 1381.1846
1491.4972 1497.9777 1505.3191
1516.1982 1643.5370 2169.0545
2886.2614 2931.0354 2982.7165
2994.9439 3023.5949 3027.0930
3034.8641 3080.3216 3207.3359

chxl201

HF = -423.2471471
ZeroPoint = 0.1568899
Energy+ZP = -423.0902572
Thermal = 0.1656678
Free Energy Correction = 0.121513

C -0.331471 1.189281 0.270066
C 0.401313 0.019999 -0.415684
C -0.311260 -1.320487 -0.065124
C -1.778125 -1.245625 -0.337010
C -2.530520 -0.094972 0.260072
C -1.828888 1.248302 -0.077055
H 0.157434 -2.145072 -0.617837
H -0.207974 1.081526 1.357937
H 0.154487 2.134313 -0.011120
H -2.207897 -1.777389 -1.186059
H -3.578223 -0.078076 -0.073369
H -2.548755 -0.188275 1.361835
H -1.949215 1.452088 -1.152300
H -2.322096 2.073711 0.462494
H -0.105175 -1.497121 1.003182
H 0.362983 0.170958 -1.503541
C 1.916130 -0.002596 0.006763
O 2.146617 -0.384177 1.186847
O 2.731052 0.385418 -0.873520

21.2587 111.6169 147.2644
189.0823 251.7842 297.7139
332.5771 423.4904 453.5810
509.5102 559.6397 715.4204
758.6301 797.2150 847.7805
855.7797 898.3053 910.2289
931.4712 981.7423 1024.4896
1074.3533 1086.5076 1129.7997
1142.3336 1185.5307 1227.8265
1275.7936 1286.1907 1309.2296
1336.1350 1338.5578 1348.5326
1362.6961 1378.6315 1392.8793
1494.1111 1500.2729 1504.0500
1515.9849 1664.9463 2948.0708
2984.4204 2995.5599 3015.0641
3024.1841 3026.8064 3033.3098
3057.5553 3062.4180 3146.3787

chxl2501

HF = -423.1993598
ZeroPoint = 0.1531287
Energy+ZP = -423.0462311
Thermal = 0.1620621
Free Energy Correction = 0.117938

C -0.418017 0.142521 -0.309731
C 2.404769 1.174424 -0.047297
C 1.799706 -1.199959 -0.479198
C 0.309979 -1.183401 -0.026135
C 0.098159 1.297120 0.479013
C 2.592183 -0.146249 0.243388
H -0.350079 0.373872 -1.382305
H 2.069110 1.485216 -1.033809
H 1.835114 -1.024048 -1.565917
H 2.842238 1.958377 0.568636
H 2.220669 -2.201627 -0.304864
H 0.239100 -1.403668 1.046474
H 0.171056 1.172225 1.559351
H -0.219668 -1.997790 -0.540126
H -0.191195 2.297599 0.154591
H 3.024788 -0.418085 1.208046
C -2.004661 -0.004340 -0.016973
O -2.301559 -0.653000 1.014852
O -2.740171 0.562655 -0.860913

-364.0711 30.5445 93.6673
184.2590 192.1142 265.1818
294.9958 340.9833 394.9478
456.3742 487.6826 543.2311
649.6700 696.1570 750.4390
787.8858 809.8815 838.5386
865.1620 907.0847 927.9917
949.3670 956.5628 994.8490
1030.2935 1106.5801 1152.5686
1201.3067 1241.7124 1249.5901
1290.0237 1299.7233 1325.3319
1363.7493 1383.8514 1441.3862
1475.2392 1501.1602 1508.9197
1589.8608 1695.7336 2995.3883
3018.6003 3024.8580 3035.1999
3078.9736 3108.8035 3126.2779
3142.2728 3195.4110 3215.3537

chxl301

HF = -423.2458795
ZeroPoint = 0.1569597
Energy+ZP = -423.0889198
Thermal = 0.1655162
Free Energy Correction = 0.121721

C 0.399710 0.000038 0.913339
C -0.477585 1.263347 0.845488
C -1.342148 1.289271 -0.434929
C -2.075140 0.000024 -0.648776
C -1.342198 -1.289238 -0.434802
C -0.477644 -1.263243 0.845616
H -2.044396 2.137038 -0.413439
H -1.144198 1.296384 1.724465
H 0.165162 2.148926 0.867325
H -3.003470 -0.000004 -1.222423
H -2.044489 -2.136966 -0.413245
H -0.652139 -1.478034 -1.278692
H -1.144245 -1.296186 1.724603
H 0.165077 -2.148841 0.867514
H -0.652089 1.477967 -1.278839
H 0.914123 0.000087 1.888944
C 1.572303 -0.000049 -0.151786
O 1.993701 1.134865 -0.504374
O 1.993409 -1.135024 -0.504515

15.4146 105.9048 167.9012
217.0928 297.2997 347.4279
378.4498 400.6501 513.3061
536.9620 549.4234 635.8032
774.1342 778.3622 825.6448
842.2492 877.0597 897.3614
961.2905 1015.3779 1033.9688
1072.0106 1082.3281 1120.8862
1160.3155 1173.0059 1195.5059
1285.3162 1305.3060 1321.1329
1340.0456 1344.3136 1354.1447
1373.3745 1396.4986 1398.4026
1484.9203 1489.4076 1493.5167
1501.8585 1662.8454 2946.0140
2948.8446 2968.1717 2968.9438
2989.5765 3012.0554 3012.9335
3097.9238 3098.3096 3128.3473

chxl701

HF = -423.1750212
ZeroPoint = 0.1523585
Energy+ZP = -423.0226627
Thermal = 0.160937
Free Energy Correction = 0.116998

C 0.377204 -0.042547 -0.373353
C -0.323495 1.316316 -0.186778
C -1.839721 1.243335 -0.239400
C -2.558106 -0.053581 0.017288
C -1.771967 -1.337093 0.093575
C -0.305516 -1.108711 0.504717
H -2.386766 0.915415 0.890810
H 0.040699 1.727811 0.765570
H 0.022804 2.020036 -0.957056
H -3.604725 -0.088685 -0.285362
H -2.261629 -2.058492 0.766439
H -1.767847 -1.807997 -0.910112
H -0.255836 -0.790613 1.557827
H 0.248726 -2.052275 0.426600
H -2.407538 2.028771 -0.738664
C 1.913518 0.014978 -0.043544
O 2.635309 -0.758800 -0.729850
O 2.256803 0.793384 0.888536
H 0.283713 -0.366816 -1.420574

-1938.4890 18.5906 100.1737
166.7629 191.0826 262.9018
315.1315 345.3246 461.8411
512.9243 565.1862 607.2946
703.9454 758.1322 776.0248
819.8182 839.8274 907.6032
910.8965 927.5627 999.4499
1047.2800 1075.2663 1085.2559
1126.8880 1183.7262 1199.0728
1239.4290 1277.9963 1284.9800
1312.5080 1339.5037 1352.3203
1357.0707 1371.9672 1379.2876
1385.6670 1497.5406 1504.0383
1514.6871 1663.4523 2157.1752
2907.4059 2996.7549 3006.8485
3016.7748 3020.2225 3044.3699
3072.7471 3122.6024 3144.3538

chxl901

HF = -423.170818
ZeroPoint = 0.1523421
Energy+ZP = -423.0184759
Thermal = 0.1603975
Free Energy Correction = 0.118190

C -0.431934 -0.071125 0.869309
C 0.541563 -1.276161 0.784772
C 1.689006 -1.072703 -0.238216
C 2.153834 0.374369 -0.244542
C 1.047900 1.332703 -0.689317
C 0.341182 1.219469 0.664430
H 2.522653 -1.749798 0.001418
H 1.001612 -1.402284 1.779027
H -0.013374 -2.190934 0.550532
H 3.195695 0.583393 -0.512869
H 1.428490 2.348185 -0.860351
H 0.455772 1.008007 -1.553638
H 1.676247 0.841820 1.041299
H -0.072295 2.123696 1.118760
H 1.316439 -1.342225 -1.237334
H -0.879108 -0.049012 1.871348
C -1.642011 -0.138627 -0.157298
O -1.451609 -0.830543 -1.193354
O -2.652062 0.533244 0.176728

-2095.6581 34.4587 108.0513
164.9453 276.1465 313.2736
376.3433 422.2899 481.2344
565.5084 602.5893 689.4261
774.4221 782.5892 825.6767
836.7635 848.8979 873.3199
916.4208 947.4748 1005.2057
1019.2314 1059.5888 1082.7962
1100.0842 1118.7670 1204.2908
1226.3548 1265.2903 1278.9523
1300.3386 1306.5015 1323.8243
1331.8567 1362.5910 1371.6753
1380.2615 1487.9758 1500.9157
1513.8737 1664.0098 1671.4375
2978.1840 3003.7938 3032.5644
3038.5859 3042.6629 3070.2442
3088.6838 3090.0975 3109.9642

chxl4801

HF = -423.2134403
ZeroPoint = 0.1522688
Energy+ZP = -423.0611715
Thermal = 0.162744
Free Energy Correction = 0.114285

C -0.568556 0.279747 -0.189407
C 3.533168 0.672110 -0.245772
C 1.668683 -1.034351 -0.414439
C 0.196218 -1.032227 0.053827
C -0.226189 1.353763 0.767235
C 2.596522 -0.102243 0.317900
H -0.393281 0.626182 -1.216955
H 3.657138 0.722049 -1.327194
H 1.719774 -0.822180 -1.492812
H 4.185891 1.307916 0.349252
H 2.054685 -2.060878 -0.284747
H 0.142469 -1.285568 1.121327
H -0.175778 1.120077 1.830759
H -0.321542 -1.848106 -0.466455
H -0.429526 2.390886 0.508407
H 2.501092 -0.099240 1.405532
C -2.176114 0.017569 -0.115835
O -2.539513 -0.817676 0.746029
O -2.845901 0.695508 -0.929551

24.2647 43.6429 82.6848
120.5810 183.4623 220.5248
243.4214 271.8623 337.5508
349.9844 455.8283 488.1589
585.9921 614.9682 693.1970
767.0143 782.3766 827.5900
867.5162 890.8118 934.1289
956.4881 1012.2731 1036.6376
1044.3463 1122.7935 1153.0975
1205.9190 1246.3884 1256.1277
1300.9471 1323.9293 1345.0070
1369.1701 1388.4630 1463.0900
1475.4534 1492.4919 1503.8544
1697.2116 1699.7162 2968.9413
3027.9355 3029.4472 3042.0018
3074.1804 3122.1588 3130.9440
3140.5839 3210.1379 3212.9782

Table S2. Geometry and electronic and zero-point energies (Hartrees) for stationary points on the potential energy surface for the reaction of 4-carboxylatocyclohexyl radical anions and dioxygen. Negative frequencies for all transitions states are reported in cm^{-1} and are presented in parentheses. The relative energies derived from this data are presented in Figure 4.

chxl1001

HF = -423.1702697
ZeroPoint = 0.1520558
Energy+ZP = -423.0182139
Thermal = 0.1600953
Free Energy Correction = 0.117785

C -0.383930 0.014305 0.388804
C 0.241307 1.302049 -0.209041
C 1.789737 1.287245 -0.129904
C 2.328681 -0.103704 -0.430788
C 1.876459 -1.154861 0.585292
C 0.464912 -1.177494 -0.008400
H 2.206170 2.023876 -0.832537
H -0.044438 1.348240 -1.269851
H -0.183181 2.186637 0.276388
H 3.321006 -0.186843 -0.888083
H 2.404418 -2.108271 0.450869
H 1.945346 -0.857599 1.643770
H 1.208545 -0.671130 -1.122090
H -0.052959 -2.114839 -0.211047
H 2.111952 1.598708 0.880901
C -1.909183 -0.089222 0.015167
O -2.273061 -1.107061 -0.630848
O -2.604518 0.882035 0.420244
H -0.344121 0.111529 1.489735

-2094.7129 29.5477 125.3098
193.6375 250.6780 306.9707
367.8327 427.1445 501.4968
526.0037 616.3399 673.5597
751.2601 805.5332 826.3919
838.4028 877.0923 886.5863
910.9017 965.6972 990.6120
1025.8312 1056.9595 1064.2055
1085.5451 1149.9893 1174.8586
1213.0881 1238.4498 1270.0416
1282.9461 1311.6222 1321.8991
1340.4898 1345.6475 1373.2018
1384.7255 1497.3995 1507.7264
1514.4029 1667.8340 1704.0486
2942.9717 2949.6665 3003.0764
3018.5859 3035.7458 3053.3161
3074.9483 3103.0883 3161.4621

chxl1402

HF = -573.5833964
ZeroPoint = 0.1600425
Energy+ZP = -573.4233539
Thermal = 0.170761
Free Energy Correction = 0.120377

C -0.271756 -1.066910 -0.654201
C 1.187288 -0.722837 -0.990034
H 1.646957 -1.333355 -1.778365
H -0.853166 -1.139834 -1.582393
C 1.642824 0.597676 -0.927308
H 2.549480 0.874933 -1.459282
H 1.905709 -1.135746 0.004938
C 0.856954 1.688614 -0.254743
H 1.219209 1.800342 0.778546
H 1.075416 2.646391 -0.751656
C -0.654811 1.389304 -0.244175
H -1.057459 1.506677 -1.261457
H -1.173576 2.113834 0.393962
C -0.961285 -0.035766 0.249297
H -0.582359 -0.125387 1.277650
H -0.324691 -2.061807 -0.192319
O 3.252040 0.087855 0.809045
O 2.870156 -1.132944 0.966279
C -2.524533 -0.233594 0.316532
O -3.062460 -0.781287 -0.683854
O -3.066437 0.220756 1.358302

-840.4730 7.8210 49.0737
118.3058 135.9529 164.6279
185.1325 226.0610 298.3544
320.8237 351.3258 457.6438
501.6780 530.5708 635.8833
671.3405 701.6242 760.6086
802.7092 814.6940 864.0958
910.8568 917.0490 928.4703
952.6506 1013.1033 1039.7040
1093.6885 1106.9703 1148.1228
1207.1281 1210.8621 1261.6650
1275.5500 1296.0524 1317.5862
1327.4578 1343.1818 1357.8882
1369.4999 1386.1887 1414.7567
1481.1158 1493.3199 1507.2975
1518.2978 1576.5235 1672.5056
3006.7184 3014.3926 3024.0435
3036.1578 3038.0706 3055.9522
3073.9484 3088.1416 3187.3019

chxl1502

HF = -573.5792148
ZeroPoint = 0.160135
Energy+ZP = -573.4190798
Thermal = 0.1706105
Free Energy Correction = 0.122408

C 0.353105 0.294374 1.670265
C -1.107487 0.429909 1.210688
H -1.833021 0.533269 2.027618
H 0.498552 1.028816 2.480683
C -1.427697 1.133730 0.043730
H -2.427984 1.540768 -0.076548
H -1.508608 -0.733880 0.768710
C -0.392742 1.462551 -0.988448
H -0.269175 0.617661 -1.681218
H -0.724281 2.322689 -1.587505
C 0.983323 1.711623 -0.339377
H 0.945744 2.641327 0.254775
H 1.727504 1.841035 -1.131060
C 1.389587 0.531196 0.553817
H 0.540293 -0.697642 2.094477
O -2.574734 -0.757652 -0.905900
O -2.224784 -1.586370 0.014553
H 2.338044 0.786676 1.051779
C 1.729818 -0.787662 -0.256984
O 1.868657 -1.820206 0.447877
O 1.874048 -0.652652 -1.502012

-958.1577 44.3890 50.8543
103.7700 131.3395 186.3058
201.2441 281.8029 306.6389
328.8571 417.9175 486.6194
509.3858 537.7646 587.4501
627.2399 674.8621 770.7134
789.6441 813.0710 845.3152
888.8164 910.0421 936.3021
966.7830 1010.2664 1044.0226
1086.8537 1108.7851 1166.9046
1178.3050 1219.4203 1249.8942
1296.3490 1301.2285 1319.6246
1335.1714 1338.3961 1354.0280
1367.1378 1384.8348 1420.3183
1482.2695 1492.9754 1502.3357
1524.3147 1573.7079 1676.0626
2968.7741 2970.6557 3004.8065
3019.4078 3054.9416 3058.6434
3092.3095 3101.9411 3189.3068

chxl1601

HF = -573.5913188
ZeroPoint = 0.1617317
Energy+ZP = -573.4295871
Thermal = 0.1729012
Free Energy Correction = 0.122862

C 1.047683 -0.129454 -0.324702
C 0.493388 1.297554 -0.214338
C -0.880635 1.418403 0.308109
C -1.757021 0.262338 0.640507
C -1.049758 -1.102441 0.755193
C 0.483198 -0.986875 0.821003
H 1.187779 1.825493 0.476324
H 0.601670 1.855091 -1.159418
H 0.747033 -0.588186 -1.276040
H -2.420501 0.458894 1.496402
H -1.435251 -1.641163 1.631395
H -1.334545 -1.692162 -0.124499
H 0.788430 -0.540019 1.780393
H 0.933615 -1.985695 0.780304
H -1.324959 2.405627 0.417651
C 2.619063 -0.130023 -0.265355
O 3.146245 0.851785 0.333284
O 3.178923 -1.126073 -0.787409
O -2.460794 0.475791 -0.569988
O -3.849501 -0.564328 -0.589443
H -3.597771 -0.972276 -1.436565

-516.6216 30.2777 45.8947
119.6763 137.6924 154.7202
168.1697 200.6776 234.7558
312.1042 344.7565 398.2297
459.4381 465.5370 527.9213
642.6127 680.2648 711.8796
760.8231 798.0907 836.7020
870.7380 908.6176 910.4309
945.8393 997.1443 997.4507
1039.4327 1066.9930 1110.4445
1141.4451 1174.7171 1211.5219
1229.2314 1276.7918 1299.0646
1330.5955 1342.7307 1357.3406
1363.7408 1386.5537 1399.3947
1417.7484 1448.5443 1502.5094
1517.7255 1665.6327 2887.9955
2995.4650 2997.2282 3008.9863
3036.7153 3043.6092 3076.1669
3086.3110 3179.6116 3737.3234

chxl1801

HF = -573.5819693
ZeroPoint = 0.1625846
Energy+ZP = -573.4193847
Thermal = 0.1737662
Free Energy Correction = 0.123450

C -1.101094 0.041285 -0.319623
C -0.383226 -1.251218 0.096162
C 0.995950 -1.067752 0.630457
C 1.617539 0.168732 0.780478
C 0.817527 1.443870 0.600923
C -0.700893 1.189896 0.623740
H -1.022760 -1.736338 0.857700
H -0.365177 -1.973532 -0.736616
H -0.803354 0.327067 -1.337596
H 2.495181 0.213319 1.422851
H 1.107088 2.169066 1.375960
H 1.098849 1.895720 -0.361669
H -1.019106 0.938928 1.647094
H -1.238680 2.099471 0.332170
H 1.573197 -1.960996 0.872512
C -2.666389 -0.121224 -0.314040
O -3.129390 -1.024780 0.438091
O -3.290453 0.698419 -1.036229
O 2.775802 0.306240 -0.798106
O 3.915119 -0.532319 -0.667065
H 4.529652 0.025274 -0.154520

-358.6136 36.7194 44.9601
68.7738 123.9550 150.4443
192.3023 201.6723 291.3052
322.6115 337.5137 383.4531
389.9678 483.3840 526.9835
649.0987 707.0930 723.7426
763.5732 804.9489 861.9444
904.0807 905.4767 920.3359
941.8099 999.4821 1027.7772
1043.8418 1071.7899 1106.7965
1143.0326 1195.0695 1205.9724
1248.4545 1276.3324 1326.7228
1343.3724 1357.5780 1362.1090
1371.1841 1385.3503 1424.8270
1459.2766 1493.0009 1515.6807
1528.1969 1663.0691 2955.4522
2998.4319 3009.6119 3015.1405
3037.8371 3044.4651 3086.0821
3135.1358 3154.9077 3644.2763

chxl1901

HF = -573.5665651
ZeroPoint = 0.1606125
Energy+ZP = -573.4059526
Thermal = 0.1709123
Free Energy Correction = 0.122596

C 1.188840 0.000122 -0.425025
C 0.430064 1.259922 0.028362
C -1.027829 1.291427 -0.469606
C -1.749359 0.000096 -0.165564
C -1.027893 -1.290985 -0.470790
C 0.429967 -1.259989 0.027302
H -1.593789 2.135329 -0.054020
H 0.453580 1.296215 1.125506
H 0.951908 2.158065 -0.327539
H 1.261704 0.000597 -1.523083
H -2.151556 -0.000445 1.117977
H -1.593911 -2.135254 -0.056030
H -1.046433 -1.410697 -1.569218
H 0.453433 -1.297171 1.124414
H 0.951766 -2.157886 -0.329288
H -1.046432 1.412180 -1.567921
C 2.655097 -0.000107 0.143511
O 2.740117 -0.001132 1.402182
O 3.577169 0.000801 -0.714166
O -3.130817 0.000284 -0.451967
O -3.440667 -0.000435 1.020208

-1757.5986 20.0963 63.0689
118.0641 167.1073 176.2268
228.2091 255.4628 340.0104
357.2475 370.3262 465.8918
508.9567 547.5703 644.0800
723.1496 765.4792 785.7354
798.4610 813.9916 877.7050
906.7189 908.8660 964.3170
984.5664 986.4450 1020.1686
1087.3606 1104.8405 1124.9877
1127.2266 1187.7904 1225.1252
1262.6937 1273.5645 1297.4082
1314.3608 1346.1456 1349.7551
1358.9952 1380.2740 1396.6606
1480.3143 1492.9411 1509.5853
1520.3216 1668.0338 1885.7799
2968.3324 2973.9938 3009.6693
3036.1658 3038.6641 3060.9888
3062.3422 3076.6968 3081.8081

chxl2001

HF = -573.5959893
ZeroPoint = 0.1615914
Energy+ZP = -573.4343979
Thermal = 0.1711421
Free Energy Correction = 0.125645

C -0.852861 -0.513400 -0.655967
C -0.001153 -1.178752 0.383411
C 0.604138 -0.236658 1.405328
C 1.563065 0.698366 0.651154
C 0.809856 1.479414 -0.436672
C -0.085446 0.630189 -1.364254
H -0.187774 0.370209 1.871835
H -0.386922 -2.124437 0.774637
H 1.168943 -1.428181 -0.258267
H -1.177139 -1.249021 -1.399508
H 2.050341 1.404263 1.337645
H 0.171398 2.196493 0.093591
H 1.536241 2.049880 -1.032674
H -0.802152 1.292871 -1.866005
H 0.543581 0.178503 -2.140567
H 1.151586 -0.779810 2.185951
C -2.230348 -0.008994 0.044520
O -2.151422 1.096063 0.634083
O -3.190366 -0.798162 -0.090063
O 2.698022 -0.073910 0.200720
O 2.279815 -1.115462 -0.711209

-1534.6384 42.0537 112.1790
154.8265 181.8094 205.2625
285.4658 353.0716 368.3294
399.8340 463.6331 514.8147
555.0797 598.0057 689.9088
743.2782 756.9674 769.7728
804.4914 826.7922 847.9619
883.9005 900.3458 947.9985
983.5123 1033.4408 1036.8894
1070.9162 1085.5354 1135.4467
1146.1644 1175.4082 1211.8535
1252.5239 1260.1273 1302.7204
1320.4019 1337.1443 1354.6467
1356.1583 1379.6916 1395.8088
1407.1167 1472.7002 1490.8905
1507.5561 1586.5965 1697.0355
3006.8653 3024.4209 3040.0763
3046.4825 3065.4753 3069.1924
3072.8681 3089.6712 3109.2960

chxl2101

HF = -573.5862666
ZeroPoint = 0.1608657
Energy+ZP = -573.4254009
Thermal = 0.1703925
Free Energy Correction = 0.124727

C 0.895271 0.137892 -0.542933
C 0.019866 -1.085129 -0.407545
C -1.310992 -0.985050 -1.119439
C -2.102164 0.156597 -0.451025
C -1.314902 1.478414 -0.497450
C 0.160274 1.399259 -0.040005
H -1.165368 -0.744922 -2.187317
H 0.557931 -2.034741 -0.428615
H -0.512078 -0.997254 0.847925
H -3.085091 0.290409 -0.923257
H -1.354430 1.810736 -1.548407
H -1.858904 2.232415 0.088674
H 0.700470 2.290649 -0.375800
H 0.205331 1.408430 1.051968
H -1.890773 -1.914817 -1.058958
O -2.478780 -0.296606 0.862393
O -1.308451 -0.541192 1.663077
H 1.091784 0.258404 -1.628215
C 2.342178 -0.062343 0.064654
O 2.886834 0.965346 0.537191
O 2.797139 -1.232192 -0.047102

-1661.4127 36.8847 87.8774
171.0409 197.3845 229.6989
302.2534 336.4355 384.0254
422.4654 468.0873 492.1984
523.6824 591.9723 628.9673
737.3450 758.1501 787.1944
814.5606 861.6460 881.8585
902.7327 920.7184 939.2773
964.0191 1028.2566 1041.0439
1074.6727 1095.0504 1106.8827
1143.7202 1176.1720 1193.5376
1214.9643 1248.5596 1295.1811
1308.3426 1324.8752 1347.0140
1352.4575 1357.4399 1380.6372
1393.1154 1483.7297 1494.4694
1514.5176 1546.5699 1678.4488
2905.0239 2974.1553 2990.3356
3041.2189 3046.8766 3064.3342
3078.2603 3127.0366 3144.5137

chxl2201

HF = -573.5881223
ZeroPoint = 0.1608957
Energy+ZP = -573.4272266
Thermal = 0.1707722
Free Energy Correction = 0.123571

C -0.655109 0.030612 -0.168434
C -0.056863 1.382180 -0.529631
C 1.455486 1.272658 -0.858135
C 2.090495 0.047944 -0.184506
C 1.472415 -1.249697 -0.729677
C -0.060313 -1.119077 -0.968366
H 1.610435 1.171304 -1.944095
H -0.605010 1.803421 -1.387064
H -0.234677 2.076418 0.297578
H -0.111410 -0.206701 1.015840
H 3.178361 0.047016 -0.343244
H 1.984795 -1.492583 -1.671638
H 1.686196 -2.060119 -0.025477
H -0.258854 -0.939983 -2.039453
H -0.587637 -2.040397 -0.708358
H 1.987525 2.181118 -0.547162
C -2.193521 0.006109 0.113848
O -2.690819 1.113648 0.436392
O -2.744178 -1.112474 -0.056051
O 1.975970 0.180891 1.258616
O 0.838368 -0.527547 1.773853

-1599.3421 11.8751 126.1634
142.0113 163.7448 218.7000
268.6612 317.5492 335.5701
343.3232 444.6565 466.8204
506.0186 541.4686 688.8426
739.5511 751.8598 775.0634
791.5570 856.2667 887.8783
901.7832 920.7310 938.5722
963.4237 1015.5392 1050.3652
1088.4624 1115.9667 1124.1062
1182.2959 1214.2342 1240.2191
1253.8109 1264.1494 1293.9910
1307.9554 1338.1757 1347.5738
1361.1026 1376.6227 1381.0390
1489.4564 1492.3454 1499.7140
1504.4737 1519.5717 1653.1582
2972.7519 2997.4821 3011.6545
3016.2595 3036.2995 3055.8463
3096.6840 3100.2857 3121.3698

chxl2301

HF = -573.5793671
ZeroPoint = 0.1638001
Energy+ZP = -573.415567
Thermal = 0.1736696
Free Energy Correction = 0.128182

C -0.723778 -1.132687 0.181480
C 0.130995 -1.137712 -1.037415
C 1.636723 -1.200585 -0.888624
C 1.774190 0.118458 -0.121396
C 1.316129 -0.045065 1.333088
C 0.143705 -1.048087 1.455894
H 2.013556 -2.084063 -0.341257
H -0.349578 -1.256561 -2.003948
H 2.747048 0.623633 -0.191515
H 2.172002 -0.386180 1.937620
H 1.023838 0.941215 1.700634
H 0.549787 -2.051493 1.662287
H -0.490431 -0.778743 2.306668
H 2.137608 -1.151697 -1.861475
O 0.786361 0.830944 -0.903802
O 0.732191 2.421526 -0.268682
H -0.159210 2.232816 0.112307
H -1.322824 -2.058658 0.203693
C -1.831038 0.024967 0.046859
O -1.647062 1.042204 0.768143
O -2.746908 -0.232924 -0.763700

-783.6582 80.2332 110.5885
131.0428 201.0577 239.9238
267.6369 302.2311 333.9845
379.4900 389.6050 423.5166
534.9610 582.5439 645.8164
661.3775 688.3716 737.4185
776.8568 825.1982 832.2494
856.5512 889.2521 923.4699
955.8362 1020.0718 1036.7795
1066.5393 1090.7844 1109.1883
1133.6800 1163.0176 1190.3667
1222.6717 1233.4186 1284.6746
1306.5641 1315.3936 1324.8050
1343.8720 1360.0658 1388.2052
1396.5689 1490.3777 1499.7436
1514.9737 1695.0209 2944.2160
2967.2113 2986.0445 3004.8616
3036.1887 3085.8044 3091.5303
3129.0916 3208.2883 3490.7114

chxl2401

HF = -573.5947922
ZeroPoint = 0.162536
Energy+ZP = -573.4322562
Thermal = 0.1730869
Free Energy Correction = 0.126143

C -0.509418 -0.349373 0.133847
C 0.137616 -1.327222 -0.810048
C 1.670777 -1.367105 -0.639548
C 2.073900 0.069885 -0.215434
C 1.649570 0.274022 1.256285
C 0.172555 -0.177375 1.452019
H 1.980082 -2.115621 0.107569
H -0.314339 -2.305908 -0.581731
H -0.152016 -1.073197 -1.832986
H -0.666006 2.065505 -0.693560
H 3.178072 0.190871 -0.274037
H 2.312349 -0.288458 1.932178
H 1.726193 1.339873 1.481206
H 0.159682 -1.173162 1.926598
H -0.387242 0.511159 2.085463
H 2.142111 -1.636745 -1.592706
C -1.982277 -0.110721 -0.074720
O -2.480872 0.709921 -0.851879
O -2.494479 -1.022341 0.646876
O 1.428435 0.955656 -1.045008
O -0.109987 2.158391 0.103460

-244.8578 64.6540 112.7802
168.1584 180.9790 193.9101
217.6855 248.0773 262.3457
323.5382 359.2049 403.3256
416.0468 461.8684 556.7563
644.6219 683.8466 730.1328
755.6341 772.3200 822.0218
842.2039 893.8397 909.8248
932.6835 993.6192 1025.6447
1052.2644 1092.0435 1110.7171
1131.4111 1176.0501 1214.8302
1245.9792 1261.6401 1272.2647
1304.7603 1330.4544 1347.2624
1358.2974 1362.8400 1400.0221
1461.9685 1476.6120 1492.4874
1511.4336 1726.1861 2858.0168
2983.8910 2997.3832 3011.3371
3020.6429 3066.6765 3116.9257
3131.6065 3148.8916 3704.4266

chxl2601

HF = -573.5550571
ZeroPoint = 0.1605452
Energy+ZP = -573.3945119
Thermal = 0.1718242
Free Energy Correction = 0.121644

C 1.331959 0.241681 0.749429
C 0.346555 1.341601 0.475740
C -0.920464 1.330570 1.013572
C -1.776886 -0.611359 0.271584
C -0.511896 -1.409086 0.055606
C 0.614934 -1.089447 1.064431
H 0.614967 2.034754 -0.318288
H -2.400137 -0.851199 1.142185
H -0.749522 -2.485196 0.099272
H -0.135594 -1.218778 -0.956609
H 0.204575 -1.092797 2.087578
H 1.366455 -1.881245 1.003155
H -1.624509 2.125938 0.760942
C 2.406444 0.114518 -0.426765
O 2.758687 1.208240 -0.935506
O 2.810879 -1.049378 -0.674825
O -2.503581 -0.520398 -0.894783
O -3.571503 0.506565 -0.732518
H -3.022020 1.314586 -0.741821
H -1.111946 0.872564 1.982522
H 1.958009 0.510269 1.620542

-511.2423 30.8925 41.8477
85.1437 153.7886 155.2272
224.0599 249.1473 286.5723
308.8963 363.7481 383.0013
433.2100 457.2373 470.8266
550.9519 595.0847 629.2342
687.4890 766.4579 822.7001
847.6744 863.8477 875.3532
930.6375 942.3693 992.5193
1010.6185 1046.7373 1086.1786
1096.5644 1149.3051 1190.4745
1215.4274 1248.7149 1261.3716
1307.8286 1328.4209 1336.8905
1339.1509 1367.2887 1381.1429
1427.5000 1497.2407 1498.3944
1563.6133 1691.0961 2941.1965
2979.5852 2992.0660 3045.1313
3086.8794 3105.3292 3113.9043
3165.2347 3193.8067 3656.1848

chxl2701

HF = -573.6019016
ZeroPoint = 0.163846
Energy+ZP = -573.4380556
Thermal = 0.1751883
Free Energy Correction = 0.124831

C -1.247558 0.058251 -0.430374
C -0.415065 -1.234380 -0.269368
C 1.051656 -1.009014 -0.442293
C 1.680098 0.155099 0.244224
C 0.863850 1.442029 0.041994
C -0.615110 1.193843 0.394551
H -0.655571 -1.620157 0.739944
H -0.768474 -2.003349 -0.969285
H -1.251956 0.360813 -1.486420
H 1.771619 -0.025457 1.336472
H 1.290660 2.247273 0.656939
H 0.950979 1.744844 -1.010258
H -0.704622 0.945097 1.462675
H -1.184870 2.118366 0.235604
H 1.704323 -1.771656 -0.859540
C -2.743615 -0.139666 0.015017
O -2.917301 -0.838778 1.051142
O -3.599414 0.454457 -0.692759
O 3.008304 0.468512 -0.239470
O 3.898888 -0.642551 0.086634
H 4.278557 -0.325861 0.926987

22.2419 56.7973 107.0152
144.0510 162.9100 199.1108
216.3323 241.3858 292.8827
311.6706 334.1479 441.2742
467.3348 514.1096 536.2810
585.1207 720.9459 764.3695
795.0311 856.2461 891.5550
893.5559 913.9354 939.9276
994.5496 1018.4137 1037.3101
1081.5678 1098.6935 1119.1271
1185.2469 1188.9681 1241.7855
1268.9949 1302.1306 1325.1611
1330.4734 1343.8181 1352.0821
1352.6902 1365.9522 1381.8054
1401.8920 1486.8697 1509.5009
1515.2644 1668.1742 2873.3812
2939.9459 3017.6369 3023.7616
3032.8065 3052.2794 3063.2006
3074.7656 3188.8998 3674.6828

chxl2801

HF = -573.6045245
ZeroPoint = 0.1650674
Energy+ZP = -573.4394571
Thermal = 0.175951
Free Energy Correction = 0.126736

C -1.229343 0.054282 -0.423746
C -0.375049 -1.230279 -0.178473
C 1.053991 -0.952728 -0.503870
C 1.679112 0.189683 0.238248
C 0.881031 1.483394 -0.025061
C -0.603247 1.247487 0.322070
H -0.514842 -1.495227 0.879220
H -0.773222 -2.058068 -0.777700
H -1.244777 0.273919 -1.499659
H 1.688623 -0.002593 1.322618
H 1.306487 2.304482 0.570062
H 0.985637 1.751765 -1.085456
H -0.707601 1.071984 1.402102
H -1.175373 2.156479 0.093595
H 1.400570 -1.097515 -1.531251
C -2.722034 -0.157318 0.042042
O -2.863928 -0.633476 1.199264
O -3.596520 0.199181 -0.790026
O 3.033550 0.443146 -0.181152
O 3.861531 -0.670388 0.272532
H 3.450678 -1.420051 -0.205732

21.4280 65.3412 115.8962
160.7493 191.4570 225.2687
241.3719 280.4758 323.8507
339.2981 410.2008 451.4245
470.2337 516.8937 558.8357
655.2738 729.5615 763.1874
800.7317 864.5812 885.7703
897.5796 907.6169 948.2207
994.4126 1014.6060 1047.8454
1063.7445 1124.1538 1138.2641
1143.8156 1200.2156 1248.1174
1269.1022 1287.4830 1313.1310
1321.9413 1329.5443 1345.0912
1347.2211 1378.7568 1397.7705
1412.0324 1503.1378 1509.5374
1516.2734 1676.5570 3003.0879
3018.2014 3027.8537 3031.3180
3038.1571 3059.9521 3075.0529
3079.3841 3111.6325 3603.5603

chxl2901

HF = -573.602843
ZeroPoint = 0.1652387
Energy+ZP = -573.4376043
Thermal = 0.175933
Free Energy Correction = 0.127540

C -1.388967 0.087599 0.869509
C -0.343247 -0.994617 1.279905
C 0.804846 -0.973959 0.322886
C 1.499273 0.345185 0.188519
C 0.484589 1.411070 -0.278978
C -0.703817 1.457599 0.701891
H 0.011065 -0.769296 2.302332
H -0.829122 -1.973470 1.283559
H 1.931440 0.665501 1.151356
H 0.984240 2.388125 -0.342716
H 0.122273 1.149765 -1.280345
H -0.344019 1.824046 1.678959
H -1.449165 2.167387 0.330038
H 0.718059 -1.581497 -0.578550
C -2.225994 -0.314463 -0.410994
O -2.944054 0.609939 -0.876861
O -2.114440 -1.504581 -0.807844
O 2.559775 0.328440 -0.785270
O 3.627322 -0.528143 -0.276572
H 3.190186 -1.403324 -0.294023
H -2.123881 0.177041 1.685333

33.1436 65.8377 115.0176
154.6371 193.3345 228.8901
300.1675 306.9566 333.8905
376.2123 411.1569 457.5082
503.4794 531.4198 555.0880
599.5652 704.4139 772.5298
821.9318 848.0950 888.6145
894.2591 910.4098 933.3829
969.5764 1028.1578 1048.4395
1089.5262 1105.7227 1118.5736
1166.7307 1199.2445 1208.3503
1275.7925 1297.2071 1313.1531
1333.3221 1339.1116 1350.4380
1353.0937 1385.1872 1392.0759
1410.5236 1483.9328 1498.5851
1515.1587 1671.0276 2953.1972
2970.9156 2982.6436 3002.5859
3029.6334 3092.5889 3104.7048
3118.3153 3158.0720 3625.8825

chxl3001

HF = -573.6003923
ZeroPoint = 0.1643569
Energy+ZP = -573.4360354
Thermal = 0.1753575
Free Energy Correction = 0.126136

C 1.096061 0.295401 0.455313
C 0.308280 -0.909835 0.997951
C -1.111544 -0.606845 1.338352
C -1.922746 0.436084 0.643981
C -1.087019 1.514122 -0.066758
C 0.261395 1.018858 -0.617027
H 0.395281 -1.692371 0.216178
H 0.818931 -1.343745 1.870766
H 1.295566 1.004633 1.271988
H -1.703668 1.961139 -0.857824
H -0.889969 2.306936 0.671364
H 0.093706 0.339268 -1.461685
H 0.834158 1.873927 -0.998334
H -1.643018 -1.243854 2.047594
C 2.482735 -0.137341 -0.144496
O 2.513458 -1.275473 -0.691055
O 3.402277 0.716299 -0.042060
O -2.949085 -0.167945 -0.230068
O -2.318304 -0.795177 -1.383042
H -1.933436 -1.602025 -0.988957
H -2.617291 0.911789 1.354813

35.8593 52.5553 110.0938
133.9029 182.2539 201.4981
244.8594 296.7990 318.5591
348.6444 385.3013 449.7977
481.3309 509.2803 594.6943
680.5186 723.6535 739.0119
763.8165 819.8421 877.2332
891.1633 901.6886 909.8737
928.9840 998.9662 1057.0244
1069.4539 1093.8294 1131.5888
1167.4999 1209.8953 1229.6469
1273.5950 1322.5371 1324.9989
1348.9034 1353.2295 1356.6239
1372.3210 1375.0460 1385.5326
1413.3902 1472.8184 1489.5017
1519.9272 1665.4617 2908.2503
2992.4204 3011.3850 3014.6582
3026.0242 3043.7951 3061.3527
3089.2404 3131.7939 3652.3922

chxl3101

HF = -573.5993184
ZeroPoint = 0.1645909
Energy+ZP = -573.4347275
Thermal = 0.1755752
Free Energy Correction = 0.126326

C 1.116016 -0.200475 0.932594
C 0.213673 1.014821 1.211412
C -0.726015 1.310883 0.086447
C -1.254729 0.275210 -0.846776
C -0.496714 -1.064247 -0.842095
C 0.238073 -1.381884 0.471141
H -0.351714 0.809228 2.147523
H 0.825033 1.902924 1.417103
H -1.207809 -1.861426 -1.094620
H 0.245892 -1.015329 -1.646676
H -0.495680 -1.623920 1.255372
H 0.870511 -2.267158 0.328226
H -1.006002 2.343416 -0.115753
C 2.215253 0.111837 -0.142355
O 3.244268 -0.610111 -0.091053
O 1.936378 1.029165 -0.968771
O -2.715676 0.096767 -0.681710
O -2.996774 -0.420794 0.654363
H -2.813105 0.370480 1.197804
H -1.277769 0.677624 -1.870543
H 1.631731 -0.492927 1.856730

42.6474 46.3915 77.2407
122.5024 165.7022 236.4616
259.8568 308.8721 328.3022
367.1909 382.0069 461.9360
474.3943 516.4629 583.1868
680.6471 719.4261 753.0204
787.0623 833.1893 854.0326
883.7750 886.0388 909.3350
921.3161 1008.5733 1068.2056
1069.6970 1086.9126 1153.8142
1175.7718 1199.1499 1215.6229
1301.3912 1309.2389 1323.4449
1339.6948 1348.5464 1361.2165
1372.4664 1388.1575 1397.2977
1417.8169 1475.1040 1494.1314
1516.1059 1653.0054 2853.2736
3006.5006 3019.0948 3038.4269
3046.7273 3053.1176 3067.2198
3092.5561 3160.3731 3633.3942

chxl3201

HF = -573.6033556
ZeroPoint = 0.1641214
Energy+ZP = -573.4392342
Thermal = 0.1752002
Free Energy Correction = 0.125890

C 1.284210 0.003446 0.429447
C 0.446589 -1.171382 0.047336
C -1.041190 -1.145906 0.246481
C -1.638780 0.198531 -0.184542
C -0.889696 1.368568 0.455692
C 0.598578 1.331832 0.055694
H 0.953586 -2.118842 -0.111730
H 1.411713 -0.008415 1.534895
H -1.598246 0.294387 -1.280580
H -1.354530 2.315693 0.146989
H -0.993163 1.296524 1.549003
H 0.697080 1.482672 -1.026769
H 1.130914 2.167411 0.522975
H -1.534024 -1.966194 -0.289518
C 2.769135 -0.125095 -0.119179
O 3.311989 -1.238172 0.100939
O 3.239689 0.896327 -0.682445
O -3.016594 0.358747 0.223351
O -3.833010 -0.626913 -0.486373
H -4.203089 -0.067769 -1.193335
H -1.299900 -1.275339 1.318715

32.5545 64.5944 112.0159
163.6107 188.4464 205.3725
223.6399 253.6633 282.4724
364.1683 421.7384 462.2137
472.7400 481.0432 518.7909
587.2281 665.6125 766.5768
801.5329 854.6397 885.2632
905.4938 908.6308 953.2404
972.2074 1030.4591 1044.9444
1071.6920 1087.0136 1131.2349
1185.3420 1197.3110 1219.0635
1263.9878 1303.7504 1307.4001
1329.9345 1333.2238 1345.8405
1353.3697 1378.8929 1385.7395
1402.5011 1493.1726 1504.1063
1517.8051 1683.1328 2855.9879
2891.3502 3005.6343 3014.7899
3044.3183 3060.9410 3067.9722
3094.3338 3202.0261 3686.2174

chxl3301

HF = -573.6110806
ZeroPoint = 0.165381
Energy+ZP = -573.4456996
Thermal = 0.175636
Free Energy Correction = 0.128548

C -0.955026 -0.974975 0.112487
C -0.194545 -0.744795 1.378169
C 1.235199 -0.300045 1.455313
C 1.942598 -0.219252 0.095979
C 1.442321 -1.340619 -0.824507
C -0.050474 -1.156464 -1.140351
H -0.766800 -0.751352 2.305678
H -1.587280 -1.863204 0.246084
H 2.024824 -1.340550 -1.756861
H 1.630315 -2.305893 -0.326633
H -0.147939 -0.270235 -1.774110
H -0.408961 -2.012415 -1.728372
H 1.334368 0.666669 1.968940
C -2.001179 0.215017 -0.094745
O -3.200131 -0.058308 0.112015
O -1.503267 1.334826 -0.439322
O 1.776979 1.029244 -0.630551
O 0.991871 2.017234 0.085286
H 0.040729 1.755615 -0.170353
H 1.815694 -1.021942 2.062172
H 3.028075 -0.313866 0.259958

47.1952 65.5073 116.7058
179.5873 216.2109 257.4295
297.8443 314.5279 348.8308
363.9158 463.5969 476.0811
525.4181 616.6217 650.4594
741.2227 765.2413 783.1036
808.1417 852.6380 878.7930
897.7454 921.9372 976.1111
980.0672 994.7195 1044.4790
1056.7096 1105.5341 1140.8784
1179.2227 1203.1408 1221.7334
1245.4556 1317.3570 1339.0515
1349.9943 1358.1494 1369.7508
1385.5796 1393.6453 1422.9722
1471.7782 1497.0945 1510.2794
1592.0484 1678.4573 2902.0702
2915.7315 2977.7167 3002.1540
3007.7268 3030.9267 3034.7607
3043.5404 3107.2820 3148.9879

chxl3401

HF = -573.6147081
ZeroPoint = 0.1651839
Energy+ZP = -573.4495242
Thermal = 0.1762009
Free Energy Correction = 0.126803

C -1.260519 -0.015779 0.225418
C -0.413765 -1.232670 0.441632
C 0.977005 -1.104289 -0.223575
C 1.645525 0.206706 0.185631
C 0.787161 1.418209 -0.187336
C -0.608604 1.309251 0.475008
H -0.952542 -2.109632 0.070700
H 1.829409 0.211490 1.273279
H 1.294195 2.343533 0.120516
H 0.674814 1.449862 -1.279336
H -0.477108 1.471261 1.565725
H -1.273769 2.102558 0.120878
H 1.620051 -1.950717 0.048098
C -2.730802 -0.116936 -0.113158
O -3.192571 -1.291309 -0.238453
O -3.349728 0.984446 -0.231407
O 2.915239 0.425672 -0.470963
O 3.864479 -0.587515 -0.003928
H 4.400584 -0.047936 0.604601
H 0.866311 -1.108647 -1.316789
H -0.257301 -1.399080 1.528620

40.2592 47.1707 103.5153
142.0898 178.8394 205.6453
239.8764 261.0408 292.8657
330.3629 432.0733 460.7555
477.9670 505.3937 548.2558
640.7688 741.9320 779.9962
798.7276 844.3100 886.2051
932.7428 939.4233 955.1092
980.4080 1021.1182 1049.2434
1085.0451 1122.5708 1133.6316
1208.9198 1253.4415 1257.3856
1283.3761 1311.7439 1320.6291
1333.7508 1348.3959 1351.3103
1362.6179 1384.7219 1405.0101
1493.8428 1499.7412 1506.3259
1525.1670 1605.1251 2886.4294
2893.6866 2981.6552 3025.9312
3036.2041 3069.7316 3079.4375
3106.4514 3107.7954 3691.1825

chxl3501

HF = -497.8831997
ZeroPoint = 0.1527528
Energy+ZP = -497.7304469
Thermal = 0.1612591
Free Energy Correction = 0.118684

C -0.665395 0.024574 0.931439
C 0.295973 -1.185534 0.980113
C 1.575497 -1.026595 0.184083
C 1.976140 0.276480 -0.390101
C 1.076783 1.492152 -0.231191
C 0.108186 1.351487 0.955690
H 0.612899 -1.374251 2.020726
H -0.252215 -2.071238 0.636499
H 3.043451 0.469629 -0.537863
H 1.703498 2.388022 -0.106035
H 0.488232 1.621540 -1.146995
H 0.683263 1.424099 1.896997
H -0.606245 2.180103 0.932931
H 2.368329 -1.738982 0.438257
C -1.749517 -0.074782 -0.219095
O -2.228620 -1.225071 -0.397588
O -2.066165 1.009942 -0.777634
O 1.484842 -0.787486 -1.231317
H -1.267670 -0.024692 1.852157

56.8424 77.7487 142.2375
256.3235 307.6842 334.7984
390.8530 430.9802 503.9817
538.9845 578.0177 680.1192
753.0547 772.0068 793.6879
831.2737 870.7057 894.8394
920.2619 978.8890 1031.6083
1043.3696 1055.7110 1064.4462
1123.7362 1164.8412 1212.4703
1214.6661 1250.7823 1295.9877
1312.0577 1326.0820 1343.2272
1362.1850 1375.9473 1389.7800
1407.5882 1465.8420 1492.8953
1493.1817 1502.0981 1674.1620
2951.7328 2967.8520 3001.1378
3011.5168 3057.6744 3076.0868
3078.4661 3089.9849 3100.3323

chxl3502

HF = -497.8902215
ZeroPoint = 0.1527653
Energy+ZP = -497.7374562
Thermal = 0.1613926
Free Energy Correction = 0.117869

C -0.640600 0.084589 -0.387917
C 0.160265 -1.225979 -0.302059
C 1.663547 -1.033753 -0.420955
C 2.286669 0.299151 -0.293808
C 1.432916 1.524082 -0.042535
C 0.021431 1.178778 0.466373
H -0.073094 -1.726760 0.645483
H -0.171835 -1.913542 -1.090597
H -0.624663 0.440141 -1.431805
H 1.957166 2.192172 0.659392
H 1.354723 2.069439 -0.997089
H 0.079523 0.841911 1.511005
H -0.612454 2.071567 0.445628
H 2.207568 -1.788170 -0.996958
C -2.162678 -0.077994 -0.014555
O -2.863382 0.945441 -0.243254
O -2.516690 -1.187464 0.465772
O 2.389117 -0.652986 0.780836
H 3.241397 0.480070 -0.799160

23.6500 86.7436 181.4565
208.3901 291.0319 327.6703
358.2517 399.5549 499.7478
542.6171 617.4253 691.5698
750.4473 766.1654 802.6770
830.1386 874.1337 908.4335
931.8179 978.6363 1014.4250
1033.7181 1051.7971 1077.2208
1143.3902 1162.7861 1182.6162
1219.5427 1256.5092 1285.8114
1295.4285 1327.2401 1350.4095
1366.6920 1373.4703 1386.2942
1396.5771 1468.5136 1489.3760
1496.6823 1517.3037 1669.2706
2980.4618 2994.4860 3018.8642
3041.7062 3045.4322 3067.0359
3082.4731 3090.7114 3099.4176

chxl3601

HF = -497.8900872
ZeroPoint = 0.1528285
Energy+ZP = -497.7372587
Thermal = 0.1614978
Free Energy Correction = 0.117735

C 0.589961 0.041219 0.325508
C -0.161893 -1.246759 -0.048267
C -1.659031 -1.092947 -0.181117
C -2.289192 0.237230 -0.297883
C -1.441820 1.500513 -0.260009
C 0.054017 1.222944 -0.502828
H 0.241798 -1.598641 -1.007804
H 0.055329 -2.041417 0.680530
H -3.248356 0.311304 -0.818959
H -1.824859 2.207822 -1.011560
H -1.584180 1.975668 0.721473
H 0.211750 1.000172 -1.569559
H 0.642139 2.119242 -0.272515
H -2.187712 -1.943986 -0.622826
C 2.145323 -0.081650 0.101009
O 2.523923 -0.894921 -0.786130
O 2.841985 0.686980 0.816456
O -2.386554 -0.515088 0.931569
H 0.435063 0.270762 1.387586

20.5408 89.2165 173.1868
189.5093 273.6751 344.9521
352.4342 401.0068 489.9616
545.7070 627.0842 721.1042
746.5940 773.4341 805.5820
823.8997 864.5608 908.7081
945.2711 978.9761 998.1983
1040.7133 1058.9862 1066.8202
1134.4087 1164.1486 1196.5120
1219.0766 1260.3662 1285.2271
1294.7604 1333.3974 1349.1759
1368.5566 1370.9091 1385.5208
1403.1049 1468.7414 1493.0221
1497.2150 1518.2195 1668.2364
3004.0144 3012.4411 3023.0419
3042.9917 3046.0529 3065.9011
3070.4291 3082.1199 3086.2537

chxl3701

HF = -497.830957
ZeroPoint = 0.1524846
Energy+ZP = -497.6784724
Thermal = 0.1611081
Free Energy Correction = 0.117606

C -0.659836 -0.037652 -0.471066
C 0.113529 -1.297771 0.105312
C 1.511902 -0.914538 -0.313355
C 1.961815 0.250958 0.416104
C 1.570990 1.506090 -0.327240
C -0.000438 1.362023 -0.177967
H -0.010439 -1.352975 1.191251
H -0.290065 -2.210763 -0.349486
H -0.715964 -0.174005 -1.558639
H 1.642187 0.289821 1.459755
H 1.911338 2.451623 0.120226
H 1.887625 1.485612 -1.377402
H -0.271320 1.623694 0.852015
H -0.493843 2.101686 -0.823064
H 1.604000 -0.838812 -1.399292
C -2.145479 -0.058800 0.067540
O -2.287648 0.288781 1.270435
O -3.013650 -0.442457 -0.759010
O 2.878997 -0.876042 0.249659

20.0810 97.1070 184.8148
256.7555 291.9942 324.7465
389.4948 405.3472 479.8887
522.9195 527.7320 684.2284
758.3853 760.3464 808.0047
837.9592 860.4569 885.8639
916.5274 936.1841 964.1142
1013.5987 1052.6590 1075.3344
1105.0576 1152.3102 1185.2699
1206.0722 1214.9715 1243.2980
1268.3224 1303.6318 1328.7584
1351.2795 1357.3642 1376.2055
1420.4658 1493.1226 1511.6009
1523.9454 1526.9881 1678.4660
3016.0105 3035.3824 3042.1900
3054.4399 3069.7851 3089.1927
3093.7826 3107.3933 3123.1431

chxl3801

HF = -497.9372331
ZeroPoint = 0.1524059
Energy+ZP = -497.7848272
Thermal = 0.1615539
Free Energy Correction = 0.116481

C -0.754274 0.000514 -0.415611
C -0.012824 -1.254358 0.070576
C 1.469595 -1.280767 -0.374317
C 2.199122 0.000422 -0.013520
C 1.468880 1.282899 -0.368199
C -0.013511 1.253522 0.076573
H -0.075685 -1.287539 1.165915
H -0.514104 -2.157944 -0.301202
H -0.775194 0.003284 -1.515888
H 2.020050 2.128702 0.060301
H 1.506401 1.382936 -1.465921
H -0.076191 1.281393 1.172094
H -0.515363 2.158543 -0.290887
H 2.021245 -2.128305 0.050112
C -2.248033 -0.000536 0.080773
O -2.396108 -0.007572 1.333091
O -3.124793 0.006114 -0.823508
O 3.301885 -0.000513 0.522958
H 1.507234 -1.375481 -1.472510

18.5656 67.3745 163.4338
172.0097 194.1443 280.2168
347.3592 426.9322 435.7355
496.6519 519.0819 650.4862
733.2815 762.9283 766.1725
767.5530 847.6665 906.3585
922.0300 946.4854 1002.3543
1015.0906 1070.8181 1106.3946
1125.4530 1181.4180 1204.1198
1268.4471 1273.4535 1277.0694
1300.5802 1332.7865 1349.6986
1356.3511 1382.4252 1387.7228
1480.3675 1490.7923 1513.0194
1525.1861 1674.0299 1759.3237
2994.1388 3001.1399 3009.0401
3036.0681 3038.5831 3073.7175
3076.5686 3081.6156 3086.2092

chxl3901

HF = -422.6822605
ZeroPoint = 0.1473871
Energy+ZP = -422.5348734
Thermal = 0.1555274
Free Energy Correction = 0.113302

C 0.366219 1.310865 -0.198960
C 1.870712 1.200583 -0.176293
H 2.443633 2.126416 -0.277329
H -0.006187 1.767541 0.730256
C 2.533223 0.041145 -0.042716
H 3.625639 0.037000 -0.053589
C 1.830012 -1.285716 0.129310
H 1.921716 -1.872645 -0.801276
H 2.344844 -1.878942 0.902918
C 0.345062 -1.107949 0.492661
H 0.264363 -0.801899 1.546466
H -0.188832 -2.060774 0.390477
C -0.343196 -0.040315 -0.379847
H -0.254884 -0.360301 -1.428611
H 0.062685 2.002860 -0.999901
C -1.877849 0.013984 -0.043822
O -2.230539 0.846723 0.836490
O -2.589220 -0.816077 -0.672916

22.5848 110.2253 192.0436
194.2189 299.8889 351.0053
396.7183 484.4803 530.8918
644.6589 677.5968 741.4474
769.2007 821.7548 871.8506
916.3612 929.1825 947.0747
986.6067 1004.1184 1047.8867
1088.1289 1099.8146 1157.8129
1203.9772 1206.0998 1270.6027
1277.6118 1326.8639 1353.0185
1365.1997 1374.2501 1383.4645
1424.1446 1490.9782 1496.5703
1514.3465 1663.0864 1708.6126
2973.9991 2993.2412 3004.6565
3012.7732 3025.5250 3041.0718
3075.9830 3096.5128 3127.3169

chxl4001

HF = -422.6802203
ZeroPoint = 0.1473683
Energy+ZP = -422.532852
Thermal = 0.1553672
Free Energy Correction = 0.113990

C -0.387569 0.153220 0.867755
C 0.529231 -1.075765 0.985212
C 1.347041 -1.296387 -0.297735
C 1.987474 -0.017196 -0.778262
C 1.582401 1.195596 -0.372886
C 0.437391 1.425543 0.582889
H 2.122704 -2.062528 -0.134106
H 1.224752 -0.934362 1.831249
H -0.078011 -1.963404 1.188389
H 2.801568 -0.097653 -1.502632
H 2.087692 2.083249 -0.761542
H 0.842056 1.851249 1.519684
H -0.248514 2.175551 0.168369
H 0.673300 -1.691251 -1.072062
C -1.574919 -0.041634 -0.164808
O -2.158801 1.016884 -0.521238
O -1.848266 -1.231632 -0.479415
H -0.895312 0.296873 1.834875

42.5215 95.1979 163.5614
275.2033 315.5575 388.6042
430.5043 512.1236 535.7010
582.3525 650.3946 726.3755
781.1871 818.5014 849.8939
892.4872 918.6944 964.1670
982.4234 1002.7373 1047.1289
1075.1905 1108.1099 1158.8871
1195.3661 1214.0292 1261.1562
1306.3581 1325.4043 1342.4519
1355.1814 1377.0062 1391.2271
1428.6597 1481.8341 1491.7049
1499.3170 1666.0405 1712.2387
2946.1632 2962.8437 2989.4045
2998.1159 3040.8598 3061.0518
3095.6305 3099.4023 3128.2363

chxl401

HF = -573.6397847
ZeroPoint = 0.1675411
Energy+ZP = -573.4722436
Thermal = 0.1779897
Free Energy Correction = 0.129189

C -1.219656 0.029596 -0.417000
C -0.418135 -1.222605 -0.017436
C 1.070711 -1.124502 -0.403754
C 1.684436 0.135746 0.198473
C 0.941764 1.399701 -0.215902
C -0.548766 1.285689 0.165137
H 1.634681 -2.001820 -0.059740
H -0.519946 -1.362294 1.067406
H -0.855658 -2.111806 -0.490846
H -1.234668 0.108267 -1.513947
H 1.753903 0.052082 1.288364
H 1.406057 2.275624 0.258837
H 1.042470 1.527613 -1.303723
H -0.658316 1.255591 1.257640
H -1.077072 2.185112 -0.178340
H 1.173334 -1.074535 -1.498003
C -2.711522 -0.082597 0.068387
O -2.862559 -0.165878 1.318411
O -3.585855 -0.077933 -0.838164
O 3.083401 0.291734 -0.269157
O 3.932791 -0.470425 0.402025

22.2723 61.6460 76.0431
164.3318 189.2134 225.6698
250.3646 289.3876 337.0342
418.4266 461.7363 468.3695
520.1086 556.1143 722.7662
765.2168 803.6101 807.6485
883.0054 889.4201 915.3851
922.9594 978.3752 1011.0798
1032.0896 1070.0681 1088.4456
1137.7170 1159.9334 1193.2736
1230.3626 1236.6533 1269.9758
1299.1965 1321.7208 1328.1551
1339.2171 1347.1273 1370.7733
1378.3241 1388.1731 1397.6053
1505.7190 1511.6065 1517.1152
1527.0864 1670.7631 3014.9205
3017.7608 3022.2214 3032.5426
3035.7452 3052.6905 3061.3087
3074.0462 3076.9474 3092.5683

chxl4101

HF = -573.6099918
ZeroPoint = 0.1633582
Energy+ZP = -573.4466336
Thermal = 0.1755301
Free Energy Correction = 0.120686

C 0.351461 -0.697834 1.007216
C -0.980342 -0.047788 1.277578
H -1.633871 -0.521943 2.014910
H 1.014517 -0.586604 1.878718
C -1.395221 1.088647 0.683321
H -2.372477 1.503645 0.938446
H -2.431052 -0.541319 -0.340012
C -0.536946 1.854708 -0.298331
H -0.937004 1.727369 -1.318633
H -0.622403 2.931768 -0.084268
C 0.934568 1.408197 -0.245080
H 1.402014 1.819945 0.661959
H 1.486555 1.807671 -1.103606
C 1.081404 -0.125129 -0.217113
H 0.625968 -0.522072 -1.137132
H 0.215135 -1.784069 0.894541
O -3.125368 -1.020773 -0.883340
O -4.290344 -0.693405 -0.327045
C 2.607714 -0.509028 -0.257819
O 3.151779 -0.751424 0.853936
O 3.123532 -0.492526 -1.406495

22.6754 25.6144 31.3201
58.7199 93.4030 109.9178
187.1726 193.0385 229.1646
303.2487 355.5434 397.9635
486.0323 531.2517 563.1842
652.3976 692.7204 742.5431
770.6048 819.5969 870.6162
911.9416 929.5054 948.0951
1001.0237 1010.6596 1045.1108
1087.0057 1102.2989 1158.5386
1193.9877 1199.9002 1208.2144
1269.5761 1275.2612 1326.6112
1347.7537 1364.8683 1372.7548
1383.4608 1429.8368 1486.8291
1496.0200 1516.0679 1528.6425
1671.3573 1689.2668 2984.6618
3003.1062 3008.3633 3015.4106
3028.7101 3041.7076 3087.2884
3107.4911 3138.3371 3199.5727

chxl4201

HF = -573.6013297
ZeroPoint = 0.1633812
Energy+ZP = -573.4379485
Thermal = 0.1756971
Free Energy Correction = 0.119873

C -0.335134 -0.927735 -0.392798
C 0.947733 -0.429417 -1.006867
H 1.501520 -1.058916 -1.706142
H -0.656882 -1.875430 -0.834273
C 1.354013 0.828064 -0.739870
H 2.244511 1.248149 -1.209349
C 0.506137 1.674624 0.178391
H 0.651415 1.341377 1.218090
H 0.824835 2.724775 0.149500
C -1.008350 1.548999 -0.158894
H -1.232256 2.241217 -0.982645
H -1.591969 1.862964 0.712867
C -1.472862 0.123987 -0.548913
H -0.189035 -1.114701 0.683849
C -2.722023 -0.394917 0.264238
O -2.882218 0.087853 1.417236
O -3.396966 -1.278651 -0.327438
H -1.756185 0.110040 -1.608509
H 2.684346 -0.492602 0.380404
O 3.475354 -0.814998 0.907561
O 4.541657 -0.435267 0.205702

21.0892 23.6313 30.1251
50.9912 57.1288 92.4189
167.5569 210.5652 232.9760
288.6095 356.4426 425.4774
467.1887 555.9681 565.6292
637.2156 708.3643 729.6048
761.2829 784.1070 869.8523
907.3759 942.9605 960.4517
987.8107 990.0086 1038.2516
1087.2823 1093.8872 1161.1809
1195.5622 1208.2303 1222.1207
1257.6162 1271.4410 1315.2935
1333.5285 1340.1375 1362.8688
1377.3582 1418.2890 1502.1820
1508.2998 1516.8477 1534.3462
1669.8798 1675.9407 2994.8452
3003.2730 3016.4847 3046.2241
3056.6932 3095.3908 3107.0487
3129.7347 3155.4142 3195.5772

chxl4301

HF = -573.6355309
ZeroPoint = 0.163137
Energy+ZP = -573.4723939
Thermal = 0.1745917
Free Energy Correction = 0.122770

C -0.074254 -1.253385 0.152885
C -1.265817 -1.733335 -0.639168
H -1.120304 -2.628332 -1.247303
H 0.108525 -1.961812 0.978776
C -2.461410 -1.127039 -0.637491
H -3.265838 -1.524094 -1.260239
H 2.449084 0.475685 -0.061170
C -2.751058 0.116748 0.163659
H -2.777777 0.986206 -0.506844
H -3.748251 0.037405 0.626072
C -1.686717 0.367120 1.245871
H -1.849411 -0.338537 2.076995
H -1.803570 1.380770 1.645600
C -0.251298 0.175142 0.723685
H 0.829906 -1.295133 -0.464799
O 3.313318 0.035668 0.422777
O 3.456241 -1.193910 -0.072541
C 0.193978 1.279219 -0.287536
O 1.414260 1.205461 -0.688129
O -0.619364 2.158988 -0.623529
H 0.441449 0.271355 1.572859

23.7088 48.8674 60.0841
76.8953 96.3744 159.9085
199.3247 260.5316 305.3280
333.4855 388.2054 414.9954
502.7898 550.8234 635.0844
652.0704 730.8887 792.2940
825.5070 866.3163 896.0883
926.1609 969.7010 987.2784
1002.5841 1051.8105 1082.3458
1104.7963 1110.4493 1170.7835
1208.1768 1210.6438 1229.0353
1263.4134 1302.3925 1326.6256
1351.0674 1367.2239 1394.0590
1403.7744 1430.6508 1488.2072
1495.6089 1502.8745 1573.4842
1668.5332 1717.0628 1986.8999
2978.6423 2985.6479 2999.2175
3019.4799 3058.5528 3081.5107
3088.5628 3112.1906 3139.8439

chxl4401

HF = -497.905006
ZeroPoint = 0.1536686
Energy+ZP = -497.7513374
Thermal = 0.16189
Free Energy Correction = 0.119436

C 0.284917 0.009454 -0.034912
C -0.295787 -1.148876 -0.893773
C -1.769205 -1.226757 -0.394455
C -1.772562 -0.096950 0.663856
C -1.778794 1.281299 -0.041054
C -0.305634 1.353977 -0.543304
H -2.512084 -1.064841 -1.187362
H -0.202056 -0.942810 -1.964126
H 0.250610 -2.073214 -0.680088
H -2.510209 -0.212935 1.465081
H -2.522973 1.340032 -0.847092
H -2.000573 2.077569 0.680150
H -0.213075 1.449624 -1.628928
H 0.235418 2.189054 -0.087005
H -1.985959 -2.192684 0.077946
C 1.835781 -0.008504 0.085173
O 2.343787 -0.239328 1.204942
O 2.394802 0.214551 -1.027444
O -0.455014 -0.169180 1.212782

21.2466 137.2635 180.2593
209.8139 320.3473 345.8921
397.2229 496.1753 554.4532
584.8877 756.5079 770.2835
771.9258 808.0205 815.8496
829.3277 865.4132 930.5726
945.5660 948.2965 979.5715
994.2340 1025.8309 1069.4287
1079.1673 1140.4161 1183.5735
1189.5320 1217.4970 1246.0129
1249.8638 1299.0616 1299.6411
1331.6113 1336.8482 1339.0349
1372.7942 1497.2763 1509.9321
1515.5353 1532.5040 1686.0994
3028.3304 3034.2337 3064.7121
3067.5190 3073.3839 3075.5743
3086.0708 3115.3177 3122.7865

chxl4501

HF = -497.8855994
ZeroPoint = 0.1537167
Energy+ZP = -497.7318827
Thermal = 0.1619143
Free Energy Correction = 0.119749

C -0.509587 0.070490 -0.640915
C 0.309060 -1.067293 -0.031246
C 1.008933 -0.644675 1.279082
C 2.091307 -0.146628 0.299594
C 1.777326 1.245118 -0.252225
C 0.242350 1.409966 -0.431634
H 0.492162 0.077906 1.917124
H -0.206854 -2.028418 -0.083414
H -0.618205 -0.164132 -1.707030
H 3.150882 -0.286606 0.554258
H 2.173382 2.022094 0.421637
H 2.310858 1.344714 -1.208498
H -0.193232 1.865881 0.463791
H 0.028310 2.098754 -1.259508
H 1.349232 -1.506237 1.863393
C -1.964492 0.041744 -0.014815
O -2.220569 0.892444 0.878643
O -2.698340 -0.876286 -0.467724
O 1.641920 -1.125694 -0.687019

37.9769 93.8951 180.4212
250.5216 323.4832 364.7585
415.7866 437.6610 553.6834
583.5068 689.7758 755.0479
802.3393 822.4965 837.1147
856.2435 892.2124 914.3175
943.0966 965.7343 972.4448
1028.2831 1051.3772 1089.7623
1112.3758 1125.6716 1185.1794
1205.0444 1233.0186 1261.8382
1271.1873 1300.3472 1315.8187
1336.2775 1348.4064 1358.5497
1375.3724 1388.5240 1496.8679
1509.8107 1534.0239 1674.9952
2994.9676 3031.0794 3033.9109
3041.1543 3054.2815 3070.7518
3094.5826 3125.0515 3132.7819

chxl4601

HF = -497.8791952
ZeroPoint = 0.1534553
Energy+ZP = -497.7257399
Thermal = 0.1615974
Free Energy Correction = 0.119860

C -0.504834 0.007771 0.726406
C 0.426273 -1.100370 0.240115
C 1.882704 -0.888648 0.726134
C 1.956990 -0.014693 -0.543756
C 1.418753 1.399632 -0.320437
C 0.234456 1.373638 0.685511
H 2.044830 -0.416663 1.702596
H -0.036620 -2.086523 0.298669
H 2.869125 -0.043474 -1.156000
H 2.219739 2.067344 0.036427
H 1.087325 1.776983 -1.296514
H 0.624677 1.608662 1.687224
H -0.502803 2.140186 0.429494
H 2.490585 -1.796215 0.635447
O 0.884678 -0.802364 -1.134583
H -0.748703 -0.229880 1.775014
C -1.900370 -0.038218 -0.020131
O -2.347681 1.052571 -0.457064
O -2.428495 -1.182093 -0.042780

62.5234 84.2050 168.2032
271.4304 318.2881 381.9931
392.1923 508.5474 530.4004
594.0620 644.6415 772.2120
780.8653 827.0700 832.7546
875.9497 878.8347 911.9670
933.6641 954.9731 979.6168
1032.2694 1057.1793 1087.0114
1107.1142 1137.5540 1177.4310
1218.2610 1219.6683 1258.1497
1278.3426 1298.8020 1323.1489
1331.3810 1346.2126 1353.2896
1379.0846 1382.1257 1491.0903
1501.6083 1518.4902 1681.0336
2981.2316 2993.8338 3010.8050
3028.7579 3051.9756 3064.5555
3097.9685 3106.3298 3140.0090

chxl4701

HF = -497.896453
ZeroPoint = 0.147778
Energy+ZP = -497.748675
Thermal = 0.1588147
Free Energy Correction = 0.108697

C -0.774878 0.104229 -0.394294
C 0.273054 -1.010674 -0.161977
C 1.690196 -0.727472 -0.725277
C 2.642054 -0.132326 0.280160
C -0.113862 2.547534 -0.316986
C -0.421258 1.389127 0.288259
H 0.321972 -1.229279 0.913134
H -0.107271 -1.922199 -0.639449
H -0.864993 0.274238 -1.475624
H 0.089503 3.454508 0.250780
H -0.086681 2.637928 -1.402983
H -0.470198 1.350067 1.377744
H 2.162649 -1.631012 -1.130421
C -2.173385 -0.444049 0.130016
O -2.286284 -0.497224 1.382164
O -2.977952 -0.792125 -0.768519
O 3.813845 -0.452642 0.401816
H 1.611284 -0.006890 -1.555997
H 2.215340 0.650349 0.939713

33.8876 38.8284 56.1260
75.0274 104.9185 166.4382
213.4826 269.4681 274.3117
338.9583 412.6931 484.8145
508.8552 629.4538 729.8127
767.4145 776.7353 818.3289
878.7857 882.9900 950.1196
963.9794 1037.2565 1039.8819
1066.5092 1094.3864 1159.5476
1200.0440 1245.5312 1261.3686
1305.0624 1322.5793 1333.6933
1357.1695 1367.7405 1423.9999
1465.3400 1474.2524 1510.9017
1680.9263 1692.1060 1777.1091
2959.5527 3007.7636 3034.8842
3042.1504 3073.8307 3083.2754
3126.2274 3148.7819 3199.7231

chxl5001

HF = -234.621922
ZeroPoint = 0.1419705
Energy+ZP = -234.4799515
Thermal = 0.1493056
Free Energy Correction = 0.110191

C 1.506608 -0.097231 -0.465508
C -2.264893 -0.978012 -0.194285
C -0.758849 1.051350 -0.156172
C 0.758839 1.051348 0.156160
C 2.264916 -0.977988 0.194295
C -1.506623 -0.097216 0.465512
H 1.406984 -0.195345 -1.548938
H -2.392223 -0.927216 -1.274613
H -0.912512 1.049767 -1.243961
H -2.786004 -1.781825 0.319897
H -1.177457 1.997802 0.218244
H 0.912502 1.049780 1.243948
H 2.392281 -0.927153 1.274616
H 1.177452 1.997793 -0.218270
H 2.786027 -1.781809 -0.319877
H -1.407034 -0.195292 1.548948

60.7905 98.2510 102.8407
263.6676 341.9179 420.8079
436.5148 619.3201 659.9689
828.7981 876.8512 937.1231
939.2374 947.2918 987.6725
1024.2882 1024.3612 1037.5910
1058.2905 1199.9491 1249.1091
1256.3817 1330.5435 1330.9772
1358.9640 1374.5579 1466.7459
1471.7969 1499.0193 1507.6773
1715.9077 1716.1257 3011.0635
3022.5939 3053.1788 3067.7474
3130.0711 3131.3254 3150.0736
3150.3062 3228.9615 3229.1891

chxl501

HF = -573.6401638
ZeroPoint = 0.1675804
Energy+ZP = -573.4725834
Thermal = 0.1778717
Free Energy Correction = 0.129369

C -1.364372 0.004438 0.878624
C -0.419254 -1.193571 1.079177
C 0.764351 -1.158026 0.093733
C 1.506865 0.169489 0.218740
C 0.595910 1.368355 -0.016043
C -0.587694 1.329346 0.970276
H 1.463026 -1.984757 0.279200
H -0.027805 -1.199885 2.111646
H -0.982859 -2.117786 0.923144
H 2.021970 0.239929 1.184339
H 1.169483 2.299183 0.094732
H 0.199296 1.337367 -1.037929
H -0.205936 1.474240 1.996312
H -1.265743 2.155721 0.739746
H 0.377172 -1.263933 -0.927159
O 2.590602 0.239857 -0.790872
O 3.702903 -0.353074 -0.386192
H -2.105664 -0.010828 1.693679
C -2.225552 -0.112981 -0.449195
O -2.584515 0.978174 -0.965965
O -2.492048 -1.286401 -0.820668

20.6364 59.0827 74.9485
163.6557 169.1917 277.6844
303.8150 335.6372 366.4054
415.1106 449.9249 531.2556
532.4163 546.1981 596.0943
771.1672 795.2973 822.8071
849.9273 887.2395 909.2093
922.3097 957.7354 1013.8921
1045.9127 1089.9651 1094.7546
1117.4501 1153.9743 1194.1908
1209.9274 1239.8931 1285.0961
1301.0112 1330.8808 1338.3746
1343.6496 1345.2306 1360.1782
1379.6448 1383.3333 1399.5412
1485.6283 1497.1276 1509.7792
1529.1034 1674.8900 2965.1933
2968.9069 3001.0629 3032.4906
3040.1242 3060.1916 3090.1069
3098.0963 3110.3964 3111.5631

chxl601

HF = -573.6102613
ZeroPoint = 0.165821
Energy+ZP = -573.4444403
Thermal = 0.1758747
Free Energy Correction = 0.129911

C -0.940698 -1.078362 0.295411
C -0.169664 -1.521741 -0.906285
C 1.323696 -1.340341 -0.956650
C 1.747100 -0.086232 -0.168258
C 1.277509 -0.170795 1.296174
C -0.017150 -0.989461 1.523650
H 1.868681 -2.197836 -0.513518
H -0.717587 -1.685171 -1.830516
H 2.843523 0.039098 -0.185662
H 2.100069 -0.627848 1.866809
H 1.164954 0.846925 1.674072
H 0.258933 -2.018563 1.805025
H -0.570508 -0.565283 2.368922
H 1.674373 -1.260563 -1.994645
O 1.169647 0.980363 -0.948230
O 1.008571 2.199346 -0.181661
H 0.063016 2.038800 0.130640
H -1.732471 -1.816424 0.501938
C -1.773959 0.255470 0.002642
O -1.377463 1.313617 0.588965
O -2.755002 0.111129 -0.751969

63.1745 103.4211 165.9612
185.7469 224.3646 272.2213
285.1929 298.2955 348.6276
399.8352 444.5042 485.1218
546.7763 586.7053 628.7995
732.1333 776.6281 796.5239
818.6105 828.2247 874.0892
892.3676 900.7616 943.8222
944.6675 995.0293 1063.0267
1069.5597 1093.2504 1146.3990
1155.9174 1220.0963 1235.3617
1266.7476 1302.6273 1322.5623
1336.8159 1350.8484 1372.5390
1377.4199 1399.2297 1401.9057
1487.2125 1498.9586 1518.0900
1565.1724 1680.9504 2909.6891
2957.1853 2972.3965 2988.6821
3019.0220 3046.1632 3076.4870
3086.6836 3136.4914 3187.8906

chxl6101

HF = -573.5887605
ZeroPoint = 0.1619132
Energy+ZP = -573.4268473
Thermal = 0.1730037
Free Energy Correction = 0.123058

C -1.350386 0.229141 -0.668529
C -0.395214 1.387773 -0.234415
C 0.949454 1.232359 -0.811984
C 1.673240 -0.051979 -0.636675
C 0.741295 -1.165838 -0.144849
C -0.574045 -1.094124 -0.940259
H -0.825878 2.367282 -0.471582
H -0.383266 1.317086 0.870012
H 2.258567 -0.366546 -1.516127
H 1.229196 -2.141132 -0.256022
H 0.539104 -1.016417 0.922476
H -0.337200 -1.182234 -2.013121
H -1.227560 -1.939468 -0.700703
H 1.450873 2.030969 -1.352374
O 2.490619 0.571457 0.323412
O 3.714243 -0.606602 0.859743
H 3.343950 -0.631709 1.759991
H -1.876377 0.511294 -1.587823
C -2.457810 -0.012319 0.435474
O -2.192001 0.391847 1.598819
O -3.474188 -0.619102 0.012113

-498.0199 26.2372 43.9062
101.3822 137.1842 167.2575
198.3624 235.1159 279.1867
294.5928 361.9122 396.0984
422.3643 491.6592 545.4568
604.0746 631.9649 710.0066
763.5016 788.7133 842.9098
885.4300 903.2757 909.4690
926.4091 965.5211 1037.6926
1060.9801 1072.0918 1092.1982
1116.1798 1174.3714 1190.1074
1200.4228 1267.6380 1290.3971
1302.4108 1327.6661 1332.2081
1354.8971 1372.6033 1401.1700
1415.0858 1484.7468 1519.9786
1525.9029 1669.5087 2941.5474
2983.1811 2988.4210 3056.4500
3056.8219 3081.2935 3093.9137
3098.9148 3196.8752 3734.0061

chxl6301

HF = -573.5739756
ZeroPoint = 0.1606563
Energy+ZP = -573.4133193
Thermal = 0.1704189
Free Energy Correction = 0.123831

C -1.258434 0.413944 0.786091
C -0.324406 -0.529516 1.564724
C 1.062510 -0.666330 1.002408
C 1.723093 0.523332 0.295813
C 0.719715 1.348092 -0.510987
C -0.524230 1.685175 0.327957
H 1.760724 -1.221050 1.641443
H -0.215297 -0.176200 2.610438
H -0.805676 -1.516311 1.619754
H 2.285579 1.161889 0.996412
H 1.214558 2.259757 -0.874141
H 0.405971 0.770496 -1.386491
H -0.226503 2.287885 1.205830
H -1.211548 2.287779 -0.272742
H 1.261526 -1.351467 -0.162445
O 2.746021 -0.107161 -0.509706
O 2.053082 -1.209742 -1.122520
H -2.061222 0.717031 1.476650
C -2.025477 -0.330478 -0.383104
O -2.226878 -1.561006 -0.196480
O -2.402817 0.392269 -1.340310

-2062.5614 33.7277 56.5227
133.8034 190.1397 242.6498
266.7955 319.5687 359.5807
428.3949 462.0903 521.2628
530.2582 550.2097 621.1179
704.6258 754.2165 777.0567
800.2833 856.5408 882.7405
897.5874 919.0038 937.0216
940.9377 1009.7436 1052.7735
1080.2102 1110.6665 1119.4160
1175.9304 1189.1069 1215.3469
1222.8259 1278.3146 1301.8970
1327.6707 1331.9593 1345.6628
1362.4220 1368.0692 1386.3926
1404.0603 1455.1320 1491.7593
1519.5699 1662.8614 1699.9090
2908.3793 2951.7397 2996.1589
3000.7008 3033.2002 3038.6008
3072.4209 3107.1102 3113.8095

chxl6401

HF = -573.5801113
ZeroPoint = 0.1606684
Energy+ZP = -573.4194429
Thermal = 0.1704811
Free Energy Correction = 0.124010

C 1.041087 0.055309 0.384319
C 0.330323 -1.241509 -0.027305
C -1.156149 -1.143600 -0.174358
C -1.781148 0.145933 -0.719087
C -1.021663 1.400525 -0.277656
C 0.498744 1.235663 -0.443744
H -1.642424 -2.046687 -0.565043
H 0.793494 -1.535952 -0.993047
H 0.591473 -2.066046 0.653126
H 0.865800 0.272747 1.447013
H -1.895446 0.121284 -1.813614
H -1.393216 2.262512 -0.849762
H -1.257998 1.584350 0.777504
H 0.749002 1.069387 -1.503203
H 1.009772 2.157490 -0.139969
H -1.932074 -0.948708 0.926702
C 2.587392 -0.069350 0.162348
O 2.931593 -0.792214 -0.820317
O 3.320603 0.580831 0.946181
O -3.138325 0.099831 -0.214904
O -2.973858 -0.284472 1.168188

-1935.0186 44.0232 67.3958
153.0199 183.1502 199.0702
264.3365 300.4002 340.9165
369.0417 476.8976 507.5817
545.2990 563.8206 676.5430
715.0103 756.0461 784.2214
793.1515 854.9523 883.4781
898.0249 910.8459 937.1174
973.3600 1014.5496 1044.3256
1073.2122 1103.4181 1136.4394
1164.1597 1193.1056 1211.3951
1231.8977 1270.7066 1285.6992
1329.8355 1333.0536 1340.6703
1353.9429 1377.1086 1382.8791
1401.7590 1457.6313 1511.1418
1516.8515 1643.9616 1700.6646
2906.0548 3011.5316 3014.2470
3022.0477 3030.2825 3037.8206
3066.8307 3073.8757 3086.4856

chxl6501

HF = -573.5763268
ZeroPoint = 0.1625899
Energy+ZP = -573.4137369
Thermal = 0.1738672
Free Energy Correction = 0.121785

C -1.426280 0.165888 0.699965
C -0.358347 -0.926324 1.016215
C 1.006002 -0.383296 1.261166
C 1.519418 0.599970 0.429576
C 0.555453 1.231424 -0.544928
C -0.795010 1.479484 0.163205
H -0.684861 -1.557803 1.851473
H -0.366178 -1.586865 0.128141
H 2.394652 1.158835 0.752351
H 0.967377 2.161030 -0.957994
H 0.398738 0.547417 -1.390517
H -0.620276 2.186310 0.988931
H -1.509600 1.956465 -0.515749
H 1.629018 -0.792151 2.055987
O 2.707409 -0.417885 -0.850509
O 4.034907 -0.466512 -0.357986
H 4.406903 0.382022 -0.663179
H -1.967227 0.416237 1.621106
C -2.522584 -0.367852 -0.308647
O -2.280856 -1.457996 -0.892802
O -3.526517 0.383985 -0.419936

-304.5946 11.5318 33.1649
43.5659 118.1580 131.3259
189.8754 253.6020 275.2356
306.9677 377.9341 391.5413
407.1364 483.4970 558.5028
613.4043 657.5635 742.7969
763.9791 791.2778 863.4555
901.5835 911.2773 933.8726
946.4503 980.3317 1012.0206
1050.3159 1072.8724 1096.8455
1138.0585 1186.9458 1204.4915
1213.9188 1279.4760 1317.7667
1330.4281 1337.3192 1353.4055
1361.0467 1373.9703 1421.5824
1490.1340 1508.9311 1520.6436
1533.7307 1662.4175 2943.7813
2996.7494 3035.4253 3041.0665
3066.6830 3071.6873 3094.4964
3151.6457 3172.4598 3640.3507

chxl6601

HF = -573.568595
ZeroPoint = 0.1607075
Energy+ZP = -573.4078875
Thermal = 0.1708005
Free Energy Correction = 0.123533

C -1.269711 0.089285 0.916326
C -0.348712 -1.113666 1.190070
C 0.718948 -1.287338 0.094939
C 1.453594 0.000665 -0.169794
C 0.620899 1.249547 -0.348270
C -0.441701 1.380670 0.759143
H 1.436183 -2.083480 0.331720
H 0.149099 -0.983356 2.166647
H -0.947345 -2.028950 1.241904
H 2.367664 0.212239 0.795284
H 1.276676 2.127935 -0.397382
H 0.117071 1.167084 -1.325289
H 0.064770 1.624303 1.708230
H -1.119983 2.205599 0.520316
H 0.188976 -1.566477 -0.830873
O 2.582055 -0.099556 -1.011326
O 3.495744 0.163345 0.156517
H -1.931592 0.226518 1.784206
C -2.235922 -0.106905 -0.318766
O -2.998101 0.867585 -0.547871
O -2.152936 -1.203245 -0.939401

-1711.9508 34.4901 73.9208
103.5459 154.8435 191.6181
286.7183 323.7995 339.2090
351.4173 419.4346 462.5332
515.7951 560.2750 628.8960
655.3973 767.9290 780.5483
799.5163 828.3217 851.5408
894.5800 915.5630 934.7929
975.7745 1004.8382 1034.2823
1091.0711 1095.4676 1113.2362
1151.1575 1163.6251 1218.6321
1248.9102 1285.7071 1307.9409
1323.4656 1340.6402 1349.1593
1367.1721 1376.8896 1399.4910
1476.7222 1494.0232 1494.3206
1507.5792 1661.6540 1869.2366
2972.8568 2980.9232 2998.1232
3009.1272 3018.5397 3068.9307
3070.9444 3093.4068 3103.9025

chxl6801

HF = -573.5838464
ZeroPoint = 0.1622029
Energy+ZP = -573.4216435
Thermal = 0.1732712
Free Energy Correction = 0.123881

C -0.914573 -0.106851 -0.529326
C -0.241443 -0.939296 0.468693
C 0.595900 -0.266147 1.518588
C 1.691838 0.336305 0.634265
C 1.143420 1.459145 -0.263194
C -0.380363 1.336169 -0.521443
H 0.042750 0.499905 2.091303
H -0.493955 -1.992992 0.537885
H 2.588289 0.654993 1.182714
H 1.353677 2.434585 0.202397
H 1.719772 1.427302 -1.195830
H -0.932915 1.865565 0.262434
H -0.647730 1.837011 -1.460880
H 1.025340 -0.985383 2.223572
O 2.034119 -0.823507 -0.157630
O 3.607623 -0.477136 -0.631854
H 3.537360 -0.991676 -1.453628
H -0.867155 -0.576977 -1.519265
C -2.542669 -0.186150 -0.186803
O -2.996661 0.787244 0.447233
O -3.074842 -1.233024 -0.607172

-556.3713 39.9579 65.5738
101.6490 122.9117 139.7990
174.2797 235.2028 261.9657
336.4218 356.6386 404.2305
425.8441 503.0672 557.1175
631.6212 650.0281 713.9112
747.0488 779.1058 817.1661
863.9051 885.8713 930.2202
961.1028 993.0676 1021.6385
1065.9051 1072.3124 1088.9760
1129.1687 1144.1787 1169.3749
1224.6535 1241.2947 1278.2188
1298.9457 1317.9807 1336.9268
1361.6484 1376.6541 1381.3360
1416.0782 1495.7954 1503.9935
1529.9801 1740.4690 2961.4002
3004.1309 3035.5666 3040.2129
3049.5066 3067.5630 3091.2202
3094.6348 3209.9666 3751.4042

chxl6901

HF = -497.8098663
ZeroPoint = 0.1480486
Energy+ZP = -497.6618177
Thermal = 0.1566977
Free Energy Correction = 0.114048

C 0.821615 0.333392 -0.729242
C 0.146103 -1.008790 -0.799224
C -1.286411 -1.145225 -0.799196
C -2.182657 -0.045787 0.121614
C -1.527149 1.322417 -0.273278
C -0.035411 1.366662 0.063568
H -1.609894 -0.782976 -1.789950
H 0.765272 -1.868133 -1.026636
H -3.179358 -0.085958 -0.410856
H -1.698335 1.524958 -1.346734
H -2.055379 2.100791 0.293665
H 0.390854 2.363178 -0.104972
H 0.060292 1.141802 1.131613
H -1.635153 -2.174527 -0.662418
O -2.219338 -0.344764 1.384804
H 1.084589 0.736239 -1.720829
C 2.018879 -0.071760 0.148257
O 3.103010 0.519492 0.199617
O 1.634740 -1.107331 0.820843

-395.3962 61.1188 101.7891
189.7042 210.3725 241.0976
336.1404 380.7682 411.7318
475.3400 511.7025 631.3674
667.9074 697.7555 740.8977
759.4732 792.1151 831.7401
860.9184 901.2056 960.3663
986.7468 1017.5365 1044.3438
1072.8054 1131.7538 1150.8537
1185.6017 1217.4786 1251.3602
1302.2552 1318.9948 1333.0156
1343.6897 1355.0567 1384.8918
1419.8092 1454.3453 1457.8674
1492.2473 1505.8761 1709.5391
2625.3391 2957.7730 2989.0737
2993.4987 3046.3490 3058.0285
3096.0134 3101.8002 3218.3751
-395.3961 61.1190 101.7891
189.7042 210.3725 241.0975
336.1405 380.7682 411.7318
475.3400 511.7025 631.3674
667.9074 697.7555 740.8977
759.4732 792.1151 831.7401
860.9184 901.2056 960.3663
986.7468 1017.5365 1044.3438
1072.8054 1131.7538 1150.8538
1185.6017 1217.4786 1251.3602
1302.2552 1318.9948 1333.0156
1343.6897 1355.0566 1384.8918
1419.8092 1454.3452 1457.8674
1492.2474 1505.8762 1709.5391
2625.3392 2957.7730 2989.0737

2993.4987 3046.3490 3058.0285
3096.0134 3101.8002 3218.3751

chxl7001

HF = -497.9399493
ZeroPoint = 0.1526327
Energy+ZP = -497.7873166
Thermal = 0.1615745
Free Energy Correction = 0.117237

C -0.814947 0.026554 0.920288
C 0.113993 -1.192785 1.028703
C 1.106379 -1.269014 -0.156108
C 1.850988 0.033573 -0.356275
C 0.983121 1.277382 -0.382723
C 0.012723 1.319383 0.821806
H 1.836221 -2.078679 -0.038226
H 0.683097 -1.146731 1.972668
H -0.483461 -2.109670 1.039140
H 1.631468 2.160327 -0.426060
H 0.374665 1.251028 -1.298901
H 0.597823 1.470338 1.744314
H -0.666321 2.169385 0.706960
H 0.502060 -1.463464 -1.053856
O 3.073186 0.085317 -0.474351
H -1.416318 0.084951 1.841176
C -1.872063 -0.076783 -0.254695
O -2.500571 0.987658 -0.495465
O -1.990164 -1.203892 -0.806833

22.5686 73.0986 140.3766
162.1330 284.8326 339.4298
387.0348 412.2962 494.0754
505.4738 537.9326 586.0067
681.3757 755.2027 767.1680
790.9906 849.1380 882.5665
898.5815 955.7593 998.4247
1030.7206 1073.5490 1103.2715
1140.9787 1155.5128 1197.7000
1261.4510 1270.0795 1288.3545
1321.4569 1336.9788 1342.1129
1360.9617 1370.0445 1393.3328
1483.3928 1494.0203 1498.4383
1509.4980 1671.4581 1748.8427
2978.2635 2983.0168 3008.1446
3030.3064 3037.5078 3087.7089
3090.8906 3098.9559 3106.6119

chxl801

HF = -423.1731147
ZeroPoint = 0.1524626
Energy+ZP = -423.0206521
Thermal = 0.1609052
Free Energy Correction = 0.117661

C 0.416449 0.110798 0.895777
C -0.459114 1.370591 0.728101
C -1.521911 1.234437 -0.345813
C -1.992512 -0.122652 -0.790036
C -1.241034 -1.356747 -0.357536
C -0.461150 -1.151896 0.952577
H -2.622200 0.666864 0.054245
H -0.925220 1.616102 1.701520
H 0.199751 2.204841 0.466697
H -2.537569 -0.143982 -1.733914
H -1.918222 -2.221573 -0.277472
H -0.494632 -1.605442 -1.130085
H -1.171383 -1.071465 1.796061
H 0.173313 -2.026111 1.127730
H -1.702591 2.063518 -1.028805
C 1.584039 0.015252 -0.171373
O 1.993589 -1.149233 -0.430743
O 2.020290 1.113714 -0.607772
H 0.939123 0.202702 1.861964

-1945.0923 30.6109 82.0272
141.6204 253.1729 270.7875
335.4164 411.3663 493.3745
527.0406 560.3737 589.0668
649.4319 758.3396 790.6644
813.9126 835.4020 878.0541
890.2030 936.0345 1002.1681
1056.7062 1068.4920 1076.6120
1142.0102 1192.6049 1198.3531
1228.0171 1280.5289 1309.4950
1316.7556 1333.4835 1343.5786
1358.1432 1376.4319 1385.8580
1391.4649 1485.2293 1495.4221
1507.6887 1665.0837 2144.7005
2913.3980 2951.7534 2985.0728
2989.9978 3010.0625 3091.3641
3098.6048 3127.5303 3149.8443