Table S1 Calculated XYZ coordinates (Å) of all the optimized structures, absolute energies (a.u.) and normal-mode frequencies (cm^{-1}) of 1-NpOH–$(Pip)_n$ (n = 0-3) clusters in the S_0, L_b and L_a states.

(Oa)

Ground state optimized

Atom	X	Y	Z
C	-1.401070	0.674586	0.000000
C	-2.291085	-0.364136	0.000000
C	-1.824764	-1.695745	0.000000
C	-0.488616	-1.968517	0.000000
C	0.453099	-0.909641	0.000000
C	1.848188	-1.148250	0.000000
C	2.737787	-0.111468	0.000000
C	2.278055	1.222446	0.000000
C	0.937808	1.490101	0.000000
C	0.000000	0.432484	0.000000
O	-1.785602	1.979409	0.000000
H	-2.745077	2.028758	0.000000
H	-3.355487	-0.162168	0.000000
H	-2.545320	-2.502130	0.000000
H	-0.130267	-2.989215	0.000000
H	2.197271	-2.173066	0.000000
H	3.800956	-0.310261	0.000000
H	2.992296	2.034331	0.000000
H	0.574031	2.507326	0.000000

Absolute energy

-461.087144695

Normal-mode frequencies

142.796

173.255

264.8346

287.8755

363.7243

434.1077

472.7694
478.9139
488.1987
533.5442
584.9592
594.0232
658.3585
733.8126
755.6819
802.0249
802.4987
824.055
885.2033
896.3396
911.0039
995.6934
1006.1373
1028.598
1049.5627
1072.1337
1112.2463
1163.0845
1174.8909
1188.8137
1227.0954
1258.0429
1276.6071
1315.2403
1399.9615
1433.451
1443.3338
1497.4903
1515.5525
1575.1964
1658.2003
1676.7054

1713.1341
3188.3765
3196.4455
3205.516
3209.0421
3220.9367
3223.2334
3237.1664
3885.3831

(Oa)
Lb state optimized

Atom	X	Y	Z
C	1.345134	0.792149	-0.031295
C	2.353500	-0.170226	-0.014468
C	2.006410	-1.546349	0.036904
C	0.674754	-1.929752	0.059808
C	-0.386481	-0.967337	0.002705
C	-1.753732	-1.334076	-0.096165
C	-2.739913	-0.337703	-0.052650
C	-2.400964	1.045928	0.030925
C	-1.077092	1.451018	0.119892
C	-0.048949	0.447721	0.042636
O	1.601310	2.114015	-0.076666
H	2.559998	2.249778	-0.090578
H	3.400110	0.142638	-0.036755
H	2.794748	-2.298615	0.053059
H	0.408100	-2.987487	0.097805
H	-2.023196	-2.388708	-0.149927
H	-3.792588	-0.626518	-0.050586
H	-3.199387	1.789062	0.022007
H	-0.794263	2.499495	0.178554

Absolute energy
-460.800728840

Normal-mode frequencies
105.8728
128.7089
235.799
286.071
350.2045
417.3427
439.7818
460.7491
463.6334
468.4684
516.1743
548.2025
571.0077
655.0546
686.1427
709.7716
725.3124
778.6216
784.7421
838.6922
859.3939
860.7123
878.2649
945.6731
1009.7664
1059.1669
1092.1773
1126.8457
1159.7428
1189.9952
1212.614
1229.763
1240.8028
1324.6163
1411.1751

1423.9303
1442.1984
1472.8199
1487.0351
1533.7043
1566.1638
1595.5685
3090.8883
3199.6172
3205.6367
3210.0329
3229.0842
3233.1774
3241.8466
3318.3061
3828.9362

(Oa)
La state optimized

Atom	X	Y	Z
C	-1.406911	0.638637	0.000000
C	-2.340905	-0.451958	0.000000
C	-1.856287	-1.733443	0.000000
C	-0.446631	-1.954817	0.000000
C	0.491203	-0.898324	0.000000
C	1.883184	-1.117089	0.000000
C	2.791851	-0.015340	0.000000
C	2.311633	1.273183	0.000000
C	0.904365	1.528086	0.000000
C	0.000000	0.451758	0.000000
O	-1.850057	1.906377	0.000000
H	-2.817890	1.908700	0.000000
H	-3.411759	-0.238671	0.000000
H	-2.536073	-2.584732	0.000000
H	-0.074115	-2.980864	0.000000
H	2.258411	-2.140754	0.000000

H	3.865232	-0.204897	0.000000
H	3.001413	2.117903	0.000000
H	0.526215	2.548140	0.000000

Absolute energy
-460.813190547

Normal-mode frequencies
111.9729
161.5045
204.0231
283.5943
311.2319
408.2578
438.4231
444.4914
460.439
489.3616
507.9836
536.1251
595.2086
681.3164
695.0391
704.3913
712.2522
778.0371
785.503
820.8911
851.9775
859.7528
921.252
950.9217
1019.2114
1040.182
1065.7475
1087.6035

1157.7002
1160.0764
1220.1646
1233.9918
1260.0969
1340.6473
1412.3177
1430.2821
1443.116
1467.6182
1478.5267
1487.279
1516.9679
1613.8856
1663.8057
3197.3142
3206.1027
3210.0892
3217.622
3231.8122
3237.7393
3251.8591
3828.8404

(Ob)

Ground state optimized

Atom	X	Y	Z
C	-1.362963	0.78037	0.000001
C	-2.322459	-0.195441	-0.000004
C	-1.954793	-1.553097	-0.000005
C	-0.640384	-1.922984	0.000001
C	0.372462	-0.936297	0.000003
C	1.744633	-1.286542	0.000004
C	2.719495	-0.331352	0.000001
C	2.368844	1.034656	-0.000005
C	1.054451	1.407156	-0.000004

C	0.02011	0.43979	0.000001
O	-1.782155	2.072836	0.000004
H	-1.030636	2.668503	0.000029
H	-3.361261	0.102358	-0.000006
H	-2.731372	-2.305742	-0.000008
H	-0.35482	-2.966282	0.000004
H	2.005438	-2.337299	0.000008
H	3.762456	-0.616603	0.000002
H	3.14385	1.788444	-0.000011
H	0.827207	2.466376	-0.000011

Absolute energy
-461.084775893

Normal-mode frequencies
70.318
173.094
211.1766
265.5462
308.7246
429.1775
472.5038
479.3576
485.2227
532.9272
585.1157
586.5481
656.8241
733.4245
748.2605
795.8688
801.9915
814.6818
883.5144
894.4557
919.6872

978.2292
1003.3469
1021.6271
1050.391
1071.9904
1116.5766
1168.4243
1185.5577
1199.8996
1216.8654
1243.4496
1296.9543
1320.1901
1407.0691
1427.745
1448.0632
1496.339
1513.9427
1574.9615
1658.2819
1682.0431
1716.0725
3182.643
3199.1398
3204.7415
3214.8917
3220.0562
3228.1304
3232.3755
3911.7194

(Ob)
Lb state optimized

Atom	X	Y	Z
C	-1.362451	0.799183	0.010943
C	-2.363091	-0.186955	-0.017105

C	-1.999055	-1.557478	-0.041886
C	-0.649282	-1.929712	-0.014492
C	0.383870	-0.966625	0.019687
C	1.751559	-1.311988	0.053498
C	2.755042	-0.342362	0.032785
C	2.404205	1.037544	-0.044764
C	1.061780	1.421237	-0.068547
C	0.022256	0.471698	-0.002945
O	-1.786033	2.078814	0.051597
H	-1.029626	2.658193	0.214714
H	-3.402923	0.134183	-0.000610
H	-2.775354	-2.320869	-0.066913
H	-0.376640	-2.986650	-0.022403
H	2.017409	-2.370565	0.088436
H	3.803090	-0.637083	0.061432
H	3.183978	1.796628	-0.093126
H	0.839332	2.488401	-0.157355

Absolute energy
-460.804108208

Normal-mode frequencies
68.5004
157.3221
216.8794
277.0497
333.3516
374.0778
391.6092
463.79
465.7549
480.2651
534.4253
568.7199
576.4159
660.3188

677.0187
703.8017
714.0607
783.0169
785.412
800.8335
889.3618
893.3054
909.6374
927.8606
1011.615
1043.4024
1093.7486
1152.7265
1156.3773
1167.7231
1222.4532
1247.3132
1302.6583
1345.373
1425.5492
1428.8789
1483.6356
1498.475
1523.6796
1578.6194
1605.2679
1632.4655
2298.4349
3178.2638
3204.1251
3210.2901
3233.4674
3244.603
3253.1478
3278.6731

3841.2943

(Ob)

La state optimized

Atom	X	Y	Z
C	-1.323898	0.811301	-0.002843
C	-2.395510	-0.139971	-0.044819
C	-2.084238	-1.474357	-0.043812
C	-0.717540	-1.873732	-0.002791
C	0.356168	-0.952170	0.011867
C	1.707939	-1.357362	0.068706
C	2.745939	-0.380880	0.056890
C	2.450332	0.958346	-0.044175
C	1.089158	1.394741	-0.128778
C	0.050532	0.444754	-0.049832
O	-1.685158	2.089131	0.125361
H	-0.891385	2.610338	0.335287
H	-3.416270	0.239406	-0.052082
H	-2.868106	-2.230146	-0.068292
H	-0.479867	-2.939401	-0.005966
H	1.944849	-2.418455	0.140000
H	3.784585	-0.706306	0.123619
H	3.249489	1.699304	-0.068980
H	0.884678	2.448195	-0.328960

Absolute energy

-460.815776624

Normal-mode frequencies

104.6079

158.0181

208.7514

280.4789

321.5988

418.7579

449.6845

458.3018
490.4235
513.2872
521.1305
540.603
615.689
647.7724
688.6497
704.2423
718.0147
764.2495
786.1867
796.2327
861.4998
882.3024
940.7853
951.1361
1027.7649
1055.7399
1079.8931
1082.128
1152.1957
1165.2251
1220.5869
1246.7284
1267.599
1346.1969
1416.0697
1432.4804
1448.8339
1461.0927
1487.8905
1498.9564
1525.8212
1617.0718
1664.6125

3193.9297
3206.8734
3208.6721
3225.32
3233.1145
3235.3842
3251.1553
3740.4374

(Ia)
Ground state optimized

Atom	X	Y	Z
C	-0.586045	0.257208	-0.558915
C	-0.35194	1.608991	-0.494577
C	-1.377248	2.493481	-0.10132
C	-2.620455	2.032247	0.220252
C	-2.895801	0.643719	0.158835
C	-4.170637	0.11845	0.479883
C	-4.414956	-1.224276	0.41481
C	-3.393866	-2.115896	0.023689
C	-2.150984	-1.642408	-0.292782
C	-1.875443	-0.257648	-0.23272
O	0.353803	-0.635259	-0.921701
H	1.238895	-0.196444	-1.027019
H	0.624591	1.9911	-0.761644
H	-1.165008	3.553603	-0.059491
H	-3.406658	2.711995	0.520609
H	-4.952004	0.80577	0.779198
H	-5.394989	-1.609092	0.663167
H	-3.599171	-3.176611	-0.024843
H	-1.359419	-2.312173	-0.596352
N	2.950844	0.289804	-1.084669
C	3.645265	-0.994938	-0.915655
C	3.262502	-1.618026	0.420801
C	3.56546	-0.658014	1.568985
C	2.902812	0.695533	1.321792

C	3.321528	1.245065	-0.034251
H	3.173606	0.677092	-1.993741
H	3.359137	-1.648431	-1.739518
H	4.734818	-0.856133	-0.954786
H	2.195773	-1.849808	0.40856
H	3.803778	-2.555875	0.548404
H	3.229879	-1.080208	2.516011
H	4.648293	-0.51687	1.646896
H	1.814752	0.586065	1.336991
H	3.171955	1.407182	2.10263
H	2.828365	2.195623	-0.236906
H	4.405921	1.425727	-0.034852

Absolute energy
-712.980899262

Normal-mode frequencies
15.554
21.6773
56.1229
74.8021
98.9566
133.2574
148.6502
178.0276
265.4616
270.1425
276.2083
324.0721
422.5917
432.8005
442.1468
455.138
480.8279
483.6703
490.7816

547.0259
566.1659
591.5708
596.6369
664.9372
737.9199
755.4474
800.9614
803.5051
808.8804
825.5956
828.6017
838.0707
885.6508
887.6605
897.266
899.1152
909.0505
915.8846
983.1351
989.6081
994.5725
1004.3196
1025.7654
1050.3428
1062.2476
1077.0352
1078.3373
1078.4296
1115.8984
1150.0868
1166.3646
1176.2461
1179.6267
1181.9666
1190.9275

1197.4039
1236.2781
1274.6873
1299.9354
1301.1155
1320.4608
1325.2362
1348.9537
1354.2125
1369.709
1388.2386
1394.4708
1420.742
1427.0594
1441.301
1456.0916
1476.7162
1488.5228
1492.3624
1500.8952
1502.4605
1506.7291
1520.2999
1533.8893
1583.0482
1655.0757
1673.7736
1709.1118
2989.2219
2992.3006
3042.7082
3061.4701
3073.1955
3106.5889
3107.375
3110.0553

3114.2114
3120.896
3171.0946
3193.0852
3197.3177
3206.251
3211.2376
3219.3287
3221.5675
3235.7546
3549.4402

(Ia)
Lb state optimized

Atom	X	Y	Z
C	-0.566865	0.243332	-0.530551
C	-0.312371	1.632766	-0.468706
C	-1.345007	2.535239	-0.099704
C	-2.62241	2.045398	0.207986
C	-2.918007	0.665716	0.155502
C	-4.194897	0.138485	0.461067
C	-4.454019	-1.228413	0.398322
C	-3.422845	-2.139807	0.020003
C	-2.147642	-1.658287	-0.287099
C	-1.856585	-0.285706	-0.233373
O	0.387885	-0.621634	-0.872166
H	1.2751	-0.156346	-0.993233
H	0.67784	1.997672	-0.742577
H	-1.142068	3.604359	-0.060709
H	-3.415626	2.73962	0.493264
H	-4.988296	0.830901	0.751667
H	-5.449139	-1.60277	0.638428
H	-3.630909	-3.207891	-0.030229
H	-1.352571	-2.345285	-0.578054
N	2.918741	0.312398	-1.07709
C	3.621472	-0.976286	-0.950593

C	3.255424	-1.632785	0.377665
C	3.580038	-0.702275	1.547142
C	2.921926	0.662939	1.341623
C	3.319032	1.242887	-0.010961
H	3.138026	0.724399	-1.984695
H	3.32295	-1.614486	-1.794441
H	4.719009	-0.830105	-1.004524
H	2.177378	-1.85844	0.372912
H	3.795356	-2.586206	0.473491
H	3.251884	-1.149533	2.496384
H	4.674423	-0.569088	1.615483
H	1.823712	0.560343	1.369792
H	3.207999	1.361911	2.140985
H	2.823812	2.209466	-0.182643
H	4.413384	1.418549	-0.034289

Absolute energy
-712.626733001

Normal-mode frequencies
16.978
24.821
59.387
80.602
103.835
119.28
139.154
166.861
228.139
264.694
278.594
320.728
365.63
385.305
423.585
441.52

452.38
467.978
472.753
490.561
540.794
558.462
573.04
576.925
642.213
685.271
709.843
717.615
767.852
785.378
797.814
818.784
818.854
843.659
883.174
892.641
902.013
917.165
923.25
931.445
934.336
972.114
1008.143
1047.509
1054.088
1062.622
1078.16
1082.719
1090.796
1154.509
1155.674
1156.229

1162.872
1168.768
1173.429
1188.11
1241.046
1267.659
1290.036
1290.609
1314.115
1318.71
1335.456
1359.155
1380.693
1387.045
1395.107
1420.555
1430.139
1448.509
1454.636
1457.279
1464.03
1470.492
1476.415
1481.928
1487.467
1521.179
1539.496
1570.401
1610.792
1623.797
2641.18
2948.322
2996.8
3004.717
3043.956
3061.062

3075.103
3109.76
3111.052
3114.888
3121.572
3129.021
3198.4
3204.041
3222.304
3228.245
3240.618
3241.929
3313.951
3528.397

(Ia)

La state optimized

Atom	X	Y	Z
C	-0.580992	0.396993	-0.52805
C	-0.419912	1.826211	-0.404415
C	-1.490732	2.584938	-0.008562
C	-2.73448	1.953314	0.27394
C	-2.931336	0.557021	0.152082
C	-4.167038	-0.060898	0.434888
C	-4.310161	-1.474441	0.302547
C	-3.241792	-2.243979	-0.097662
C	-1.97648	-1.64619	-0.386533
C	-1.823909	-0.252672	-0.264607
O	0.444149	-0.356433	-0.890225
H	1.31799	0.175413	-0.905563
H	0.540153	2.271908	-0.665299
H	-1.402244	3.667183	0.083535
H	-3.578196	2.56888	0.592647
H	-5.006977	0.553459	0.759688
H	-5.271774	-1.939637	0.521376
H	-3.352488	-3.324561	-0.1995

H	-1.131726	-2.252483	-0.705106
N	2.825156	0.80469	-0.706654
C	3.784021	-0.237152	-1.116827
C	3.528591	-1.512784	-0.320315
C	3.629536	-1.235841	1.180295
C	2.691243	-0.093577	1.571487
C	2.96981	1.141702	0.721234
H	2.987113	1.642793	-1.266975
H	3.657081	-0.415204	-2.193867
H	4.824051	0.105104	-0.947612
H	2.519727	-1.886377	-0.559411
H	4.249851	-2.283762	-0.628058
H	3.39256	-2.142167	1.755473
H	4.668601	-0.957333	1.430826
H	1.646147	-0.406091	1.414574
H	2.803994	0.163847	2.634433
H	2.257585	1.945052	0.960089
H	3.991056	1.516745	0.930118

Absolute energy
-712.637105985

Normal-mode frequencies
14.956
18.4181
50.4211
89.174
105.0548
132.0374
147.8546
171.0016
210.796
263.8279
274.3657
322.8326
332.514

419.4925
441.3363
447.6297
451.0378
453.4038
473.5897
498.915
523.6211
550.0795
563.9497
604.0252
683.9467
691.0705
703.2391
717.8057
775.6807
786.3784
804.1978
816.0684
828.5238
843.8847
854.6911
863.2022
900.4774
902.1381
922.6748
928.016
947.6342
972.1334
1026.8156
1044.0701
1062.5696
1070.0555
1075.9517
1077.3244
1090.0418

1116.1674
1154.3989
1155.7634
1159.658
1171.7044
1176.2597
1192.3689
1225.4567
1251.9821
1291.3322
1292.4267
1317.6806
1325.8417
1336.2853
1358.3962
1368.5917
1383.1374
1388.5881
1418.4883
1421.1196
1433.0487
1446.3519
1448.5761
1457.9119
1464.3064
1468.7141
1474.767
1476.3891
1486.703
1492.9478
1503.2327
1573.8607
1620.2078
1662.898
2730.1925
3004.5313

3008.1508
3045.2095
3071.377
3071.9794
3108.955
3115.5354
3117.2371
3126.4587
3128.5725
3201.1528
3203.4512
3214.6484
3221.1408
3230.2388
3240.1044
3254.9579
3522.9284

(Ib)

Ground state optimized

Atom	X	Y	Z
C	-0.556887	-1.16633	-0.913248
C	-0.903781	-2.412143	-0.457683
C	-2.008086	-2.580693	0.400276
C	-2.746114	-1.508318	0.813517
C	-2.423702	-0.209021	0.355023
C	-3.166116	0.929062	0.75497
C	-2.857914	2.173663	0.284756
C	-1.794717	2.3432	-0.627774
C	-1.053655	1.266675	-1.028834
C	-1.333511	-0.029838	-0.535687
O	0.509227	-1.032526	-1.734199
H	-0.304774	-3.257217	-0.767506
H	-2.258243	-3.575331	0.74448
H	-3.583883	-1.634562	1.4865
H	-3.991141	0.790418	1.442456

H	-3.435928	3.031999	0.599321
H	-1.576701	3.32792	-1.018964
H	-0.253621	1.392914	-1.74556
H	2.361792	0.809425	-0.897647
N	3.414459	-0.181134	-0.628114
C	3.00522	-1.064447	0.542694
C	2.718436	-0.216588	1.7793
C	1.68209	0.85688	1.456357
C	2.125157	1.684086	0.258463
C	2.632808	1.374574	-1.694071
H	3.555938	-0.779722	-1.527781
H	4.366623	0.31536	-0.394358
H	2.110087	-1.625696	0.263866
H	3.797451	-1.786457	0.742837
H	2.372965	-0.84478	2.600227
H	3.644787	0.263987	2.110467
H	0.722148	0.387143	1.227176
H	1.525546	1.515832	2.310845
H	1.356566	2.408582	-0.00919
H	3.039667	2.236096	0.51833
H	1.068061	-0.257151	-1.456053

Absolute energy
-712.979639120

Normal-mode frequencies
18.592
29.647
56.578
93.723
98.046
142.337
174.989
184.366
263.139
281.228

282.831
302.254
418.847
436.873
442.926
454.629
475.444
482.189
489.053
543.993
566.384
586.752
595.414
665.71
733.775
760.163
800.624
805.035
808.711
826.028
828.758
837.68
879.103
897.983
898.365
901.212
909.762
923.647
957.514
981.661
998.391
1007.555
1024.097
1049.903
1063.123
1075.895

1077.491
1080.697
1115.787
1151.607
1166.321
1175.418
1181.605
1186.259
1195.71
1197.069
1236.37
1270.741
1297.78
1302.935
1316.583
1327.7
1349.418
1355.954
1369.265
1387.706
1392.436
1419.589
1428.494
1439.97
1468.732
1477.618
1486.259
1490.981
1493.711
1500.393
1502.867
1515.753
1517.229
1566.689
1656.06
1676.998

1708.699
2989.069
2992.324
3039.946
3068.285
3068.483
3107.362
3109.578
3111.701
3114.292
3117.272
3135.151
3193.705
3199.067
3202.4
3214.112
3217.414
3225.109
3226.047
3541.658

(Ib)

Lb state optimized

Atom	X	Y	Z
C	0.499105	1.054005	-0.957242
C	0.827789	2.391887	-0.657252
C	1.978579	2.682611	0.121075
C	2.763672	1.642897	0.636546
C	2.471399	0.287262	0.360561
C	3.242431	-0.786516	0.854808
C	3.00516	-2.102521	0.457362
C	1.987394	-2.381059	-0.50527
C	1.189776	-1.34708	-0.999258
C	1.339677	-0.023997	-0.540278
O	-0.633739	0.81818	-1.622358
H	0.151243	3.17387	-0.998991

H	2.227993	3.717732	0.351513
H	3.631704	1.87443	1.257534
H	4.056794	-0.566307	1.549012
H	3.617656	-2.911964	0.853003
H	1.848009	-3.398645	-0.870111
H	0.44272	-1.557412	-1.767046
H	-1.96353	-1.194497	-0.47131
N	-3.373023	-0.822898	-0.677476
C	-3.614867	0.582461	-0.135144
C	-3.249795	0.65212	1.348349
C	-1.814829	0.170106	1.566224
C	-1.617114	-1.216058	0.96219
C	-1.799721	-2.12444	-0.859249
H	-3.588554	-0.868453	-1.754577
H	-4.045979	-1.539285	-0.164916
H	-2.989651	1.289765	-0.70338
H	-4.667157	0.859885	-0.295139
H	-3.374726	1.676603	1.727944
H	-3.94097	0.009718	1.922763
H	-1.108477	0.875986	1.098185
H	-1.571654	0.133723	2.638215
H	-0.571876	-1.5421	1.057379
H	-2.258512	-1.944081	1.498682
H	-1.056345	-0.042302	-1.273948

Absolute energy
-712.626409840

Normal-mode frequencies
31.365
35.856
51.147
107.999
113.117
138.804
164.075

174.393
239.698
273.431
282.884
309.047
368.565
398.332
425.076
442.738
454.232
466.12
474.324
481.883
534.75
558.542
573.548
584.718
656.141
687.637
708.139
723.697
783.345
793.791
804.33
816.815
821.077
843.534
892.131
893.381
902.553
904.682
922.311
926.836
932.662
971.409
1004.254

1040.641
1056.452
1062.501
1076.813
1084.323
1098.702
1151.391
1155.473
1157.099
1161.035
1166.645
1174.414
1188.205
1242.92
1264.671
1289.636
1291.045
1315.362
1318.411
1335.789
1357.06
1382.306
1387.163
1404.492
1420.888
1426.661
1447.647
1455.254
1458.815
1459.982
1466.351
1472.201
1484.59
1485.304
1514.609
1523.884

1579.469
1591.318
1624.931
2243.159
2788.882
2993.41
2999.82
3041.166
3070.354
3074.428
3110.296
3113.26
3122.926
3123.777
3125.944
3197.433
3201.35
3206.244
3226.88
3237.665
3245.729
3256.06
3519.093

(Ib)

La state optimized

Atom	X	Y	Z
C	0.534522	1.015076	-0.956373
C	0.845401	2.401459	-0.711808
C	1.922801	2.714444	0.076055
C	2.720099	1.668279	0.612439
C	2.486777	0.297815	0.333377
C	3.299362	-0.732641	0.859931
C	3.067929	-2.085834	0.477552
C	2.067841	-2.402414	-0.413788
C	1.222919	-1.380704	-0.950935

C	1.405923	-0.040875	-0.539262
O	-0.616244	0.764288	-1.543823
H	0.169936	3.148172	-1.128062
H	2.168608	3.751932	0.300959
H	3.577693	1.925276	1.23792
H	4.105185	-0.479037	1.548181
H	3.699543	-2.87325	0.89094
H	1.914482	-3.438438	-0.719786
H	0.505228	-1.60947	-1.738156
H	-1.855142	-1.1777	-0.371927
N	-3.291519	-1.029987	-0.659215
C	-3.743936	0.374596	-0.271982
C	-3.456269	0.641184	1.20643
C	-1.978643	0.393539	1.513919
C	-1.562533	-1.003167	1.065035
C	-1.529321	-2.102211	-0.657901
H	-3.450000	-1.212666	-1.731426
H	-3.878258	-1.780577	-0.094738
H	-3.196777	1.103383	-0.892067
H	-4.815658	0.487224	-0.491656
H	-3.740251	1.669211	1.474369
H	-4.075011	-0.034123	1.823692
H	-1.360309	1.142296	0.99224
H	-1.777011	0.500503	2.589555
H	-0.485735	-1.168838	1.209938
H	-2.113959	-1.76021	1.655883
H	-1.046486	-0.124211	-1.16407

Absolute energy
-712.640072724

Normal-mode frequencies
31.141
39.082
52.581
102.007

115.716
143.138
179.008
187.196
223.834
272.024
280.772
315.276
341.023
427.666
438.671
447.888
454.929
467.2
478.656
507.102
531.772
552.684
563.434
615.804
680.731
701.685
704.85
719.017
775.739
785.971
791.153
815.351
831.179
843.386
865.361
881.243
900.517
905.785
928.125
942.973

944.551
970.85
1030.773
1057.186
1061.258
1072.6
1074.468
1078.138
1087.095
1151.173
1153.53
1158.034
1163.145
1175.273
1184.354
1189.779
1225.483
1244.992
1289.993
1290.668
1319.703
1329.876
1335.806
1355.843
1377.865
1383.139
1387.254
1416.228
1417.752
1431.4
1444.389
1451.337
1455.126
1459.488
1463.721
1471.652

1475.015
1486.529
1497.715
1510.437
1593.975
1610.458
1651.908
2231.786
3012.817
3014.272
3045.824
3067.977
3072.362
3111.94
3113.826
3123.622
3125.836
3129.94
3198.043
3201.821
3215.173
3225.96
3226.856
3232.421
3244.642
3524.728

(Ic)

Ground state optimized

Atom	X	Y	Z
C	1.678456	-1.411102	0.254426
C	2.763262	-2.109649	-0.198874
C	3.9214	-1.423732	-0.620855
C	3.97527	-0.061771	-0.584995
C	2.863379	0.683481	-0.120039
C	2.883244	2.097686	-0.070033

C	1.800603	2.798612	0.380241
C	0.639814	2.11932	0.80595
C	0.582921	0.753298	0.77567
C	1.692269	0.009338	0.309125
O	0.535487	-2.029046	0.673376
H	0.653804	-2.980397	0.603338
H	2.732047	-3.192237	-0.232499
H	4.76858	-1.994805	-0.975078
H	4.861993	0.467009	-0.908272
H	3.776949	2.613697	-0.397388
H	1.830329	3.879462	0.411609
H	-0.212254	2.683551	1.160443
H	-0.313971	0.237378	1.093114
N	-2.383681	-0.832554	0.534495
C	-2.134604	-0.630256	-0.886938
C	-2.765546	0.683688	-1.327069
C	-4.260705	0.686177	-1.012825
C	-4.503815	0.354966	0.458513
C	-3.804248	-0.946089	0.831669
H	-1.868469	-1.636671	0.866552
H	-1.056969	-0.614609	-1.051726
H	-2.553992	-1.448833	-1.495639
H	-2.272265	1.498327	-0.790439
H	-2.596159	0.839766	-2.3933
H	-4.706814	1.648051	-1.268398
H	-4.755198	-0.068505	-1.633184
H	-4.101959	1.155026	1.084725
H	-5.572374	0.276096	0.663977
H	-3.925142	-1.152867	1.89504
H	-4.276471	-1.772997	0.274863

Absolute energy
-712.967200464

Normal-mode frequencies
12.9696

28.3335
31.8038
66.1739
73.767
90.3793
154.654
179.7639
257.2468
263.4657
267.979
291.2129
350.9145
417.3082
440.7072
442.3991
454.2149
475.1276
479.8647
488.4582
534.47
562.5993
586.1117
595.9616
658.9109
732.5941
760.8505
783.5782
803.1183
804.1433
827.4481
831.4246
840.296
879.4793
888.5911
895.7065
898.7518

918.8797
923.1532
982.9699
997.6875
1015.016
1047.4407
1052.5041
1062.3493
1070.2391
1076.8611
1077.4223
1112.9648
1160.8386
1167.046
1173.7975
1174.462
1181.9099
1193.4572
1197.9907
1227.4643
1260.3217
1283.9892
1290.5016
1298.6787
1316.3066
1322.081
1352.5408
1367.0304
1382.296
1385.478
1400.923
1426.5437
1433.328
1445.2512
1474.7215
1484.9147

1486.6168
1496.2268
1502.248
1504.345
1515.7438
1516.8801
1576.4077
1657.1593
1677.2917
1713.0568
2944.4752
2949.0963
3038.802
3057.3208
3059.5641
3099.3886
3101.8952
3106.0257
3106.895
3109.6672
3187.8605
3194.5394
3204.0234
3205.0346
3214.8325
3222.5531
3223.0217
3579.2549
3878.2254

(Ic)

Lb state optimized

Atom	X	Y	Z
C	-1.64877	-1.370236	-0.200488
C	-2.77497	-2.197024	0.132334
C	-3.967688	-1.59413	0.433226

C	-4.066457	-0.17081	0.413133
C	-2.97167	0.660318	0.09029
C	-3.066287	2.065119	0.075824
C	-1.936327	2.87277	-0.257774
C	-0.738898	2.273761	-0.569387
C	-0.604953	0.848663	-0.566596
C	-1.710821	0.044808	-0.232971
O	-0.461413	-1.946333	-0.487965
H	-0.549263	-2.906011	-0.395697
H	-2.660652	-3.28298	0.133508
H	-4.842521	-2.191519	0.687902
H	-5.023187	0.296345	0.653255
H	-4.019753	2.531505	0.326481
H	-2.033098	3.95835	-0.261688
H	0.131411	2.878451	-0.827923
H	0.353886	0.395949	-0.821882
N	2.378756	-0.720044	-0.592729
C	2.278909	-0.719815	0.861937
C	2.979523	0.517644	1.414253
C	4.437081	0.556717	0.950791
C	4.521492	0.432108	-0.571547
C	3.760729	-0.803296	-1.045359
H	1.821373	-1.481224	-0.975394
H	1.213209	-0.714959	1.134285
H	2.741672	-1.627069	1.312808
H	2.446547	1.409547	1.044645
H	2.919616	0.526119	2.513063
H	4.930472	1.47894	1.292913
H	4.982847	-0.286897	1.410433
H	4.0651	1.319832	-1.039198
H	5.570233	0.380211	-0.901451
H	3.770505	-0.863136	-2.143336
H	4.276249	-1.710082	-0.655897

Absolute energy
-712.616756125

Normal-mode frequencies
12.471
22.437
32.177
70.515
81.332
88.973
130.093
166.634
203.839
258.11
263.701
283.911
312.808
374.528
414.409
436.693
438.704
445.184
451.645
462.878
486.8
506.706
536.486
554.625
591.287
678.746
698.609
711.0
728.684
783.947
787.664
794.555
819.997
846.341

847.549
858.009
873.961
891.378
905.834
921.828
928.39
961.101
973.878
1018.096
1040.048
1059.986
1071.216
1075.241
1078.328
1090.137
1160.034
1161.101
1162.527
1164.542
1167.613
1202.343
1220.938
1237.595
1267.725
1279.084
1288.14
1313.238
1331.657
1335.985
1362.352
1375.293
1382.113
1410.69
1420.532
1429.884

1442.118
1446.37
1451.857
1461.682
1466.021
1470.598
1474.027
1481.378
1483.964
1488.269
1518.504
1613.571
1661.76
2936.723
2940.774
3038.173
3057.708
3061.299
3100.584
3102.775
3107.038
3111.82
3115.032
3198.797
3206.471
3212.284
3215.69
3224.811
3234.686
3238.298
3562.299
3824.961

(Ic)

La state optimized

Atom	X	Y	Z

C	-1.648707	-1.370225	-0.200449
C	-2.774862	-2.197088	0.132318
C	-3.967629	-1.594277	0.433179
C	-4.066486	-0.170961	0.413105
C	-2.971751	0.660238	0.090284
C	-3.066457	2.065035	0.075812
C	-1.936535	2.872758	-0.25772
C	-0.739056	2.273834	-0.569302
C	-0.605023	0.848741	-0.566538
C	-1.71085	0.044817	-0.232949
O	-0.461295	-1.946228	-0.487874
H	-0.549091	-2.905921	-0.395724
H	-2.660477	-3.283037	0.133473
H	-4.842438	-2.191721	0.687808
H	-5.023249	0.296125	0.653232
H	-4.019963	2.531366	0.326422
H	-2.033379	3.958332	-0.2616
H	0.131229	2.878582	-0.827784
H	0.353885	0.396121	-0.821754
N	2.378667	-0.719818	-0.592759
C	2.278906	-0.719636	0.861926
C	2.979737	0.517687	1.414264
C	4.43728	0.556556	0.950748
C	4.521594	0.432003	-0.5716
C	3.76062	-0.80326	-1.045446
H	1.821226	-1.480976	-0.975372
H	1.213222	-0.714624	1.134331
H	2.741553	-1.626981	1.312722
H	2.446891	1.409695	1.044721
H	2.919868	0.526127	2.513077
H	4.930823	1.478692	1.292886
H	4.982938	-0.28716	1.410328
H	4.065309	1.319815	-1.03919
H	5.570307	0.379965	-0.90157
H	3.770342	-0.863028	-2.143426
H	4.276005	-1.710153	-0.656062

Absolute energy
-712.616756124

Normal-mode frequencies
12.6052
22.4286
32.0232
70.5293
81.3812
88.9464
130.0859
166.6074
203.7673
258.1215
263.7332
283.9137
312.8287
374.4635
414.4306
436.6982
438.7359
445.189
451.651
462.8818
486.7959
506.7048
536.4858
554.6236
591.2998
678.7331
698.6018
711.0049
728.701
784.0082
787.6598
794.5609

820.006
846.3364
847.5321
857.9779
874.0106
891.4406
905.8314
921.8203
928.3856
961.1074
973.9246
1018.107
1040.0518
1059.9953
1071.2466
1075.232
1078.3331
1090.1374
1160.0357
1161.1162
1162.5344
1164.5794
1167.6152
1202.3318
1220.9346
1237.5865
1267.7364
1279.0965
1288.1444
1313.2294
1331.7427
1335.918
1362.3462
1375.322
1382.1207
1410.6839

1420.5617
1429.8623
1442.126
1446.3785
1451.8583
1461.6958
1465.9944
1470.5855
1474.0332
1481.3561
1483.9753
1488.2778
1518.5084
1613.5782
1661.7669
2936.7677
2940.8282
3038.2088
3057.7143
3061.2886
3100.6269
3102.7985
3107.0473
3111.8228
3114.9986
3198.8073
3206.4668
3212.2792
3215.6845
3224.7638
3234.6928
3238.3007
3562.3619
3824.9814

(IIa)

Ground state optimized

Atom	X	Y	Z
C	1.040808	-1.737509	-1.102556
C	1.744329	-1.571331	-2.270245
C	3.029964	-0.997586	-2.2596
C	3.600612	-0.567204	-1.094303
C	2.911962	-0.733133	0.130437
C	3.459996	-0.2953	1.362747
C	2.793179	-0.489288	2.540072
C	1.546903	-1.154596	2.548976
C	0.985646	-1.576643	1.375973
C	1.634796	-1.352208	0.138734
O	-0.194331	-2.276004	-1.130118
H	-0.807636	-1.708455	-0.565395
H	1.28085	-1.881534	-3.196233
H	3.559371	-0.880217	-3.195833
H	4.578492	-0.104196	-1.089661
H	4.426585	0.192723	1.353157
H	3.226667	-0.150561	3.47134
H	1.043601	-1.337244	3.488806
H	0.039553	-2.09995	1.379141
N	-1.744997	-0.429497	0.035187
C	-2.666963	-0.185855	-1.07518
C	-3.658864	-1.337051	-1.180868
C	-4.404318	-1.528377	0.138579
C	-3.419156	-1.684141	1.295814
C	-2.444547	-0.51493	1.315825
H	-1.037376	0.31001	0.095093
H	-2.082271	-0.102588	-1.992117
H	-3.213352	0.759506	-0.935472
H	-3.106334	-2.247305	-1.428366
H	-4.359036	-1.147503	-1.995071
H	-5.067776	-2.391637	0.08106
H	-5.034921	-0.653013	0.324392
H	-2.852087	-2.611207	1.171413
H	-3.947659	-1.746311	2.24773

H	-1.700432	-0.631256	2.105039
H	-2.998693	0.414122	1.520448
N	0.443496	1.660929	0.539417
C	0.998246	2.104238	-0.737614
C	-0.098431	2.756572	-1.569879
C	-0.750721	3.903763	-0.801083
C	-1.23207	3.425822	0.567369
C	-0.088306	2.76727	1.327716
H	1.145386	1.153756	1.066387
H	1.411258	1.236833	-1.254449
H	1.816402	2.826966	-0.590753
H	-0.853815	2.00213	-1.807763
H	0.315834	3.11052	-2.51449
H	-1.576658	4.328946	-1.372351
H	-0.015943	4.702686	-0.659655
H	-2.034022	2.691979	0.437695
H	-1.636903	4.256102	1.147249
H	-0.4356	2.374832	2.284374
H	0.68328	3.524808	1.537521

Absolute energy
-964.870867075

Normal-mode frequencies
19.812
27.102
45.33
50.583
55.922
60.424
67.317
74.555
79.875
84.48
118.166
151.821

190.163
196.696
261.85
267.8
269.56
274.447
289.883
320.511
417.893
431.362
441.206
444.285
455.414
456.216
458.674
476.58
482.768
490.263
544.699
568.296
586.136
593.327
599.863
667.571
734.651
762.966
802.015
806.483
810.806
826.751
830.24
831.519
838.621
841.17
863.21
885.013

896.098
899.773
900.263
901.602
906.983
924.754
926.203
966.842
981.093
985.889
1002.093
1007.067
1011.983
1025.09
1049.143
1060.348
1062.412
1073.721
1076.809
1078.479
1080.1
1111.769
1118.308
1155.545
1158.408
1167.145
1171.152
1175.972
1180.13
1186.109
1188.348
1196.996
1200.483
1209.376
1237.427
1272.126

1288.165
1296.385
1299.273
1300.631
1320.622
1321.91
1323.875
1352.217
1353.015
1357.667
1366.3
1373.603
1382.81
1384.532
1386.468
1390.218
1419.136
1425.753
1426.886
1442.001
1476.312
1478.062
1484.323
1487.619
1488.37
1489.673
1496.897
1497.019
1500.939
1501.486
1507.526
1515.717
1518.015
1529.445
1544.721
1564.395

1652.508
1672.627
1704.982
2900.108
2963.165
2964.778
2971.946
2979.195
3040.068
3041.527
3046.95
3053.337
3056.078
3060.257
3093.098
3097.532
3100.179
3101.395
3104.388
3104.993
3107.233
3108.096
3109.395
3112.495
3194.206
3197.237
3205.471
3213.274
3218.825
3226.47
3228.969
3325.42
3551.75

(IIa)
Lb state optimized

Atom	X	Y	Z
C	0.547969	-2.110108	-0.817917
C	1.192837	-2.233246	-2.082987
C	2.543737	-1.829512	-2.242601
C	3.245305	-1.242183	-1.186872
C	2.651888	-1.055844	0.096766
C	3.30447	-0.41693	1.169436
C	2.715481	-0.307432	2.428478
C	1.435633	-0.923057	2.664924
C	0.774104	-1.560775	1.620313
C	1.302052	-1.585424	0.31901
O	-0.695452	-2.380325	-0.672699
H	-1.24811	-1.133599	0.002934
H	0.603434	-2.621673	-2.913173
H	3.034163	-1.951574	-3.208928
H	4.278599	-0.91826	-1.335447
H	4.304558	-0.007133	1.001101
H	3.243847	0.189858	3.241084
H	1.009775	-0.926485	3.669028
H	-0.179317	-2.065904	1.800765
N	-1.677274	-0.144008	0.162781
C	-2.494991	0.11131	-1.044848
C	-3.592233	-0.941366	-1.152072
C	-4.43608	-0.986504	0.123634
C	-3.545976	-1.1931	1.351682
C	-2.465815	-0.121141	1.411844
H	-0.857778	0.549148	0.229302
H	-1.814964	0.067458	-1.907165
H	-2.91353	1.129304	-0.971382
H	-3.104126	-1.915182	-1.317719
H	-4.216719	-0.725098	-2.030469
H	-5.183828	-1.789245	0.055789
H	-4.991745	-0.038423	0.233376
H	-3.057455	-2.180331	1.293143
H	-4.136876	-1.170417	2.278222
H	-1.762898	-0.275924	2.242317

H	-2.9108	0.882751	1.517196
N	0.546119	1.530715	0.336851
C	1.090491	1.727243	-1.014147
C	0.235586	2.731581	-1.780497
C	0.123569	4.051175	-1.015571
C	-0.372873	3.800406	0.409072
C	0.51754	2.778251	1.106058
H	1.147592	0.864956	0.829166
H	1.112959	0.749261	-1.52067
H	2.136293	2.091912	-0.96262
H	-0.774076	2.308815	-1.925667
H	0.662986	2.892435	-2.781019
H	-0.54105	4.751903	-1.542334
H	1.118803	4.526685	-0.968782
H	-1.406243	3.410578	0.376298
H	-0.395718	4.735337	0.988168
H	0.148309	2.54959	2.116826
H	1.539446	3.194832	1.212612

Absolute energy
-964.444095571

Normal-mode frequencies
24.63
32.981
44.436
57.255
60.903
69.029
75.511
88.955
101.055
108.404
142.414
148.533
168.533

202.616
248.245
259.46
267.071
283.924
289.184
320.142
347.434
414.69
419.231
424.326
450.343
450.952
451.793
453.994
458.292
466.99
483.454
535.648
569.346
581.647
585.619
619.396
642.235
686.155
714.105
747.841
767.977
775.118
807.296
814.047
817.516
835.856
842.038
848.859
859.516

885.573
893.25
901.77
906.464
908.683
914.754
933.272
953.047
961.956
967.907
968.495
994.464
1012.938
1046.911
1060.542
1063.053
1075.745
1076.352
1086.306
1090.023
1125.63
1137.328
1137.752
1148.286
1149.977
1155.34
1158.156
1165.032
1171.915
1197.665
1210.708
1223.65
1235.257
1248.598
1281.782
1286.28

1290.217
1306.309
1313.92
1315.817
1323.196
1333.296
1335.614
1357.227
1369.416
1376.244
1380.391
1386.169
1390.064
1393.039
1400.549
1418.966
1422.974
1443.869
1444.222
1449.653
1452.166
1455.531
1460.42
1462.503
1464.852
1466.709
1471.356
1477.136
1483.091
1484.954
1497
1515.407
1534.441
1562.998
1582.861
1598.934

1672.827
2068.714
2337.314
2583.813
2994.688
2998.552
3039.863
3048.355
3048.675
3052.71
3054.312
3057.393
3065.235
3076.908
3098.472
3101.245
3108.203
3110.921
3116.162
3120.569
3126.012
3130.051
3131.311
3136.099
3178.016
3180.844
3189.751
3213.99
3220.942
3233.569
3237.339
3522.056

(IIa)

La state optimized

Atom	X	Y	Z

C	0.77589	-2.239846	-0.591377
C	1.447411	-2.492407	-1.855245
C	2.671731	-1.918841	-2.12046
C	3.270131	-1.085046	-1.156243
C	2.682102	-0.837734	0.124311
C	3.289099	0.043607	1.066677
C	2.694394	0.187426	2.357322
C	1.534219	-0.487063	2.685184
C	0.877411	-1.325866	1.734141
C	1.464667	-1.477645	0.441513
O	-0.420266	-2.618056	-0.421174
H	-1.106316	-1.218203	0.156996
H	0.918815	-3.119229	-2.57411
H	3.174835	-2.094471	-3.071933
H	4.23274	-0.618435	-1.376407
H	4.228592	0.536516	0.820579
H	3.171865	0.832189	3.097494
H	1.115748	-0.382987	3.68898
H	0.031745	-1.953824	2.012798
N	-1.594246	-0.27586	0.142121
C	-2.376469	-0.228269	-1.113943
C	-3.402211	-1.354949	-1.126431
C	-4.297639	-1.289368	0.112407
C	-3.451513	-1.286678	1.387484
C	-2.431245	-0.156173	1.355547
H	-0.811995	0.482143	0.152823
H	-1.662499	-0.323737	-1.943699
H	-2.859571	0.761033	-1.176477
H	-2.851033	-2.309008	-1.145822
H	-3.997946	-1.292382	-2.048182
H	-4.996661	-2.137514	0.120974
H	-4.908665	-0.370119	0.077994
H	-2.909108	-2.243253	1.47431
H	-4.08191	-1.183488	2.281955
H	-1.747435	-0.185837	2.214494
H	-2.926395	0.828542	1.329154

N	0.430251	1.595887	0.219367
C	0.99431	1.897743	-1.102542
C	0.017213	2.745116	-1.910498
C	-0.353774	4.020001	-1.151008
C	-0.861517	3.678186	0.250894
C	0.157147	2.815072	0.987028
H	1.123582	1.047096	0.738846
H	1.208311	0.941482	-1.604033
H	1.957083	2.435937	-0.995268
H	-0.897017	2.156164	-2.10339
H	0.456041	2.986207	-2.889809
H	-1.104641	4.600659	-1.707158
H	0.54237	4.658152	-1.059932
H	-1.813252	3.121595	0.171613
H	-1.067678	4.591707	0.827834
H	-0.207607	2.519219	1.981931
H	1.089962	3.3945	1.137855

Absolute energy
-964.468669421

Normal-mode frequencies
24.047
31.013
43.333
52.166
55.593
68.289
79.15
83.831
107.545
111.132
144.651
153.482
185.803
191.447

223.081
253.881
260.02
282.979
291.393
305.848
347.768
416.984
420.365
450.429
451.691
452.795
455.526
458.013
472.79
486.532
531.413
542.923
556.164
567.921
577.554
611.169
644.65
662.74
699.212
723.876
766.409
781.925
812.661
813.257
816.022
836.418
840.381
849.969
857.864
876.747

880.923
902.089
906.754
909.346
912.553
937.517
949.823
958.321
961.893
967.879
1007.561
1031.708
1053.574
1060.365
1064.149
1075.703
1076.867
1078.757
1088.266
1089.87
1114.2
1132.466
1143.928
1149.025
1153.264
1154.649
1164.622
1174.352
1199.339
1213.308
1215.299
1217.178
1227.993
1282.284
1284.943
1289.902

1304.37
1314.758
1328.061
1331.379
1334.471
1336.819
1356.897
1361.476
1369.853
1374.851
1380.272
1386.547
1389.394
1394.549
1414.876
1416.082
1418.296
1443.165
1445.094
1451.731
1454.732
1458.161
1461.026
1463.815
1465.068
1467.569
1473.867
1481.68
1483.45
1485.461
1509.571
1536.059
1570.546
1595.628
1611.437
1633.002

1669.262
2363.22
2809.923
3001.552
3008.974
3037.234
3044.801
3046.107
3050.946
3062.504
3066.108
3070.19
3073.712
3102.705
3103.111
3109.668
3111.267
3114.917
3121.334
3127.626
3130.763
3136.85
3144.171
3183.939
3201.151
3206.633
3217.683
3225.769
3230.137
3234.58
3485.513

(IIb)

Ground state optimized

Atom	X	Y	Z
C	1.44508	0.334114	-0.097424

C	1.213573	0.734967	-1.391399
C	2.240698	0.666083	-2.355116
C	3.481009	0.198547	-2.031341
C	3.751965	-0.224145	-0.706514
C	5.022536	-0.717082	-0.323212
C	5.264097	-1.117322	0.960648
C	4.244679	-1.043509	1.933238
C	3.005887	-0.573053	1.596798
C	2.731955	-0.156338	0.274394
O	0.502325	0.367563	0.862208
H	-0.354521	0.767526	0.519873
H	0.232994	1.101464	-1.66734
H	2.030317	0.989668	-3.365889
H	4.267355	0.144354	-2.772356
H	5.803149	-0.770357	-1.071764
H	6.240927	-1.491144	1.236774
H	4.448443	-1.359602	2.947237
H	2.216954	-0.505221	2.331909
N	-1.960834	1.285197	0.266153
C	-2.372206	2.031551	-0.921074
C	-1.657103	3.376281	-0.962703
C	-1.922786	4.163377	0.318881
C	-1.554066	3.32823	1.542983
C	-2.283135	1.992771	1.508051
H	-2.376603	0.355163	0.292332
H	-2.134227	1.435319	-1.804155
H	-3.4588	2.200924	-0.922051
H	-0.582098	3.204426	-1.063401
H	-1.983413	3.939192	-1.837785
H	-1.366279	5.100685	0.311955
H	-2.985249	4.422447	0.36808
H	-0.477455	3.138487	1.550079
H	-1.801048	3.859463	2.462567
H	-1.980385	1.360095	2.343098
H	-3.36559	2.165387	1.591853
N	-1.860553	-1.70292	0.701112

C	-1.488314	-1.919097	-0.695508
C	-2.746139	-2.098578	-1.53529
C	-3.584531	-3.256098	-0.99629
C	-3.86812	-3.06687	0.492646
C	-2.569164	-2.850352	1.258033
H	-1.026967	-1.492899	1.238423
H	-0.908454	-1.060379	-1.037765
H	-0.849076	-2.807515	-0.811552
H	-3.332497	-1.174946	-1.496524
H	-2.475268	-2.270585	-2.577632
H	-4.51563	-3.351241	-1.555895
H	-3.030895	-4.189639	-1.137459
H	-4.506565	-2.19122	0.635557
H	-4.397474	-3.930868	0.896218
H	-2.77258	-2.658094	2.311273
H	-1.963451	-3.768198	1.197008

Absolute energy
-964.868016089

Normal-mode frequencies
10.1311
17.4461
27.9616
31.0326
39.8047
50.5223
61.5527
75.4275
83.1686
93.5272
110.7047
142.441
151.9043
183.9547
261.4325

263.4633
265.9451
273.1137
286.3514
330.6096
417.6398
424.0933
433.6807
443.3505
451.2404
455.254
456.924
482.5616
484.4244
491.9748
548.4458
567.5145
584.3919
592.984
597.069
668.9175
738.0717
756.3223
803.2723
803.7554
817.3053
825.7163
827.4283
827.951
834.4385
841.1713
847.2585
886.1297
893.1461
894.1904
898.8665

899.06
900.3537
910.5379
927.2014
929.9857
981.1441
982.8819
994.5452
1003.7008
1024.4321
1050.4029
1052.308
1061.0213
1062.8503
1075.4719
1077.6966
1078.0982
1079.1749
1106.8737
1116.1222
1156.1596
1159.4551
1166.2773
1172.3341
1175.4449
1177.291
1180.6639
1182.0272
1196.3484
1200.0438
1204.3535
1236.3743
1273.9987
1290.8336
1298.1285
1299.5476

1300.9803
1318.6309
1324.0157
1325.5224
1352.1023
1353.6241
1358.4108
1368.2484
1373.5157
1384.3282
1386.1797
1386.4776
1390.5939
1422.3368
1426.1306
1430.1693
1441.9165
1461.3585
1476.5942
1482.2703
1487.0024
1490.0241
1490.691
1497.1453
1499.0867
1501.8463
1502.6648
1506.5067
1514.6803
1518.7064
1522.678
1541.8945
1586.691
1653.8397
1673.7745
1708.2517

2943.3404
2966.9538
2975.087
2986.7012
2995.6042
3039.8833
3043.043
3046.9927
3057.0963
3058.5322
3060.0812
3085.2879
3101.3793
3101.7066
3103.3923
3105.1733
3105.7728
3106.9708
3109.3511
3110.8131
3113.7163
3192.8557
3196.7304
3206.3427
3207.7962
3219.331
3220.1002
3234.4766
3451.2158
3546.0288

(IIb)

Lb state optimized

Atom	X	Y	Z
C	-1.391763	0.399464	0.079018
C	-1.145755	0.813833	1.410669

C	-2.17778	0.75274	2.384693
C	-3.443186	0.263931	2.027799
C	-3.727405	-0.165814	0.713397
C	-4.993421	-0.665223	0.321886
C	-5.244343	-1.070131	-0.985316
C	-4.219997	-0.988029	-1.975412
C	-2.956719	-0.502342	-1.626581
C	-2.671559	-0.093018	-0.315344
O	-0.436791	0.441266	-0.846222
H	0.445396	0.822338	-0.472262
H	-0.150382	1.173739	1.673514
H	-1.980818	1.080053	3.4042
H	-4.23558	0.211147	2.777472
H	-5.783993	-0.727746	1.07321
H	-6.230276	-1.449606	-1.254187
H	-4.423422	-1.301535	-2.998515
H	-2.166861	-0.429563	-2.374858
N	1.97991	1.254824	-0.241289
C	2.41379	1.997284	0.943748
C	1.737542	3.365446	0.975025
C	2.025648	4.137988	-0.31335
C	1.638162	3.302506	-1.534336
C	2.333245	1.9466	-1.487137
H	2.369136	0.302948	-0.263648
H	2.156145	1.408458	1.83788
H	3.514255	2.130711	0.942419
H	0.648283	3.221735	1.076615
H	2.079479	3.929017	1.855633
H	1.4889	5.097755	-0.313701
H	3.103778	4.372773	-0.362965
H	0.547932	3.135558	-1.541777
H	1.899493	3.824551	-2.466457
H	2.017603	1.310631	-2.327353
H	3.430371	2.086573	-1.562428
N	1.799772	-1.66671	-0.670409
C	1.341781	-2.002207	0.679337

C	2.544767	-2.309397	1.565486
C	3.376475	-3.443056	0.963229
C	3.748867	-3.12361	-0.485553
C	2.499789	-2.78772	-1.294395
H	0.985722	-1.403651	-1.228965
H	0.768382	-1.149079	1.075542
H	0.659193	-2.878078	0.674634
H	3.167936	-1.401303	1.64847
H	2.206385	-2.568541	2.579696
H	4.278656	-3.627745	1.565221
H	2.78141	-4.373024	0.984498
H	4.426505	-2.253592	-0.508951
H	4.279561	-3.969475	-0.94758
H	2.768892	-2.506484	-2.322702
H	1.855637	-3.690964	-1.35216

Absolute energy
-964.438928067

Normal-mode frequencies
12.365
21.993
33.022
35.156
41.703
55.812
68.288
74.378
83.151
101.018
117.535
124.53
152.187
173.832
234.412
259.968

263.898
267.62
288.708
330.584
367.574
388.301
417.889
426.552
442.647
450.364
453.658
455.229
467.927
473.163
491.517
539.73
563.023
576.727
583.192
586.225
645.907
684.378
711.01
718.696
778.217
785.029
798.337
819.27
819.744
828.249
839.7
848.68
852.394
882.843
893.695
902.919

906.002
907.63
913.883
934.259
934.875
939.46
945.342
972.296
972.77
1009.485
1051.929
1059.967
1062.285
1070.174
1078.486
1079.489
1082.673
1090.211
1153.955
1155.881
1157.193
1159.303
1162.31
1164.768
1167.352
1169.078
1173.864
1193.552
1203.841
1205.653
1241.739
1265.758
1281.512
1288.207
1289.523
1290.452

1313.416
1317.64
1321.859
1334.906
1337.305
1362.199
1365.893
1378.68
1378.899
1382.477
1384.44
1401.102
1417.396
1424.255
1431.143
1444.458
1447.601
1452.248
1455.323
1457.527
1465.703
1466.62
1466.91
1470.129
1477.464
1486.197
1486.285
1489.136
1518.873
1525.172
1542.877
1575.948
1615.684
1623.788
2513.515
2595.215

2968.899
2982.805
2996.415
2998.657
3042.912
3044.72
3046.749
3057.354
3057.7
3061.12
3092.205
3096.32
3104.887
3105.366
3108.015
3111.065
3111.303
3115.115
3117.539
3120.649
3196.958
3201.812
3221.039
3226.508
3241.336
3241.861
3284.042
3390.705
3521.526

(IIb)

La state optimized

Atom	X	Y	Z
C	0.897957	-1.472144	0.066055
C	0.551293	-1.596217	1.462916
C	1.512787	-1.374792	2.41606

C	2.825334	-1.004865	2.012209
C	3.199102	-0.853299	0.653429
C	4.491004	-0.436376	0.264889
C	4.807599	-0.289078	-1.117302
C	3.854415	-0.522854	-2.081572
C	2.527705	-0.915229	-1.716159
C	2.2128	-1.098851	-0.354696
O	-0.018791	-1.674056	-0.854266
H	-0.957676	-1.410034	-0.465777
H	-0.456557	-1.926799	1.717605
H	1.284966	-1.488593	3.475553
H	3.58287	-0.826198	2.778358
H	5.237784	-0.228398	1.03108
H	5.815603	0.011601	-1.405684
H	4.104939	-0.415461	-3.137835
H	1.774399	-1.128546	-2.471938
N	-2.133248	-0.454647	-0.122539
C	-2.954724	-0.513625	1.087888
C	-3.840385	-1.754621	1.053992
C	-4.704868	-1.758033	-0.208466
C	-3.835829	-1.600869	-1.457724
C	-2.948824	-0.365783	-1.339622
H	-1.480272	0.349509	-0.095823
H	-2.286882	-0.52328	1.962135
H	-3.590869	0.391249	1.16836
H	-3.195425	-2.650039	1.061346
H	-4.466596	-1.792991	1.957375
H	-5.301794	-2.679886	-0.265807
H	-5.41861	-0.916923	-0.157206
H	-3.190165	-2.487671	-1.574511
H	-4.4589	-1.52835	-2.36109
H	-2.264351	-0.288444	-2.197553
H	-3.579084	0.546492	-1.323483
N	0.077115	1.510049	-0.571176
C	0.806389	2.033922	0.58607
C	-0.171815	2.734445	1.523411

C	-0.917248	3.849151	0.786984
C	-1.563129	3.313563	-0.492454
C	-0.528013	2.590111	-1.350407
H	0.720744	0.971028	-1.157649
H	1.305375	1.196581	1.092986
H	1.593821	2.751787	0.274415
H	-0.894957	1.98858	1.899368
H	0.365134	3.135705	2.395816
H	-1.672713	4.313052	1.438698
H	-0.19743	4.641807	0.5172
H	-2.366203	2.60106	-0.230068
H	-2.026418	4.129228	-1.067598
H	-0.999562	2.159124	-2.246467
H	0.232788	3.322116	-1.694703

Absolute energy
-964.453152493

Normal-mode frequencies
15.2507
30.3236
34.9028
40.8257
51.4872
61.2946
66.7958
70.9001
83.0971
98.6504
122.2847
127.1399
174.1298
197.6674
220.7827
264.0709
266.9565

272.5465
284.4848
323.8512
345.5559
422.3617
433.2329
444.1983
452.0991
452.7824
453.6981
454.8143
462.7622
473.7418
504.9057
525.1202
551.9539
565.9124
588.6849
615.3301
687.9561
697.5215
710.646
720.2806
781.7869
791.7326
801.4284
818.2163
819.5528
833.2147
839.4076
848.803
855.7446
861.9919
872.0007
896.7204
903.5295

906.3115
908.979
931.3696
942.3271
950.575
967.912
969.8429
975.9957
1029.6
1052.6451
1058.1537
1061.0116
1068.0428
1074.9587
1076.9287
1079.5084
1081.91
1090.9655
1154.7643
1155.924
1157.2254
1160.7747
1165.4454
1166.2534
1167.6008
1174.4907
1197.1368
1203.07
1225.5858
1248.9827
1250.9847
1276.8784
1286.5217
1287.7055
1289.6524
1311.8498

1319.4825
1332.3773
1333.5165
1335.3728
1360.2178
1365.8388
1374.3462
1374.7107
1378.5747
1380.0322
1382.8083
1414.7348
1418.8985
1420.1653
1436.5581
1443.5234
1447.2459
1450.6316
1454.5497
1460.6069
1462.5807
1463.7628
1465.4613
1468.7339
1472.2377
1483.6572
1487.0589
1491.8303
1501.4636
1505.5357
1540.4471
1597.6971
1628.438
1659.7389
2337.0741
2977.3522

2982.1053
2990.2257
2995.2099
3038.2865
3040.572
3046.0281
3048.6207
3056.2662
3057.4453
3097.7287
3103.9983
3105.4648
3105.8159
3107.1749
3110.1214
3112.2638
3117.1882
3119.3892
3132.4416
3200.0742
3201.848
3216.4285
3217.1857
3229.0899
3237.9373
3244.517
3248.7733
3483.7342

(IIc)

Ground state optimized

Atom	X	Y	Z
C	-1.734773	0.331294	-0.3677
C	-2.056637	1.638089	-0.635818
C	-3.403001	2.05648	-0.626933
C	-4.412106	1.177864	-0.358258

C	-4.112317	-0.178737	-0.081611
C	-5.124724	-1.126986	0.2017
C	-4.813592	-2.430085	0.469704
C	-3.46823	-2.855392	0.46976
C	-2.465904	-1.965703	0.200016
C	-2.763816	-0.613189	-0.082368
O	-0.468788	-0.128301	-0.363647
H	0.204344	0.606578	-0.432842
H	-1.26638	2.340599	-0.864484
H	-3.629289	3.092486	-0.841526
H	-5.444948	1.499742	-0.354217
H	-6.155981	-0.79684	0.202025
H	-5.599586	-3.141632	0.684274
H	-3.233685	-3.88889	0.685489
H	-1.430973	-2.278077	0.198716
N	1.740975	1.422027	-0.243496
C	1.868386	1.647073	1.197742
C	1.096699	2.897273	1.595339
C	1.60417	4.103996	0.808868
C	1.560011	3.824626	-0.692106
C	2.293492	2.531139	-1.020161
H	2.200046	0.54453	-0.494355
H	1.477833	0.770561	1.716285
H	2.923465	1.765101	1.487118
H	0.035879	2.735563	1.384504
H	1.194955	3.067035	2.667936
H	1.0209	4.993122	1.049412
H	2.638064	4.311666	1.102524
H	0.520929	3.735452	-1.017279
H	2.00378	4.649332	-1.250997
H	2.200196	2.292189	-2.079325
H	3.363589	2.664246	-0.801812
N	2.116333	-1.586527	-0.768468
C	1.96271	-2.078027	0.598685
C	3.284677	-1.93384	1.340081
C	4.390983	-2.684118	0.600262

C	4.458311	-2.242675	-0.860718
C	3.090579	-2.370077	-1.519917
H	1.212862	-1.578621	-1.227061
H	1.169606	-1.505543	1.079301
H	1.661653	-3.1378	0.613217
H	3.539666	-0.871495	1.400565
H	3.182591	-2.305357	2.36047
H	5.353281	-2.534538	1.090892
H	4.177664	-3.757022	0.637973
H	4.773448	-1.196996	-0.912733
H	5.192018	-2.835537	-1.408253
H	3.122624	-2.001108	-2.544949
H	2.811069	-3.434869	-1.557341

Absolute energy
-964.866051434

Normal-mode frequencies
9.2953
12.5375
22.1289
35.2952
40.3957
44.9305
55.2532
65.3618
70.5619
85.9254
114.9589
127.5985
148.8188
177.0075
260.1674
265.9753
267.8544
271.6458

284.4161
320.8561
420.6178
423.4523
432.7858
445.7021
452.5397
455.1202
456.2393
480.5764
482.7965
493.4252
546.8391
570.2814
585.1066
596.3262
600.2066
664.0695
738.8308
756.124
802.8804
803.4168
813.6
825.3895
826.1143
827.4602
837.6107
840.4937
859.6481
885.2835
890.1032
897.728
898.4571
900.502
904.4303
908.8738

924.9151
943.5418
980.6604
982.9742
994.1619
995.4203
1003.6918
1024.4863
1049.5445
1060.4114
1063.3578
1071.6269
1077.3576
1077.7843
1079.0988
1092.7287
1115.4319
1157.9927
1158.7723
1165.707
1172.5021
1175.6989
1178.4963
1180.2159
1181.8974
1195.9628
1198.074
1207.0928
1237.2436
1273.6245
1290.518
1293.1384
1298.9979
1301.9843
1319.7836
1322.9736

1325.4355
1352.1022
1352.6806
1356.1307
1367.4414
1373.4512
1382.8979
1384.6921
1386.202
1388.7772
1420.061
1426.2675
1428.7725
1438.7732
1454.2824
1475.2759
1482.4029
1485.4644
1487.3148
1488.7608
1496.8748
1497.5121
1499.9013
1502.4028
1506.9711
1515.8379
1521.2586
1526.9955
1537.0588
1580.5003
1654.6764
1672.7319
1708.0271
2961.6754
2966.1378
2976.1996

2978.5459
3042.1755
3042.5503
3051.2597
3055.0166
3057.4935
3064.5623
3076.1469
3101.4871
3102.3183
3104.706
3105.0471
3106.1909
3107.3408
3109.2117
3110.5873
3113.1391
3115.4616
3194.3412
3198.3334
3205.7182
3212.4913
3218.6718
3222.0683
3230.5514
3406.3188
3551.6068

(IIc)

Lb state optimized

Atom	X	Y	Z
C	-1.692359	0.346629	-0.281608
C	-1.96292	1.725649	-0.429572
C	-3.300499	2.20009	-0.383875
C	-4.356707	1.298745	-0.190826
C	-4.128699	-0.086871	-0.039511

C	-5.17043	-1.022534	0.158837
C	-4.911181	-2.382542	0.310955
C	-3.568625	-2.866441	0.271376
C	-2.512201	-1.973347	0.07713
C	-2.742301	-0.596988	-0.083459
O	-0.446903	-0.123487	-0.330113
H	0.253672	0.617194	-0.392759
H	-1.129689	2.405155	-0.60596
H	-3.501546	3.26369	-0.503123
H	-5.38445	1.66628	-0.156783
H	-6.199178	-0.656629	0.192528
H	-5.735946	-3.078891	0.461515
H	-3.369496	-3.930652	0.392038
H	-1.483803	-2.336102	0.048096
N	1.725905	1.355177	-0.257155
C	1.938647	1.651165	1.163728
C	1.251103	2.961235	1.532132
C	1.771194	4.100139	0.653734
C	1.631384	3.745255	-0.827701
C	2.282847	2.398035	-1.122727
H	2.157397	0.444741	-0.47937
H	1.5289	0.816603	1.752329
H	3.021589	1.726184	1.394339
H	0.164263	2.8399	1.385548
H	1.415853	3.182329	2.596912
H	1.241388	5.037502	0.878229
H	2.837906	4.272605	0.882369
H	0.563965	3.696147	-1.099528
H	2.087893	4.521627	-1.459542
H	2.118542	2.105228	-2.169464
H	3.377827	2.487127	-0.968367
N	2.054841	-1.602809	-0.72426
C	1.871118	-2.132984	0.627547
C	3.183302	-2.025717	1.397713
C	4.29715	-2.767682	0.656307
C	4.393396	-2.286727	-0.792864

C	3.033472	-2.382169	-1.478583
H	1.150941	-1.597867	-1.198682
H	1.067879	-1.559209	1.1118
H	1.552552	-3.197633	0.60647
H	3.451704	-0.959175	1.494448
H	3.057008	-2.426346	2.414598
H	5.260703	-2.641449	1.172013
H	4.071307	-3.848718	0.660889
H	4.721825	-1.233554	-0.810857
H	5.138055	-2.874633	-1.350078
H	3.087476	-1.986468	-2.502992
H	2.739344	-3.451304	-1.548212

Absolute energy
-964.436707895

Normal-mode frequencies
12.689
20.156
26.282
38.965
46.993
47.99
70.783
74.352
79.358
91.343
112.168
122.51
138.757
167.904
226.816
260.453
266.173
270.162
290.251

317.602
368.043
385.979
420.624
422.645
445.038
450.813
453.709
454.635
468.491
472.943
492.377
537.932
565.33
574.155
577.532
594.094
647.941
684.557
711.125
720.245
775.761
785.06
796.72
817.495
819.591
826.726
840.973
847.5
857.175
885.312
891.727
903.244
905.024
909.519
915.405

930.215
931.905
935.465
969.278
974.085
994.472
1008.037
1049.325
1054.258
1060.639
1064.799
1075.62
1078.76
1080.798
1091.27
1107.998
1153.894
1154.825
1158.447
1160.243
1161.907
1166.966
1168.073
1176.187
1180.347
1198.022
1212.051
1241.725
1266.302
1280.897
1284.41
1287.653
1290.297
1313.685
1316.393
1321.986

1335.006
1335.883
1360.936
1368.662
1376.005
1377.297
1381.406
1383.3
1398.441
1419.583
1423.044
1430.246
1443.651
1449.212
1451.319
1452.602
1459.016
1464.487
1466.414
1467.501
1468.278
1479.382
1484.242
1485.412
1489.6
1520.109
1537.507
1543.555
1568.825
1607.623
1620.808
2391.057
2751.644
2962.857
2970.851
2984.127

2988.082
3043.866
3044.827
3051.35
3052.943
3057.77
3065.44
3104.114
3105.546
3108.191
3108.289
3109.828
3112.03
3113.947
3114.728
3116.015
3118.367
3198.153
3203.872
3216.549
3227.755
3240.077
3243.536
3271.653
3333.003
3535.05

(IIc)

La state optimized

Atom	X	Y	Z
C	-1.675453	0.41463	-0.341408
C	-1.932018	1.832413	-0.396049
C	-3.217355	2.283038	-0.240147
C	-4.267473	1.346189	-0.028678
C	-4.053479	-0.052569	0.020271
C	-5.10267	-0.973229	0.231343

C	-4.82765	-2.371501	0.277644
C	-3.54101	-2.834097	0.121203
C	-2.458645	-1.924343	-0.090122
C	-2.717555	-0.542108	-0.142007
O	-0.44679	-0.042298	-0.478937
H	0.292628	0.690161	-0.485817
H	-1.095394	2.504563	-0.585876
H	-3.443788	3.34798	-0.283934
H	-5.28695	1.716866	0.097039
H	-6.119332	-0.602512	0.361977
H	-5.646535	-3.073396	0.439531
H	-3.335492	-3.904874	0.157248
H	-1.440502	-2.287467	-0.214785
N	1.728615	1.324468	-0.279591
C	1.917563	1.619129	1.146845
C	1.296689	2.967434	1.495342
C	1.889804	4.071823	0.61917
C	1.755582	3.714658	-0.862096
C	2.349695	2.337831	-1.138985
H	2.131985	0.394326	-0.483148
H	1.448469	0.809912	1.726484
H	2.996588	1.633987	1.402029
H	0.206455	2.908473	1.338166
H	1.458839	3.184554	2.56119
H	1.406126	5.036757	0.829862
H	2.960119	4.190078	0.864022
H	0.691065	3.713184	-1.150614
H	2.256262	4.46486	-1.491766
H	2.193653	2.045907	-2.187115
H	3.443312	2.37462	-0.961131
N	1.981868	-1.628908	-0.741163
C	1.692973	-2.172721	0.588337
C	2.949643	-2.105225	1.449928
C	4.096824	-2.86251	0.778298
C	4.305907	-2.363701	-0.652731
C	2.996778	-2.420314	-1.434623

H	1.113217	-1.609609	-1.27774
H	0.867599	-1.590092	1.02289
H	1.354196	-3.228953	0.527912
H	3.235248	-1.04687	1.581845
H	2.742393	-2.516006	2.44924
H	5.023892	-2.765441	1.362627
H	3.847606	-3.937907	0.75029
H	4.657535	-1.317887	-0.63123
H	5.075659	-2.959867	-1.165199
H	3.13201	-2.013649	-2.447233
H	2.685156	-3.481181	-1.539213

Absolute energy
-964.448102142

Normal-mode frequencies
a14.4049
17.3908
25.9296
40.1903
45.8639
48.6292
75.492
78.2566
84.8313
92.7237
122.6021
125.4414
149.2458
171.8622
211.1793
260.1054
266.5403
270.9807
294.2197
325.5873

329.0234
420.6698
422.8356
445.1609
450.122
450.7474
453.0142
454.3971
462.0363
473.2399
501.414
528.2326
553.1161
566.2021
591.3459
608.5559
685.023
693.7906
697.2206
721.3418
775.1724
786.4512
798.8522
815.3104
818.985
828.976
839.5327
847.6926
856.8901
859.7723
867.9411
894.053
903.2056
905.801
911.2339
924.7932

935.9443
947.7679
968.1766
973.0629
1003.5864
1030.877
1046.9274
1060.3308
1064.2956
1072.0423
1076.1975
1077.6577
1078.6492
1089.6535
1107.1468
1121.0459
1155.3394
1158.8502
1159.2013
1161.1109
1166.8667
1167.6026
1179.272
1190.3069
1197.658
1220.8914
1225.9774
1250.3879
1280.2366
1284.4852
1288.8043
1291.3412
1315.0586
1321.4113
1335.0592
1335.8963

1336.7673
1360.3686
1370.1962
1371.2121
1376.1752
1378.8268
1381.5782
1383.1995
1417.0924
1420.1158
1424.0676
1436.8975
1443.4804
1449.0084
1451.3733
1452.4561
1457.6892
1463.8907
1466.3242
1466.851
1468.0591
1473.927
1483.0503
1483.7293
1489.5102
1500.1138
1503.2379
1543.9042
1555.9919
1617.465
1663.3162
2451.2201
2973.4026
2976.2734
2994.6886
2996.38

3046.6263
3046.7727
3049.323
3051.8226
3062.1021
3062.5359
3102.1904
3104.6056
3109.1332
3111.2429
3111.5769
3112.7686
3113.7738
3114.4179
3116.5347
3120.0321
3199.8788
3205.1641
3216.0719
3222.7538
3229.2275
3240.7893
3245.9429
3291.1174
3529.4353

(IId)

Ground state optimized

Atom	X	Y	Z
C	-0.837123	-1.792628	0.137533
C	-0.591573	-1.879402	1.486804
C	-1.551903	-1.437696	2.418988
C	-2.745163	-0.913035	2.005052
C	-3.034476	-0.818783	0.620793
C	-4.246178	-0.261351	0.14293
C	-4.49095	-0.158583	-1.197201

C	-3.535818	-0.610473	-2.133955
C	-2.355946	-1.152925	-1.707215
C	-2.079446	-1.269351	-0.325162
O	0.081008	-2.154198	-0.780975
H	-0.919958	0.815219	1.166699
H	0.351254	-2.292962	1.820294
H	-1.334163	-1.517162	3.475929
H	-3.481053	-0.571272	2.720892
H	-4.977102	0.083273	0.863707
H	-5.420721	0.270141	-1.54618
H	-3.742344	-0.523388	-3.19196
H	-1.610635	-1.500805	-2.407768
N	1.290033	0.191958	0.111355
C	2.039243	-0.479511	-0.081989
C	2.969785	-0.542833	1.041824
C	4.012723	-1.622664	0.788018
C	4.743943	-1.354302	-0.526291
C	3.748378	-1.192977	-1.673621
H	2.711706	-0.130516	-1.332923
H	2.401068	-0.754148	1.948172
H	3.478547	0.423236	1.18641
H	3.507027	-2.590657	0.734734
H	4.716704	-1.663491	1.619889
H	5.450531	-2.1561	-0.742042
H	5.326998	-0.433122	-0.427412
H	3.231839	-2.140706	-1.848067
H	4.26382	-0.925924	-2.596722
H	1.956149	-0.059888	-2.116281
H	3.207618	0.849483	-1.255702
N	0.951512	-1.746523	-0.491649
C	-0.296165	1.43284	0.659148
C	0.429925	2.296439	1.584228
C	1.453282	3.119918	0.811321
C	0.767429	3.92485	-0.291655
C	-0.078178	3.012655	-1.178972
H	-1.046867	2.198529	-0.332091

H	0.923838	1.66949	2.329127
H	-0.247126	2.979317	2.121075
H	2.185921	2.440105	0.364794
H	1.992177	3.779372	1.492814
H	1.505012	4.465702	-0.885625
H	0.117079	4.675177	0.169022
H	0.573979	2.323141	-1.722674
H	-0.628195	3.596736	-1.917661
H	-1.617273	1.502189	-0.94749
H	-1.763462	2.882651	0.149591

Absolute energy
-964.868498096

Normal-mode frequencies
15.513
19.568
33.17
41.489
46.024
53.454
61.284
67.533
77.48
80.906
112.555
137.353
185.207
194.162
261.392
263.751
265.487
274.38
287.481
321.581
418.946

428.301
434.831
444.952
453.356
454.916
457.042
476.796
485.567
489.514
540.971
568.093
584.234
592.668
600.872
670.269
736.543
762.104
802.789
807.689
813.087
823.239
825.935
829.183
835.827
840.538
847.943
878.181
885.766
898.514
898.947
901.113
902.315
915.964
921.777
928.415
981.861

983.815
1001.15
1009.844
1016.791
1030.178
1048.512
1060.511
1063.018
1073.853
1075.96
1077.315
1079.155
1113.586
1116.46
1157.76
1158.014
1167.225
1172.786
1175.663
1178.1
1180.198
1186.022
1196.609
1199.345
1208.511
1236.607
1272.588
1289.51
1296.158
1299.221
1301.653
1318.437
1322.053
1325.897
1352.374
1354.444

1361.166
1367.308
1374.39
1383.623
1385.757
1386.291
1388.623
1423.7
1426.124
1427.555
1438.225
1463.409
1476.642
1481.286
1486.209
1489.049
1491.22
1495.861
1497.465
1498.952
1503.418
1504.019
1514.882
1517.168
1531.691
1546.656
1575.633
1650.358
1667.982
1704.206
2962.252
2965.6
2966.311
2970.851
3008.136
3040.907

3042.681
3049.079
3052.636
3055.843
3057.678
3084.321
3096.789
3099.69
3100.851
3104.506
3105.497
3108.173
3108.653
3108.723
3111.609
3193.088
3196.026
3206.954
3207.364
3218.977
3220.342
3235.898
3348.802
3551.512

(IId)

Lb state optimized

Atom	X	Y	Z
C	-0.797186	-1.508443	0.033736
C	-0.470914	-1.736544	1.425319
C	-1.438719	-1.559653	2.380382
C	-2.744504	-1.153446	1.983578
C	-3.120666	-0.986351	0.626966
C	-4.421448	-0.59686	0.242708
C	-4.742398	-0.434587	-1.136363
C	-3.787424	-0.648605	-2.104328

C	-2.458511	-1.031836	-1.744063
C	-2.128974	-1.195674	-0.387332
O	0.154833	-1.556766	-0.87256
H	-0.728958	0.845851	1.033708
H	0.53503	-2.080109	1.669785
H	-1.223154	-1.734176	3.434235
H	-3.504712	-0.996279	2.751795
H	-5.169729	-0.406248	1.012277
H	-5.752963	-0.137487	-1.419172
H	-4.038318	-0.527321	-3.158962
H	-1.697298	-1.206509	-2.501667
N	1.620731	0.42517	0.362528
C	2.207326	-0.37542	0.065587
C	3.092315	-0.790424	1.158059
C	3.85502	-2.047858	0.756432
C	4.645445	-1.799728	-0.529791
C	3.726539	-1.270506	-1.632165
H	2.958182	-0.042703	-1.152452
H	2.479244	-0.9612	2.054999
H	3.81128	0.017348	1.399401
H	3.131146	-2.864839	0.593465
H	4.522774	-2.358192	1.573426
H	5.151011	-2.7199	-0.856882
H	5.43501	-1.054568	-0.327757
H	2.999039	-2.049963	-1.915409
H	4.302397	-1.01853	-2.534543
H	2.237629	0.286867	-1.915336
H	3.660578	0.793123	-0.96267
N	1.070732	-1.260626	-0.425311
C	-0.059599	1.533174	0.680236
C	-0.07349	2.697499	1.568231
C	0.928641	3.736281	1.077021
C	0.601988	4.14785	-0.358942
C	0.522574	2.913261	-1.257508
H	-0.454238	1.88863	-0.688485
H	0.177602	2.362771	2.58532

H	-1.081065	3.161941	1.608512
H	1.941181	3.297801	1.114416
H	0.92269	4.609217	1.746784
H	1.348364	4.86076	-0.739987
H	-0.372775	4.666242	-0.370922
H	1.524328	2.454345	-1.328715
H	0.2178	3.189016	-2.27791
H	-0.462826	0.969285	-1.294838
H	-1.482926	2.304231	-0.716862

Absolute energy
-964.452274324

Normal-mode frequencies
19.158
26.448
28.572
42.442
46.175
55.998
67.481
72.292
89.864
96.25
115.577
124.553
173.665
193.939
214.337
257.488
266.88
268.308
281.475
326.774
345.513
414.959

434.196
442.756
449.631
451.001
453.414
458.132
460.076
473.835
501.461
524.87
552.161
557.891
589.289
611.024
688.601
697.8
716.261
719.565
780.196
791.381
811.474
816.386
819.494
828.145
839.02
848.637
856.719
860.107
866.31
896.559
904.629
906.592
908.938
923.515
942.19
949.946

969.768
970.999
986.538
1028.774
1050.43
1059.599
1062.429
1068.976
1075.775
1076.843
1085.543
1087.304
1092.379
1152.541
1153.57
1158.678
1159.879
1163.656
1165.429
1168.139
1176.762
1200.324
1206.025
1225.19
1246.272
1250.258
1281.127
1287.715
1289.345
1290.896
1315.77
1319.439
1327.896
1335.262
1337.195
1360.147

1366.649
1370.457
1378.387
1379.203
1381.799
1383.862
1414.717
1419.096
1426.722
1437.177
1442.578
1448.323
1452.028
1454.012
1455.561
1464.084
1465.741
1466.774
1469.053
1473.19
1485.649
1486.644
1487.453
1496.299
1504.937
1546.536
1601.09
1636.44
1657.212
2184.695
2979.251
2989.553
3001.608
3005.106
3044.005
3045.925

3047.853
3050.756
3053.621
3061.778
3100.889
3101.241
3105.705
3108.784
3111.485
3112.082
3113.244
3114.864
3115.861
3120.677
3199.572
3201.808
3215.06
3216.775
3228.37
3236.162
3249.479
3253.915
3514.119

(IId)

La state optimized

Atom	X	Y	Z
C	-0.796877	-1.508591	0.03436
C	-0.470657	-1.735807	1.426119
C	-1.438553	-1.558395	2.381
C	-2.744354	-1.152556	1.98388
C	-3.120442	-0.98628	0.627145
C	-4.421205	-0.597084	0.242572
C	-4.742092	-0.435681	-1.136627
C	-3.787032	-0.650257	-2.104391
C	-2.458133	-1.033205	-1.743822

C	-2.128655	-1.196198	-0.386965
O	0.155201	-1.557348	-0.871849
H	-0.729131	0.846006	1.033763
H	0.535307	-2.079093	1.670885
H	-1.223043	-1.732222	3.434982
H	-3.504622	-0.995042	2.751966
H	-5.169531	-0.406002	1.011981
H	-5.752653	-0.138807	-1.419681
H	-4.037862	-0.529626	-3.159118
H	-1.69688	-1.208338	-2.501281
N	1.620723	0.425106	0.362727
C	2.207476	-0.375391	0.065915
C	3.092968	-0.789815	1.158181
C	3.855841	-2.047176	0.756638
C	4.645719	-1.799229	-0.529961
C	3.726271	-1.270567	-1.632155
H	2.95777	-0.042827	-1.152516
H	2.480289	-0.960483	2.055412
H	3.811827	0.018209	1.399011
H	3.13211	-2.86439	0.594194
H	4.523986	-2.357093	1.57347
H	5.15139	-2.719374	-0.856969
H	5.435177	-1.053813	-0.328445
H	2.998872	-2.050298	-1.914911
H	4.301739	-1.018707	-2.534816
H	2.236824	0.286329	-1.91521
H	3.660016	0.793244	-0.963248
N	1.071058	-1.261135	-0.424605
C	-0.059916	1.53332	0.680006
C	-0.073829	2.697837	1.567761
C	0.928018	3.736691	1.076122
C	0.601002	4.147922	-0.35985
C	0.52162	2.913139	-1.258143
H	-0.454898	1.888459	-0.688704
H	0.177548	2.363371	2.584869
H	-1.081484	3.162099	1.608155

H	1.940639	3.298378	1.113387
H	0.92207	4.609752	1.745722
H	1.34718	4.860882	-0.741192
H	-0.373852	4.666148	-0.371737
H	1.523437	2.454369	-1.329455
H	0.216582	3.188619	-2.278541
H	-0.463472	0.969008	-1.294901
H	-1.483658	2.3039	-0.716941

Absolute energy
-964.452274352

Normal-mode frequencies
19.09
26.493
28.574
42.49
46.226
56.048
67.455
72.201
89.765
96.342
115.556
124.513
173.77
193.921
214.356
257.521
266.885
268.325
281.498
326.785
345.491
414.985
434.221

442.793
449.662
451.014
453.416
458.145
460.028
473.855
501.505
524.865
552.185
557.902
589.193
611.013
688.614
697.846
716.275
719.57
780.142
791.412
811.507
816.384
819.49
828.177
839.088
848.659
856.764
860.08
866.288
896.564
904.626
906.589
908.994
923.498
942.233
949.94
969.726

970.986
986.529
1028.767
1050.418
1059.556
1062.421
1068.935
1075.761
1076.858
1085.532
1087.293
1092.358
1152.537
1153.579
1158.674
1159.876
1163.649
1165.422
1168.136
1176.73
1200.286
1206.013
1225.198
1246.114
1250.259
1281.123
1287.708
1289.342
1290.89
1315.735
1319.435
1328.002
1335.234
1337.137
1360.181
1366.589

1370.511
1378.379
1379.218
1381.807
1383.867
1414.751
1419.08
1426.705
1437.183
1442.57
1448.319
1452.035
1454.07
1455.536
1464.057
1465.753
1466.775
1469.055
1473.144
1485.641
1486.635
1487.439
1496.311
1504.938
1546.48
1601.107
1636.475
1657.216
2185.062
2979.236
2989.526
3001.589
3005.024
3043.944
3046.035
3047.886

3050.769
3053.572
3061.692
3100.855
3101.185
3105.758
3108.608
3111.474
3112.051
3113.218
3114.834
3115.885
3120.681
3199.562
3201.807
3215.037
3216.762
3228.4
3236.129
3249.497
3254.237
3514.156

(IIe)

Ground state optimized

Atom	X	Y	Z
C	1.0916	-1.482454	0.545999
C	0.971889	-2.692502	-0.086613
C	2.063902	-3.245383	-0.784961
C	3.255865	-2.583062	-0.861476
C	3.420024	-1.341479	-0.202396
C	4.641916	-0.626116	-0.244829
C	4.791453	0.553035	0.428338
C	3.727017	1.072774	1.196197
C	2.53102	0.41324	1.248475
C	2.339687	-0.792841	0.534731

O	0.028325	-0.9573	1.202315
H	-0.108639	-0.003467	0.930796
H	0.021407	-3.206847	-0.044974
H	1.942241	-4.200305	-1.278562
H	4.088299	-2.997684	-1.414568
H	5.461624	-1.038168	-0.819953
H	5.73174	1.08594	0.386965
H	3.864179	1.992272	1.749437
H	1.716391	0.799737	1.845499
N	-0.81341	1.389052	0.145081
C	-0.569469	1.279807	-1.297196
C	0.780495	1.882306	-1.660364
C	0.859169	3.335002	-1.197062
C	0.535503	3.437468	0.291635
C	-0.805171	2.783081	0.593971
H	-1.717864	0.966232	0.365022
H	-0.603663	0.223828	-1.571237
H	-1.357235	1.797932	-1.864816
H	1.571317	1.300709	-1.181176
H	0.930144	1.812747	-2.738348
H	1.847458	3.747664	-1.401782
H	0.137748	3.933645	-1.762756
H	1.316121	2.933875	0.865233
H	0.511851	4.480112	0.611214
H	-1.012823	2.800674	1.663971
H	-1.600377	3.354917	0.092391
N	-2.957407	-0.673465	0.950555
C	-2.888569	-1.435629	-0.292598
C	-3.757971	-0.765551	-1.347713
C	-5.196729	-0.642708	-0.848332
C	-5.238203	0.05369	0.510852
C	-4.309387	-0.644918	1.495962
H	-2.294347	-1.055734	1.614315
H	-1.845524	-1.480724	-0.607296
H	-3.235475	-2.471689	-0.150425
H	-3.355015	0.230697	-1.553294

H	-3.71953	-1.332943	-2.278465
H	-5.811724	-0.107757	-1.572718
H	-5.623534	-1.645582	-0.74723
H	-4.911245	1.091087	0.400512
H	-6.255293	0.068333	0.904521
H	-4.292406	-0.115905	2.448628
H	-4.690959	-1.660862	1.685401

Absolute energy
-964.864835797

Normal-mode frequencies
14.046
27.318
30.103
39.878
51.448
61.764
64.092
64.852
81.778
92.536
118.917
133.25
175.172
186.791
261.213
265.694
268.553
278.543
290.586
303.681
416.255
421.541
437.051
446.262

452.659
455.823
456.412
474.565
482.216
492.183
544.182
571.948
584.636
587.246
597.241
664.922
734.815
760.519
802.603
805.536
819.347
822.369
828.983
829.666
833.259
841.113
849.666
882.307
887.921
897.928
899.742
901.522
903.505
919.124
921.557
929.867
981.392
983.846
998.879
1008.446

1014.213
1025.619
1050.215
1061.072
1064.096
1072.343
1076.384
1078.099
1080.738
1109.013
1115.897
1157.944
1158.921
1167.643
1173.938
1175.904
1179.821
1185.736
1186.184
1195.119
1197.279
1208.373
1237.804
1272.953
1291.69
1298.004
1298.714
1303.305
1314.867
1322.296
1327.491
1352.266
1355.575
1359.569
1368.034
1374.701

1383.007
1386.337
1387.655
1391.372
1421.53
1426.565
1430.036
1440.103
1473.722
1475.7
1480.521
1485.724
1486.727
1486.995
1495.733
1496.09
1496.466
1500.455
1506.39
1515.251
1516.777
1520.015
1538.397
1566.694
1655.885
1675.897
1708.106
2962.687
2965.249
2972.568
2976.34
3039.408
3041.216
3042.164
3052.073
3055.691

3070.426
3071.258
3093.412
3100.207
3101.524
3103.369
3104.359
3105.743
3108.148
3109.275
3114.789
3118.275
3193.021
3198.469
3202.063
3212.332
3216.044
3222.923
3223.847
3394.773
3554.908

(IIe)

Lb state optimized

Atom	X	Y	Z
C	-1.019977	-1.491249	-0.64919
C	-0.885926	-2.787575	-0.111303
C	-1.970587	-3.379812	0.587685
C	-3.160972	-2.666369	0.781966
C	-3.339743	-1.367544	0.25429
C	-4.523496	-0.617039	0.420295
C	-4.706539	0.612282	-0.214891
C	-3.695011	1.12163	-1.084283
C	-2.499755	0.418878	-1.254079
C	-2.252704	-0.77932	-0.558167
O	0.037134	-0.934947	-1.249005

H	0.103496	0.059532	-0.986593
H	0.069466	-3.298364	-0.226378
H	-1.863397	-4.3813	1.002748
H	-3.980482	-3.120795	1.342815
H	-5.317835	-1.028857	1.047218
H	-5.632804	1.167735	-0.072101
H	-3.861307	2.051817	-1.627969
H	-1.738224	0.797335	-1.939086
N	0.729819	1.353231	-0.213203
C	0.481148	1.216562	1.229871
C	-0.856467	1.835623	1.622067
C	-0.921804	3.298497	1.182585
C	-0.621406	3.415305	-0.311849
C	0.712612	2.756328	-0.64319
H	1.658256	0.94967	-0.415358
H	0.499415	0.14329	1.478696
H	1.29101	1.708517	1.807861
H	-1.671432	1.269568	1.144395
H	-0.989115	1.748696	2.710712
H	-1.910138	3.724151	1.410522
H	-0.177535	3.88637	1.749513
H	-1.423287	2.916974	-0.879541
H	-0.59656	4.469407	-0.626679
H	0.908816	2.788177	-1.724869
H	1.525316	3.321006	-0.141464
N	2.934931	-0.584213	-0.916015
C	2.883642	-1.463985	0.251412
C	3.694436	-0.850928	1.388254
C	5.136192	-0.60263	0.940344
C	5.165431	0.219543	-0.34957
C	4.297673	-0.436504	-1.419733
H	2.318488	-0.964737	-1.634841
H	1.82835	-1.594415	0.534299
H	3.292561	-2.471545	0.019894
H	3.22786	0.106103	1.678944
H	3.666969	-1.510448	2.268561

H	5.710244	-0.100981	1.733548
H	5.626744	-1.574973	0.756816
H	4.771928	1.230962	-0.151113
H	6.196389	0.331681	-0.717278
H	4.273564	0.179561	-2.330113
H	4.742442	-1.417839	-1.69168

Absolute energy
-964.436490227

Normal-mode frequencies
14.046
27.318
30.103
39.878
51.448
61.764
64.092
64.852
81.778
92.536
118.917
133.25
175.172
186.791
261.213
265.694
268.553
278.543
290.586
303.681
416.255
421.541
437.051
446.262
452.659

455.823
456.412
474.565
482.216
492.183
544.182
571.948
584.636
587.246
597.241
664.922
734.815
760.519
802.603
805.536
819.347
822.369
828.983
829.666
833.259
841.113
849.666
882.307
887.921
897.928
899.742
901.522
903.505
919.124
921.557
929.867
981.392
983.846
998.879
1008.446
1014.213

1025.619
1050.215
1061.072
1064.096
1072.343
1076.384
1078.099
1080.738
1109.013
1115.897
1157.944
1158.921
1167.643
1173.938
1175.904
1179.821
1185.736
1186.184
1195.119
1197.279
1208.373
1237.804
1272.953
1291.69
1298.004
1298.714
1303.305
1314.867
1322.296
1327.491
1352.266
1355.575
1359.569
1368.034
1374.701
1383.007

1386.337
1387.655
1391.372
1421.53
1426.565
1430.036
1440.103
1473.722
1475.7
1480.521
1485.724
1486.727
1486.995
1495.733
1496.09
1496.466
1500.455
1506.39
1515.251
1516.777
1520.015
1538.397
1566.694
1655.885
1675.897
1708.106
2962.687
2965.249
2972.568
2976.34
3039.408
3041.216
3042.164
3052.073
3055.691
3070.426

3071.258
3093.412
3100.207
3101.524
3103.369
3104.359
3105.743
3108.148
3109.275
3114.789
3118.275
3193.021
3198.469
3202.063
3212.332
3216.044
3222.923
3223.847
3394.773
3554.908

(IIe)

La state optimized

Atom	X	Y	Z
C	-0.972276	-1.470813	-0.767917
C	-0.737872	-2.804632	-0.272075
C	-1.692482	-3.402608	0.511108
C	-2.8953	-2.702127	0.801217
C	-3.192618	-1.425403	0.262566
C	-4.393188	-0.733608	0.544385
C	-4.654765	0.521446	-0.07721
C	-3.764399	1.059931	-0.979597
C	-2.54338	0.37816	-1.283745
C	-2.23922	-0.825655	-0.61924
O	0.037814	-0.840527	-1.329754
H	0.090461	0.191932	-0.985162

H	0.214903	-3.2765	-0.513173
H	-1.537199	-4.401887	0.917084
H	-3.64589	-3.180675	1.433972
H	-5.109796	-1.167512	1.241573
H	-5.578316	1.05144	0.159979
H	-3.98409	2.011503	-1.46703
H	-1.85666	0.764701	-2.0363
N	0.657336	1.330225	-0.219387
C	0.374451	1.177071	1.219957
C	-0.988887	1.750063	1.592867
C	-1.099668	3.209536	1.151378
C	-0.787122	3.336932	-0.33953
C	0.574406	2.732328	-0.658657
H	1.615711	0.981266	-0.391615
H	0.425898	0.103209	1.461313
H	1.160744	1.691068	1.808624
H	-1.782762	1.159061	1.111579
H	-1.124782	1.660608	2.680855
H	-2.107357	3.594918	1.36397
H	-0.386447	3.826161	1.728042
H	-1.561172	2.809133	-0.916084
H	-0.794713	4.391358	-0.65391
H	0.778029	2.763601	-1.738773
H	1.36277	3.324643	-0.152996
N	2.944873	-0.464536	-0.900092
C	2.890056	-1.393415	0.229064
C	3.667077	-0.814029	1.406395
C	5.111361	-0.518736	0.997576
C	5.147369	0.359896	-0.254183
C	4.314577	-0.265862	-1.368975
H	2.353037	-0.828578	-1.648006
H	1.832835	-1.554308	0.48767
H	3.321371	-2.38276	-0.036655
H	3.175835	0.120372	1.728579
H	3.636004	-1.5112	2.256933
H	5.660084	-0.041621	1.822994

H	5.624701	-1.472348	0.781427
H	4.729691	1.353687	-0.019683
H	6.182244	0.508674	-0.596655
H	4.293876	0.388683	-2.252037
H	4.784308	-1.22508	-1.674427

Absolute energy
-964.449031648

Normal-mode frequencies
17.092
28.425
32.589
42.53
56.914
65.566
68.333
79.534
96.575
106.339
128.29
133.609
177.502
180.207
222.259
258.569
265.551
270.878
299.904
311.014
334.881
412.943
420.896
437.42
445.163
447.069

449.507
453.042
465.023
479.502
504.325
534.549
547.517
566.394
579.309
614.176
685.817
698.513
706.531
716.583
781.295
785.906
793.346
807.224
819.714
822.119
831.14
847.952
856.175
865.319
876.84
894.422
898.486
903.334
906.175
936.548
938.041
942.495
966.753
972.73
990.74
1029.37

1051.983
1055.765
1061.773
1071.576
1075.44
1077.792
1078.868
1084.798
1095.039
1149.087
1152.659
1157.304
1159.228
1162.73
1166.976
1167.149
1178.895
1196.285
1204.85
1225.485
1243.92
1260.774
1280.335
1286.386
1294.29
1297.549
1312.388
1328.156
1334.353
1335.293
1338.923
1359.929
1368.934
1372.748
1375.815
1381.184

1382.826
1389.389
1413.827
1418.304
1422.684
1433.703
1440.509
1443.299
1444.559
1451.971
1453.881
1461.096
1462.938
1464.332
1465.377
1466.184
1481.139
1482.978
1487.523
1494.884
1505.518
1541.45
1603.918
1604.768
1643.731
1863.505
2963.459
2970.054
2996.664
3000.003
3035.311
3044.51
3053.479
3055.594
3078.715
3081.104

3092.87
3105.902
3106.473
3107.651
3109.852
3112.721
3113.963
3116.296
3134.289
3137.497
3196.107
3202.479
3212.402
3221.993
3224.252
3230.33
3239.622
3286.47
3530.794

(IIf)
Ground state optimized

Atom	X	Y	Z
C	1.700176	0.322829	-0.408499
C	2.170781	1.551373	-0.794493
C	3.558464	1.802089	-0.82851
C	4.455871	0.833709	-0.484758
C	3.99852	-0.447286	-0.08703
C	4.893326	-1.482826	0.27419
C	4.430085	-2.710421	0.655322
C	3.043452	-2.96753	0.696532
C	2.150277	-1.990525	0.354363
C	2.60781	-0.713419	-0.044456
O	0.3872	0.019488	-0.35568
H	-0.206482	0.799254	-0.506014
H	1.468666	2.321892	-1.084897

H	3.905701	2.779229	-1.136599
H	5.520123	1.026029	-0.51325
H	5.956774	-1.281689	0.241812
H	5.127092	-3.491437	0.927984
H	2.688539	-3.942564	1.001097
H	1.08587	-2.179958	0.385213
N	-1.74621	1.693464	-0.277977
C	-2.188232	2.901622	-0.98102
C	-1.247894	4.057566	-0.671143
C	-1.148057	4.283542	0.835792
C	-0.774441	2.986214	1.549502
C	-1.748398	1.877745	1.178218
H	-2.360726	0.920646	-0.51516
H	-2.204534	2.692165	-2.05
H	-3.208028	3.177504	-0.676807
H	-0.258918	3.826867	-1.073429
H	-1.60005	4.958238	-1.174817
H	-0.421965	5.065823	1.056964
H	-2.116113	4.631439	1.209719
H	0.234327	2.678403	1.259402
H	-0.773658	3.126386	2.630552
H	-1.455367	0.936251	1.643605
H	-2.754204	2.133065	1.540876
N	-1.982731	-1.718319	0.344795
C	-3.191192	-1.350515	1.059543
C	-4.23523	-2.449409	0.90005
C	-4.506817	-2.711858	-0.580175
C	-3.204021	-2.998423	-1.325149
C	-2.202376	-1.876613	-1.083084
H	-1.214445	-1.083929	0.518498
H	-2.949044	-1.201001	2.112149
H	-3.629736	-0.403775	0.687544
H	-3.851265	-3.358364	1.368328
H	-5.154423	-2.169532	1.416737
H	-5.209337	-3.537209	-0.700599
H	-4.979638	-1.826177	-1.017983

H	-2.771322	-3.932783	-0.960863
H	-3.388943	-3.110562	-2.394361
H	-1.245848	-2.087894	-1.559101
H	-2.600683	-0.95543	-1.550079

Absolute energy
-964.860788828

Normal-mode frequencies
14.4855
18.6487
21.2008
37.9301
42.2045
46.3318
58.7371
68.8281
73.5239
96.4927
100.1804
125.1103
149.1148
177.6437
258.2612
261.2338
268.7659
270.0473
275.5589
321.1276
411.955
419.6864
433.7797
445.867
447.2384
451.9214
455.9734

481.0331
483.8618
492.9131
545.3662
569.7925
574.2575
595.8609
596.555
663.722
737.9075
757.6421
789.7097
803.1133
804.6305
823.5711
826.3492
828.6702
830.399
840.6833
842.0631
876.4178
884.2811
892.4688
898.4966
900.3366
900.9995
903.9455
914.6549
925.8653
941.1526
981.6264
981.9349
996.4959
1009.4136
1034.3099
1050.1786

1061.3082
1062.0558
1068.8839
1077.1682
1078.4123
1078.7634
1080.4193
1115.4845
1154.6184
1165.1655
1166.3168
1169.6746
1174.386
1177.069
1179.5302
1182.5504
1196.134
1197.7504
1204.5119
1236.0851
1275.1615
1290.2349
1293.448
1301.5178
1302.4164
1319.7499
1322.6887
1325.3939
1334.7627
1352.8978
1356.5852
1365.9112
1373.7901
1383.9061
1384.6666
1386.1722

1391.0047
1408.2585
1424.5552
1428.523
1436.5858
1447.967
1475.8127
1477.9481
1485.7
1487.3717
1489.4251
1491.6513
1495.3564
1496.1975
1498.9678
1500.5155
1504.2989
1510.5154
1517.4062
1521.632
1576.4319
1655.9799
1673.0551
1707.9169
2897.1725
2904.8832
2989.4326
2991.0476
3036.2873
3043.8534
3058.6501
3061.891
3063.3441
3067.2775
3097.5087
3100.9316

3107.7267
3108.7005
3109.5992
3110.6997
3112.2655
3113.738
3116.0941
3116.8468
3193.4871
3197.7726
3205.891
3207.9911
3215.9984
3219.9684
3225.0847
3226.4991
3524.8658
3580.5739

(IIf)

Lb state optimized

Atom	X	Y	Z
C	1.639672	0.355412	-0.420157
C	2.120468	1.637625	-0.760586
C	3.516163	1.902739	-0.757215
C	4.415921	0.882161	-0.416026
C	3.971828	-0.412895	-0.0722
C	4.852831	-1.463506	0.279185
C	4.378351	-2.726744	0.625332
C	2.9776	-2.994472	0.638298
C	2.072971	-1.984437	0.295422
C	2.523223	-0.703272	-0.065608
O	0.334595	0.071682	-0.428732
H	-0.270969	0.868319	-0.548369
H	1.404924	2.404058	-1.060646
H	3.880724	2.892366	-1.027143

H	5.489212	1.083231	-0.415642
H	5.927186	-1.266456	0.276883
H	5.083786	-3.514531	0.890104
H	2.613096	-3.982846	0.914368
H	0.999261	-2.182855	0.312937
N	-1.75513	1.67949	-0.258105
C	-2.257338	2.864473	-0.965126
C	-1.345304	4.056454	-0.697341
C	-1.212767	4.30988	0.805152
C	-0.776001	3.034314	1.526606
C	-1.722884	1.886213	1.197823
H	-2.36784	0.885165	-0.460025
H	-2.298458	2.635919	-2.039164
H	-3.285468	3.11134	-0.632172
H	-0.351237	3.848663	-1.126738
H	-1.740735	4.944482	-1.211965
H	-0.502052	5.126699	0.997159
H	-2.190187	4.634693	1.203448
H	0.241956	2.752784	1.205439
H	-0.745171	3.188877	2.614752
H	-1.382433	0.952708	1.669993
H	-2.735919	2.111704	1.587718
N	-1.864018	-1.745297	0.343828
C	-3.069879	-1.437048	1.09293
C	-4.077451	-2.572463	0.930132
C	-4.376904	-2.808049	-0.551597
C	-3.080763	-3.017973	-1.337312
C	-2.118027	-1.861766	-1.083712
H	-1.124511	-1.065457	0.508846
H	-2.808486	-1.300736	2.152837
H	-3.557543	-0.489531	0.750848
H	-3.639668	-3.484573	1.366802
H	-5.000648	-2.343486	1.483698
H	-5.053673	-3.666225	-0.678846
H	-4.903327	-1.924684	-0.95666
H	-2.595321	-3.950347	-1.006629

H	-3.288315	-3.110546	-2.414002
H	-1.159297	-2.016682	-1.597401
H	-2.571863	-0.934754	-1.514646

Absolute energy
-964.429229771

Normal-mode frequencies
19.161
19.634
23.98
42.48
45.336
48.54
60.73
69.57
74.864
96.587
104.232
118.14
138.917
167.944
227.726
257.389
261.653
269.873
277.763
316.925
369.088
387.756
413.076
418.205
443.343
445.96
450.134
452.966

468.115
473.568
498.896
533.827
564.071
567.46
573.396
584.554
647.597
688.502
709.581
718.319
779.593
784.731
800.89
810.51
815.403
820.273
830.727
846.416
847.654
873.561
881.618
899.758
905.163
907.272
922.228
927.311
931.48
937.627
960.842
966.104
973.532
990.65
1011.114
1052.559

1059.999
1061.225
1071.708
1077.799
1079.181
1082.479
1092.835
1153.786
1155.97
1158.607
1159.777
1162.439
1167.988
1169.318
1170.811
1171.809
1197.371
1208.007
1238.828
1269.434
1278.649
1283.504
1288.483
1291.533
1307.611
1314.784
1320.469
1335
1337.218
1352.737
1364.917
1370.062
1373.708
1380.399
1381.777
1385.551

1417.216
1420.915
1428.877
1434.061
1442.085
1444.878
1451.962
1453.838
1458.891
1463.194
1466.298
1466.626
1477.102
1479.529
1480.878
1484.753
1493.832
1509.402
1530.952
1552.53
1601.371
1631.903
2639.525
2878.355
2887.881
2984.737
2997.055
3020.424
3034.527
3045.835
3055.786
3062.547
3063.395
3064.476
3097.453
3101.809

3108.485
3114.486
3114.878
3116.361
3117.605
3118.761
3119.205
3121.581
3195.635
3200.204
3204.272
3220.819
3240.976
3242.27
3320.013
3498.363
3577.911

(IIf)

La state optimized

Atom	X	Y	Z
C	1.614092	0.42609	-0.340147
C	2.021509	1.749837	-0.734737
C	3.360123	2.03823	-0.794988
C	4.313208	1.030173	-0.47037
C	3.944434	-0.281164	-0.088278
C	4.892698	-1.275603	0.228798
C	4.463667	-2.579559	0.617027
C	3.121841	-2.876061	0.686294
C	2.135957	-1.889443	0.370704
C	2.548302	-0.601067	-0.016783
O	0.330196	0.112574	-0.270809
H	-0.327071	0.874216	-0.440647
H	1.254045	2.478998	-0.995297
H	3.703351	3.027865	-1.095174
H	5.376148	1.275137	-0.519962

H	5.954571	-1.03444	0.176098
H	5.207696	-3.338953	0.859348
H	2.794248	-3.872627	0.984946
H	1.075075	-2.126725	0.440707
N	-1.804876	1.604607	-0.265119
C	-2.322172	2.746803	-1.032318
C	-1.501663	3.996643	-0.733505
C	-1.473966	4.283719	0.768515
C	-1.009522	3.048826	1.541447
C	-1.872842	1.844554	1.185938
H	-2.366384	0.776595	-0.482245
H	-2.278246	2.494423	-2.100792
H	-3.382268	2.937118	-0.772875
H	-0.473037	3.847981	-1.101276
H	-1.920098	4.849059	-1.288334
H	-0.824221	5.144106	0.98425
H	-2.490173	4.557352	1.10244
H	0.039504	2.819212	1.285952
H	-1.049281	3.225247	2.625787
H	-1.515028	0.940019	1.699522
H	-2.918264	2.023739	1.50615
N	-1.781698	-1.826878	0.461578
C	-3.077439	-1.536758	1.048872
C	-4.02599	-2.706235	0.796836
C	-4.133498	-2.987889	-0.703118
C	-2.745282	-3.180281	-1.316825
C	-1.850939	-1.990426	-0.981973
H	-1.08329	-1.125539	0.699129
H	-2.952085	-1.36524	2.128362
H	-3.548512	-0.614221	0.623181
H	-3.62051	-3.592917	1.310132
H	-5.016314	-2.491479	1.226245
H	-4.767508	-3.868011	-0.887664
H	-4.628312	-2.130496	-1.194889
H	-2.280272	-4.088646	-0.901221
H	-2.815242	-3.307448	-2.40757

H	-0.831192	-2.133025	-1.365409
H	-2.267989	-1.088324	-1.495968

Absolute energy
-964.439262038

Normal-mode frequencies
16.8943
19.2892
26.0982
41.9024
47.369
52.163
60.1333
74.9981
79.7548
102.383
111.2704
124.142
143.2543
165.9824
207.6681
259.0298
261.3327
270.2704
281.3443
324.2901
325.9
412.3409
417.6956
443.4296
446.5037
448.0098
450.2123
454.1473
456.8234

473.9397
497.3923
525.6888
547.9736
564.3293
577.5183
599.6004
683.7328
695.2664
718.4821
719.5032
781.3815
786.8169
797.426
813.933
820.9522
829.5232
831.836
846.8532
847.9815
856.1983
862.1987
872.2246
901.8766
906.2105
906.7969
920.5648
929.9231
939.2315
953.3919
967.6093
974.3301
1030.7728
1044.7129
1054.5033
1058.7406

1061.112
1070.6576
1077.5414
1078.0421
1079.2786
1087.1735
1091.3159
1155.22
1157.6105
1159.1982
1161.7211
1163.6726
1170.0644
1171.7434
1172.9802
1199.0061
1207.7986
1226.6995
1256.0718
1279.5298
1282.0601
1288.1358
1291.8851
1307.6708
1314.8426
1324.3001
1335.4171
1337.1175
1352.4558
1361.3743
1369.5538
1374.1937
1379.9119
1381.1986
1384.4983
1413.3486

1416.7231
1421.572
1439.1696
1441.4791
1442.5409
1446.3641
1452.3088
1454.3972
1457.9102
1461.9913
1465.9388
1466.8053
1472.5868
1477.3114
1480.0777
1481.9515
1488.7237
1492.1262
1497.3372
1516.96
1613.7657
1663.2734
2794.4073
2872.0561
2885.0963
3003.6545
3005.8881
3036.6603
3048.5907
3057.815
3061.9569
3065.3651
3068.5258
3097.1265
3105.8611
3110.8248

3115.3544
3116.3034
3118.8026
3119.5446
3120.6717
3121.9118
3123.4137
3202.859
3205.4321
3216.6469
3219.4025
3228.7864
3238.1455
3240.1017
3497.4353
3578.2184

(IIIa)
Ground state optimized

Atom	X	Y	Z
C	-1.123447	-1.468556	-0.965527
C	-0.550638	-0.926224	-2.091773
C	-1.330388	-0.178438	-2.998004
C	-2.661912	0.033042	-2.780593
C	-3.282151	-0.507892	-1.627542
C	-4.650043	-0.284987	-1.338435
C	-5.217759	-0.779045	-0.197751
C	-4.446165	-1.531632	0.713083
C	-3.124676	-1.775274	0.458057
C	-2.514749	-1.269462	-0.712649
O	-0.428256	-2.160817	-0.04729
H	0.567912	-1.96405	-0.133292
H	0.504897	-1.075876	-2.278011
H	-0.853982	0.234017	-3.878141
H	-3.25543	0.611076	-3.476295
H	-5.238368	0.294585	-2.038778

H	-6.262852	-0.594265	0.011251
H	-4.905716	-1.918699	1.612305
H	-2.522887	-2.356449	1.142693
N	2.138417	-1.48566	-0.054087
C	3.085007	-2.376978	-0.722563
C	2.981873	-3.774449	-0.124843
C	3.227252	-3.729632	1.38246
C	2.290141	-2.723819	2.049512
C	2.413788	-1.361751	1.380066
H	2.141365	-0.546375	-0.459146
H	2.852104	-2.394744	-1.788077
H	4.115268	-2.008338	-0.61282
H	1.979397	-4.164511	-0.320174
H	3.695067	-4.439459	-0.612859
H	3.099234	-4.720281	1.819275
H	4.263923	-3.430316	1.567376
H	1.256301	-3.067256	1.957583
H	2.514078	-2.634473	3.113055
H	1.698398	-0.648601	1.794642
H	3.425372	-0.962682	1.54775
N	1.674713	1.476836	-0.342412
C	1.293853	2.241915	-1.522593
C	2.483197	2.336187	-2.470397
C	3.681862	2.963142	-1.759003
C	3.988008	2.227544	-0.454735
C	2.73527	2.138068	0.407544
H	0.877163	1.298012	0.265907
H	0.450564	1.745724	-2.003198
H	0.97097	3.262001	-1.255584
H	2.741698	1.327036	-2.804781
H	2.214992	2.917592	-3.35355
H	4.556358	2.969993	-2.410661
H	3.44887	4.007569	-1.528467
H	4.329612	1.212069	-0.677262
H	4.786564	2.731303	0.09161
H	2.928698	1.566699	1.316709

H	2.438822	3.154992	0.714556
N	-0.74645	0.677144	1.473883
C	-1.621286	1.536961	0.675679
C	-1.375612	2.994154	1.045206
C	-1.592319	3.213303	2.541154
C	-0.745393	2.234033	3.351429
C	-1.017561	0.804782	2.902153
H	-0.857878	-0.289855	1.190206
H	-1.409148	1.365335	-0.382395
H	-2.683073	1.291042	0.836388
H	-0.344442	3.255536	0.78653
H	-2.032725	3.638538	0.460031
H	-1.360494	4.242621	2.817289
H	-2.64867	3.049226	2.776022
H	0.315088	2.45206	3.195826
H	-0.951348	2.335388	4.417789
H	-0.379572	0.103259	3.441451
H	-2.063748	0.548904	3.134266

Absolute energy
-1216.76167852

Normal-mode frequencies
11.0374
21.173
24.4528
34.5991
39.9823
41.7712
50.5682
52.022
60.3732
62.0258
65.7254
70.7896
84.8183

92.2165
104.9401
120.8112
130.5719
141.1562
171.1825
189.303
264.4602
267.5775
269.6874
275.9916
277.2212
280.2647
281.9071
341.7888
423.706
426.7124
429.3126
436.5563
447.1482
452.3534
455.136
457.6991
458.4024
459.7572
482.2666
487.1883
490.5295
547.1464
570.5249
582.8645
588.4503
598.505
601.6284
669.2402
737.5526

758.9193
801.8228
804.98
809.8338
827.8307
829.4727
830.4329
830.7315
837.2246
838.8277
840.9327
853.5307
863.9545
886.1215
893.1907
897.1167
898.3414
900.5725
901.3831
902.448
905.1624
912.2558
924.5104
949.9797
981.6364
983.9222
984.7939
989.1233
1000.1444
1009.1425
1028.4711
1049.844
1059.7438
1061.0368
1061.9992
1064.9882

1074.0541
1076.7021
1078.1236
1078.2793
1082.1713
1086.3176
1114.1569
1121.2105
1156.3959
1157.2671
1160.5092
1167.0673
1173.8733
1174.6186
1175.694
1177.2482
1179.4804
1185.6168
1189.7141
1198.5606
1202.002
1206.0389
1214.7479
1237.4561
1273.6519
1288.7137
1292.5461
1298.2113
1299.155
1300.4519
1301.8438
1319.8948
1321.7752
1324.1033
1327.0528
1351.8152

1352.9873
1354.4257
1361.7086
1368.9992
1369.5047
1374.1625
1382.9105
1384.5469
1384.8382
1385.8743
1387.1615
1389.9727
1423.7643
1425.2365
1426.8943
1428.0863
1442.9989
1467.2497
1477.6651
1478.2283
1484.6957
1486.0486
1486.806
1489.847
1494.9951
1495.9657
1497.0982
1498.1548
1499.3709
1501.8416
1506.8101
1508.7264
1514.0191
1515.4275
1518.4894
1527.0466

1533.3947
1550.3547
1596.5314
1651.0054
1671.766
1705.8449
2725.507
2951.1692
2954.0972
2964.8424
2970.1899
2981.4083
2987.8362
3040.6401
3041.167
3041.4136
3046.4079
3047.9562
3050.1784
3052.3769
3058.4342
3059.991
3088.3984
3089.7448
3092.5454
3094.7949
3095.0897
3100.3212
3100.4177
3102.7365
3105.0299
3105.0854
3105.7219
3107.6954
3110.1698
3110.2101

3112.8983
3192.7429
3193.8393
3206.3482
3208.1586
3217.1258
3218.7605
3230.168
3370.7484
3443.7727
3551.6917

(IIIa)
Lb state optimized

Atom	X	Y	Z
C	-1.061977	1.601066	0.889671
C	-0.465631	1.242911	2.139625
C	-1.233806	0.605214	3.148001
C	-2.571835	0.262831	2.906006
C	-3.209372	0.567217	1.67813
C	-4.532663	0.172432	1.381356
C	-5.122629	0.454888	0.155156
C	-4.379603	1.168838	-0.841712
C	-3.076254	1.57842	-0.579792
C	-2.451786	1.295541	0.647625
O	-0.354628	2.138018	-0.053182
H	0.953291	1.705494	-0.034665
H	0.56761	1.54217	2.327357
H	-0.7819	0.375601	4.113396
H	-3.146567	-0.251517	3.680124
H	-5.095304	-0.372572	2.144134
H	-6.146646	0.141507	-0.046154
H	-4.844487	1.40727	-1.798725
H	-2.506528	2.129445	-1.331204
N	2.028069	1.333127	-0.186803
C	2.954904	2.246296	0.506394

C	2.74811	3.662843	-0.018632
C	2.946993	3.709376	-1.535471
C	2.032801	2.695748	-2.228
C	2.244705	1.301659	-1.649795
H	2.06693	0.337364	0.171163
H	2.751918	2.18195	1.584497
H	3.989797	1.905076	0.33178
H	1.719384	3.972352	0.228694
H	3.4382	4.34895	0.492545
H	2.749574	4.722295	-1.914006
H	4.000258	3.476792	-1.773049
H	0.979056	2.976963	-2.070364
H	2.217256	2.674188	-3.311615
H	1.533257	0.569859	-2.059622
H	3.270269	0.942604	-1.846089
N	1.777372	-1.423165	0.254637
C	1.374599	-1.912317	1.575534
C	2.579248	-1.904928	2.511081
C	3.720705	-2.740273	1.92783
C	4.048208	-2.290729	0.502267
C	2.786825	-2.286733	-0.356257
H	0.959132	-1.344538	-0.367693
H	0.576993	-1.259832	1.9595
H	0.969185	-2.944359	1.509583
H	2.914346	-0.860801	2.644182
H	2.287365	-2.281989	3.50235
H	4.613962	-2.682583	2.567485
H	3.412235	-3.800264	1.904772
H	4.462555	-1.267173	0.524527
H	4.810864	-2.943621	0.052159
H	3.001678	-1.91525	-1.370168
H	2.413669	-3.327934	-0.458819
N	-0.709141	-0.731081	-1.386407
C	-1.558506	-1.549233	-0.509739
C	-1.328875	-3.026462	-0.814522
C	-1.620849	-3.321245	-2.28683

C	-0.822278	-2.378752	-3.188901
C	-1.069977	-0.927312	-2.790623
H	-0.852589	0.252845	-1.146189
H	-1.307369	-1.315334	0.537213
H	-2.631917	-1.300309	-0.643083
H	-0.276664	-3.28259	-0.591836
H	-1.960761	-3.644425	-0.159448
H	-1.398662	-4.371757	-2.527857
H	-2.698004	-3.168631	-2.474324
H	0.255738	-2.593421	-3.083344
H	-1.087848	-2.531091	-4.245915
H	-0.465371	-0.24709	-3.410808
H	-2.137327	-0.675743	-2.965438

Absolute energy
-1216.25672515

Normal-mode frequencies
18.108
18.859
30.929
35.277
40.073
48.417
51.89
61.663
66.812
69.763
75.174
79.759
87.393
101.315
114.591
123.45
133.102
145.323

172.818
190.829
230.998
262.359
264.423
275.671
278.248
280.774
291.808
348.572
354.957
401.655
415.635
426.752
427.663
447.102
450.625
454.603
455.43
456.587
459.373
465.864
473.052
479.571
540.583
569.835
572.358
578.596
587.629
589.345
640.943
690.666
712.867
731.764
760.012
778.992

794.49
818.083
819.156
820.967
833.633
841.196
842.557
849.108
854.938
861.128
883.559
890.327
897.698
903.408
905.289
907.353
910.432
918.124
935.752
940.417
957.451
969.149
970.134
971.839
983.235
1004.141
1014.943
1050.154
1055.49
1060.518
1063.982
1076.201
1076.776
1077.965
1082.255
1088.745

1091.342
1113.68
1137.758
1142.553
1144.395
1153.384
1156.187
1157.219
1161.791
1165.552
1167.801
1168.831
1171.473
1183.533
1200.058
1205.747
1207.953
1223.431
1241.454
1255.753
1278.681
1280.511
1286.615
1289.616
1290.956
1308.342
1311.185
1316.618
1326.427
1333.396
1334.906
1335.65
1359.746
1363.499
1369.407
1375.431

1376.926
1378.681
1379.795
1380.848
1386.981
1391.007
1405.315
1417.823
1420.134
1432.025
1444.087
1444.591
1448.212
1450.642
1451.237
1451.472
1458.278
1459.068
1463.772
1464.537
1466.1
1466.595
1467.873
1474.013
1482.669
1484.618
1488.901
1503.681
1511.999
1527.599
1530.113
1541.17
1556.553
1579.962
1597.505
1651.327

1742.572
2178.58
2841.96
2972.795
2973.975
2975.545
2993.897
3036.722
3042.13
3043.291
3043.939
3046.353
3047.37
3048.106
3048.658
3054.08
3069.686
3072.602
3083.744
3092.262
3098.118
3105.326
3106.605
3108.4
3110.521
3112.057
3112.851
3118.839
3119.586
3123.045
3126.574
3129.531
3131.366
3184.04
3192.049
3199.496

3204.58
3223.035
3231.893
3237.128
3335.102
3517.795

(IIIa)
La state optimized

Atom	X	Y	Z
C	-1.179969	1.610378	0.992037
C	-0.68315	1.32889	2.327978
C	-1.469713	0.656127	3.233779
C	-2.765678	0.239573	2.846354
C	-3.309642	0.494635	1.556953
C	-4.582177	0.004082	1.169252
C	-5.065129	0.26759	-0.143499
C	-4.308813	0.989572	-1.042107
C	-3.017679	1.483983	-0.679212
C	-2.525837	1.226287	0.620868
O	-0.400166	2.134707	0.119955
H	1.010926	1.657544	0.023105
H	0.316026	1.692172	2.580512
H	-1.111624	0.449033	4.24276
H	-3.383882	-0.302641	3.565527
H	-5.174632	-0.572848	1.87911
H	-6.047182	-0.107141	-0.437502
H	-4.697537	1.193117	-2.041822
H	-2.423051	2.083531	-1.365666
N	2.02771	1.369904	-0.264243
C	2.972864	2.299172	0.388225
C	2.640035	3.729164	-0.023444
C	2.675139	3.874147	-1.546382
C	1.735709	2.858951	-2.201075
C	2.072643	1.445447	-1.74448
H	2.164105	0.34589	0.018825

H	2.88663	2.158262	1.474556
H	3.996662	2.023431	0.085485
H	1.628028	3.965123	0.344406
H	3.345045	4.420982	0.458754
H	2.392731	4.89601	-1.835872
H	3.706286	3.710642	-1.906749
H	0.694428	3.073444	-1.912376
H	1.800447	2.910061	-3.297182
H	1.352264	0.704008	-2.11805
H	3.084653	1.149576	-2.069072
N	1.932626	-1.351075	0.169093
C	1.589783	-1.706985	1.549806
C	2.844724	-1.68763	2.416864
C	3.909307	-2.625498	1.84507
C	4.181	-2.299181	0.375369
C	2.87826	-2.300789	-0.418375
H	1.072554	-1.304953	-0.405691
H	0.844001	-0.987024	1.921324
H	1.127751	-2.715189	1.594325
H	3.241093	-0.656897	2.446871
H	2.590344	-1.967612	3.449665
H	4.836804	-2.567833	2.433671
H	3.547239	-3.665833	1.919555
H	4.641714	-1.298498	0.298952
H	4.888826	-3.019462	-0.060875
H	3.054699	-2.017104	-1.467044
H	2.456174	-3.327519	-0.421104
N	-0.666113	-0.801198	-1.243389
C	-1.457524	-1.636293	-0.3242
C	-1.173359	-3.110566	-0.594394
C	-1.490398	-3.460735	-2.0487
C	-0.753865	-2.512015	-2.995219
C	-1.057438	-1.062548	-2.631896
H	-0.898287	0.176864	-1.044257
H	-1.190874	-1.365252	0.709966
H	-2.541989	-1.43183	-0.436073

H	-0.105886	-3.319029	-0.393515
H	-1.762175	-3.733547	0.095136
H	-1.231141	-4.508001	-2.265869
H	-2.576868	-3.355751	-2.211523
H	0.334981	-2.67916	-2.911443
H	-1.036888	-2.705316	-4.040917
H	-0.505882	-0.373773	-3.291301
H	-2.1393	-0.863086	-2.7759

Absolute energy
-1216.27391359

Normal-mode frequencies
11.597
24.12
27.611
36.194
43.104
48.614
54.313
60.71
68.407
71.187
79.245
82.376
91.638
101.414
106.879
132.967
140.704
157.162
186.142
190.801
220.818
256.197
261.862

278.023
282.194
286.171
298.2
341.397
351.064
421.717
426.944
430.25
448.416
451.197
454.029
455.906
456.447
459.257
467.156
471.642
476.455
517.678
544.038
557.997
566.88
584.492
591.944
624.724
665.466
683.589
696.3
723.976
776.776
782.109
797.925
816.114
818.621
820.039
834.68

839.284
842.735
849.436
857.075
860.755
863.172
870.326
899.364
903.994
905.312
907.422
911.144
915.698
924.693
941.81
944.877
965.834
970.694
972.024
1001.854
1015.763
1029.801
1051.81
1058.949
1061.872
1064.442
1072.017
1075.88
1076.297
1078.504
1084.656
1088.516
1103.307
1128.692
1137.098
1144.754

1155.382
1156.527
1157.881
1158.41
1163.668
1170.554
1171.49
1175.026
1200.042
1207.738
1212.814
1218.791
1224.353
1237.666
1279.988
1282.154
1286.828
1290.466
1291.299
1309.093
1311.964
1317.017
1321.877
1326.928
1332.683
1335.246
1336.014
1358.594
1362.593
1365.776
1370.766
1375.421
1377.021
1381.394
1382.09
1387.128

1391.863
1412.854
1413.695
1418.215
1419.087
1420.659
1443.493
1445.356
1449.682
1450.212
1451.941
1456.915
1460.16
1462.487
1463.947
1465.053
1465.75
1466.99
1469.41
1477.799
1483.583
1484.502
1487.667
1507.208
1508.928
1529.5
1543.554
1555.849
1580.403
1602.737
1634.474
1669.195
2272.424
2654.576
2985.651
2987.759

2989.723
3004.869
3033.727
3039.165
3042.247
3042.908
3046.555
3050.884
3052.13
3058.977
3064.881
3070.688
3076.598
3080.701
3092.523
3094.739
3097.38
3104.9
3107.299
3109.461
3110.383
3112.332
3114.424
3121.844
3129.562
3131.688
3134.19
3137.489
3187.672
3189.945
3198.355
3208.238
3223.616
3224.682
3244.028
3249.406

3482.836

(IIIb)

Ground state optimized

Atom	X	Y	Z
C	-1.425476	-1.593932	-0.270414
C	-1.095691	-1.654835	-1.602516
C	-2.064803	-1.382084	-2.589044
C	-3.345584	-1.051702	-2.249486
C	-3.721908	-0.994912	-0.884438
C	-5.034864	-0.651888	-0.479851
C	-5.373929	-0.604894	0.843486
C	-4.41543	-0.900533	1.835873
C	-3.136286	-1.227479	1.480187
C	-2.761861	-1.278862	0.117943
O	-0.534533	-1.788163	0.717604
H	0.41485	-1.69427	0.376533
H	-0.080528	-1.900863	-1.886762
H	-1.777856	-1.432055	-3.631083
H	-4.085245	-0.835749	-3.008886
H	-5.769528	-0.429424	-1.243594
H	-6.382093	-0.342422	1.134755
H	-4.696383	-0.863831	2.879588
H	-2.389468	-1.453775	2.228105
N	2.034838	-1.376686	0.155895
C	2.72619	-1.979921	-0.98262
C	2.550569	-3.492194	-0.955617
C	3.069203	-4.060698	0.364068
C	2.403735	-3.359404	1.546611
C	2.573954	-1.849251	1.43519
H	2.103846	-0.355365	0.102612
H	2.317874	-1.55244	-1.899718
H	3.8003	-1.739921	-0.95889
H	1.487117	-3.726387	-1.05989
H	3.070861	-3.941335	-1.802162
H	2.896956	-5.136103	0.411264

H	4.151885	-3.907507	0.417132
H	1.336187	-3.592177	1.559327
H	2.82708	-3.707207	2.489376
H	2.036636	-1.341392	2.237189
H	3.639683	-1.595602	1.530689
N	2.233413	1.68813	0.226907
C	2.582805	2.507773	-0.928389
C	3.929649	2.069322	-1.488792
C	5.006552	2.148368	-0.40932
C	4.577795	1.358233	0.824877
C	3.208442	1.823672	1.304601
H	1.297709	1.907399	0.565341
H	1.80212	2.401156	-1.681942
H	2.639518	3.575646	-0.661962
H	3.842146	1.037757	-1.842296
H	4.1949	2.689544	-2.345817
H	5.961099	1.782035	-0.78862
H	5.155115	3.19592	-0.129013
H	4.518942	0.295782	0.569484
H	5.309553	1.463053	1.626871
H	2.87246	1.224225	2.152151
H	3.288386	2.866543	1.649408
N	-0.852253	1.513425	0.788446
C	-0.949178	1.66715	-0.663002
C	-0.965906	3.148998	-1.015603
C	-2.132336	3.845819	-0.317871
C	-2.08363	3.583312	1.18589
C	-2.020016	2.086277	1.456168
H	-0.7793	0.527987	1.019577
H	-0.096858	1.161201	-1.122128
H	-1.858877	1.192652	-1.061858
H	-0.026567	3.605381	-0.68882
H	-1.032449	3.271874	-2.097854
H	-2.120673	4.916854	-0.523963
H	-3.071932	3.451557	-0.717417
H	-1.194878	4.05629	1.611976

H	-2.956576	4.01233	1.679722
H	-1.942949	1.888166	2.525439
H	-2.950777	1.617683	1.098968

Absolute energy
-1216.75899932

Normal-mode frequencies
11.597
24.12
27.611
36.194
43.104
48.614
54.313
60.71
68.407
71.187
79.245
82.376
91.638
101.414
106.879
132.967
140.704
157.162
186.142
190.801
220.818
256.197
261.862
278.023
282.194
286.171
298.2
341.397

351.064
421.717
426.944
430.25
448.416
451.197
454.029
455.906
456.447
459.257
467.156
471.642
476.455
517.678
544.038
557.997
566.88
584.492
591.944
624.724
665.466
683.589
696.3
723.976
776.776
782.109
797.925
816.114
818.621
820.039
834.68
839.284
842.735
849.436
857.075
860.755

863.172
870.326
899.364
903.994
905.312
907.422
911.144
915.698
924.693
941.81
944.877
965.834
970.694
972.024
1001.854
1015.763
1029.801
1051.81
1058.949
1061.872
1064.442
1072.017
1075.88
1076.297
1078.504
1084.656
1088.516
1103.307
1128.692
1137.098
1144.754
1155.382
1156.527
1157.881
1158.41
1163.668

1170.554
1171.49
1175.026
1200.042
1207.738
1212.814
1218.791
1224.353
1237.666
1279.988
1282.154
1286.828
1290.466
1291.299
1309.093
1311.964
1317.017
1321.877
1326.928
1332.683
1335.246
1336.014
1358.594
1362.593
1365.776
1370.766
1375.421
1377.021
1381.394
1382.09
1387.128
1391.863
1412.854
1413.695
1418.215
1419.087

1420.659
1443.493
1445.356
1449.682
1450.212
1451.941
1456.915
1460.16
1462.487
1463.947
1465.053
1465.75
1466.99
1469.41
1477.799
1483.583
1484.502
1487.667
1507.208
1508.928
1529.5
1543.554
1555.849
1580.403
1602.737
1634.474
1669.195
2272.424
2654.576
2985.651
2987.759
2989.723
3004.869
3033.727
3039.165
3042.247

3042.908
3046.555
3050.884
3052.13
3058.977
3064.881
3070.688
3076.598
3080.701
3092.523
3094.739
3097.38
3104.9
3107.299
3109.461
3110.383
3112.332
3114.424
3121.844
3129.562
3131.688
3134.19
3137.489
3187.672
3189.945
3198.355
3208.238
3223.616
3224.682
3244.028
3249.406
3482.836

(IIIb)

Lb state optimized

Atom	X	Y	Z

C	1.383714	-1.550913	0.180492
C	1.038566	-1.73377	1.541308
C	2.03034	-1.60625	2.549245
C	3.349564	-1.280657	2.202565
C	3.735558	-1.085675	0.857386
C	5.047581	-0.723058	0.473885
C	5.390995	-0.530945	-0.861703
C	4.409154	-0.699754	-1.885761
C	3.10079	-1.0502	-1.546181
C	2.723232	-1.241951	-0.206017
O	0.471408	-1.611531	-0.782119
H	-0.505186	-1.579335	-0.404763
H	0.006178	-1.972058	1.797214
H	1.761819	-1.757519	3.59386
H	4.104588	-1.173686	2.984434
H	5.800911	-0.593268	1.254452
H	6.411563	-0.255275	-1.12645
H	4.682443	-0.558471	-2.931
H	2.34445	-1.181422	-2.321687
N	-2.031684	-1.383022	-0.178672
C	-2.660737	-2.058216	0.959157
C	-2.398713	-3.559451	0.880758
C	-2.914502	-4.120668	-0.44581
C	-2.325507	-3.341009	-1.622744
C	-2.58821	-1.846841	-1.457131
H	-2.152678	-0.355764	-0.099471
H	-2.251962	-1.629428	1.887043
H	-3.754727	-1.87362	0.965399
H	-1.311212	-3.733546	0.954899
H	-2.872702	-4.068155	1.733135
H	-2.673901	-5.190338	-0.531382
H	-4.01558	-4.036197	-0.469005
H	-1.235438	-3.500296	-1.666813
H	-2.749716	-3.690383	-2.575504
H	-2.108106	-1.27434	-2.264706
H	-3.678877	-1.652454	-1.505239

N	-2.227636	1.610148	-0.19242
C	-2.555382	2.31188	1.046467
C	-3.929712	1.873564	1.544936
C	-4.991285	2.122798	0.472684
C	-4.578507	1.470576	-0.847573
C	-3.180686	1.929902	-1.253139
H	-1.27222	1.841381	-0.497006
H	-1.782126	2.085591	1.795576
H	-2.561508	3.414143	0.900829
H	-3.891766	0.795982	1.782071
H	-4.180859	2.406051	2.474475
H	-5.973166	1.750778	0.801426
H	-5.096803	3.211118	0.317787
H	-4.567108	0.373145	-0.724515
H	-5.300919	1.705337	-1.643652
H	-2.858023	1.427405	-2.177468
H	-3.20725	3.020968	-1.463152
N	0.795689	1.58808	-0.722335
C	1.046171	1.647019	0.719668
C	1.03003	3.101294	1.181037
C	2.077486	3.911528	0.415198
C	1.877029	3.748469	-1.092369
C	1.856222	2.269943	-1.465694
H	0.770495	0.607783	-1.009484
H	0.266726	1.05687	1.230221
H	2.022674	1.189647	0.986651
H	0.02958	3.528355	0.992036
H	1.211798	3.152058	2.26537
H	2.036085	4.973083	0.702383
H	3.082624	3.542726	0.685055
H	0.915251	4.201416	-1.387378
H	2.672824	4.265509	-1.649441
H	1.667389	2.143434	-2.541977
H	2.849436	1.822898	-1.247265

Absolute energy

-1216.25574166

Normal-mode frequencies
9.119
24.882
30.23
34.142
36.775
39.12
51.252
56.031
61.739
68.019
74.501
76.8
81.502
101.555
106.831
119.217
124.036
135.784
169.759
178.789
234.851
262.952
265.667
268.246
278.195
283.308
289.838
337.96
364.786
388.619
420.679
424.308
430.694

445.946
452.676
453.448
455.092
455.729
456.491
468.913
473.558
485.039
542.26
564.242
577.612
580.327
583.569
587.625
645.001
686.525
711.174
720.756
776.933
783.804
796.514
820.178
820.483
821.371
828.212
839.257
842.81
848.167
854.862
859.701
888.165
892.347
902.65
903.028
905.491

906.625
908.32
912.667
933.246
935.541
936.881
969.058
972.693
973.201
974.76
996.378
1007.577
1052.517
1060.213
1061.933
1064.488
1076.27
1077.425
1079.143
1079.595
1090.334
1092.207
1101.289
1154.525
1154.977
1155.801
1156.978
1158.277
1161.64
1164.664
1167.925
1168.888
1171.288
1172.681
1176.294
1199.717

1207.142
1210.995
1242.781
1256.883
1263.66
1280.135
1282.299
1286.15
1288.912
1289.363
1293.411
1312.735
1313.623
1317.087
1325.118
1333.535
1333.914
1335.641
1360.868
1366.289
1367.852
1373.82
1376.963
1378.03
1380.55
1382.337
1385.123
1402.617
1415.897
1418.901
1421.774
1430.557
1443.095
1443.814
1448.593
1451.475

1451.799
1455.424
1458.391
1460.989
1463.815
1465.423
1466.341
1468.121
1472.411
1480.75
1481.798
1485.09
1485.958
1500.043
1522.335
1541.668
1544.062
1561.61
1581.451
1614.399
1624.373
2246.159
2342.707
2961.941
2965.706
2978.296
2982.369
2985.998
2995.355
3043.542
3044.974
3045.578
3048.408
3049.874
3050.192
3052.498

3052.921
3065.291
3074.665
3096.43
3097.124
3099.659
3101.943
3103.681
3104.527
3106.532
3108.45
3109.847
3111.951
3112.538
3112.655
3116.123
3121.391
3195.083
3201.117
3206.797
3215.237
3225.075
3237.684
3240.733
3253.45
3378.914
3531.034

(IIIb)

La state optimized

Atom	X	Y	Z
C	1.355123	-1.603527	0.133217
C	1.082276	-1.837868	1.532207
C	2.103239	-1.721762	2.440454
C	3.403359	-1.35982	1.992438
C	3.710153	-1.1187	0.6299

C	4.993081	-0.712687	0.199858
C	5.244054	-0.495234	-1.1861
C	4.241491	-0.668324	-2.113665
C	2.92815	-1.058919	-1.704526
C	2.668122	-1.276581	-0.337903
O	0.383338	-1.626738	-0.748027
H	-0.609422	-1.57403	-0.326442
H	0.068196	-2.106396	1.830006
H	1.927956	-1.900066	3.501062
H	4.206143	-1.263581	2.726649
H	5.782327	-0.567553	0.937488
H	6.24092	-0.191381	-1.50808
H	4.442039	-0.506894	-3.173858
H	2.133956	-1.211791	-2.432401
N	-2.051273	-1.351269	-0.097062
C	-2.668089	-1.937991	1.097728
C	-2.480264	-3.452715	1.097431
C	-3.050851	-4.064808	-0.183163
C	-2.451885	-3.382226	-1.413661
C	-2.655755	-1.872905	-1.333851
H	-2.146964	-0.315207	-0.084112
H	-2.209522	-1.477295	1.98638
H	-3.750346	-1.701487	1.125035
H	-1.402765	-3.682683	1.160189
H	-2.958681	-3.886249	1.98788
H	-2.860816	-5.147496	-0.209116
H	-4.147023	-3.930698	-0.190922
H	-1.369537	-3.586523	-1.466365
H	-2.905457	-3.769674	-2.33739
H	-2.176441	-1.364566	-2.183258
H	-3.738232	-1.63991	-1.362947
N	-2.151193	1.632094	-0.286496
C	-2.564531	2.345774	0.921231
C	-4.001863	1.978695	1.279048
C	-4.93939	2.291604	0.112194
C	-4.436317	1.624377	-1.168477

C	-2.982241	2.004861	-1.43147
H	-1.16543	1.839849	-0.501857
H	-1.880685	2.07796	1.740701
H	-2.498871	3.446776	0.784437
H	-4.045013	0.899163	1.507291
H	-4.313069	2.517784	2.18627
H	-5.967443	1.97315	0.340534
H	-4.969335	3.384835	-0.04034
H	-4.501576	0.527678	-1.058854
H	-5.061937	1.905608	-2.028764
H	-2.598191	1.48966	-2.324476
H	-2.927472	3.09615	-1.632058
N	0.899814	1.58356	-0.585154
C	0.995794	1.529237	0.874748
C	0.991385	2.947251	1.439163
C	2.156348	3.748862	0.855736
C	2.117959	3.702782	-0.672609
C	2.069422	2.257639	-1.156458
H	0.876115	0.629784	-0.95254
H	0.139979	0.947401	1.259782
H	1.91928	1.011021	1.207644
H	0.040481	3.440034	1.171543
H	1.04971	2.91374	2.537975
H	2.133786	4.787918	1.217668
H	3.105549	3.305007	1.203691
H	1.218597	4.229732	-1.034335
H	2.995693	4.211068	-1.099075
H	1.995809	2.212932	-2.252725
H	3.00692	1.737343	-0.867932

Absolute energy
-1216.26847792

Normal-mode frequencies
9.468
31.322

33.317
38.728
40.678
44.776
50.058
61.675
64.333
69.777
75.707
81.601
87.763
104.876
109.189
120.491
134.574
141.404
174.03
183.766
214.593
260.204
265.074
268.318
281.083
285.813
292.937
333.66
342.375
421.187
425.604
429.318
447.254
450.933
452.28
454.24
454.721
456.851

458.031
467.296
475.367
504.043
529.8
555.068
566.633
579.46
587.405
610.171
685.209
694.197
708.926
720.336
781.163
786.526
799.603
817.221
818.325
822.506
831.096
836.966
842.084
848.783
855.54
860.186
861.628
866.828
897.556
903.496
904.322
906.188
907.163
911.496
926.698
937.509

948.18
969.67
972.14
976.918
981.166
1005.597
1029.022
1049.441
1060.42
1062.791
1065.347
1071.167
1076.022
1077.772
1078.692
1081.259
1089.864
1099.407
1117.184
1153.609
1154.656
1157.013
1159.275
1159.668
1164.923
1168.845
1169.794
1170.208
1170.762
1182.964
1197.709
1206.071
1210.089
1224.315
1248.313
1278.862

1283.034
1287.738
1289.238
1290.93
1293.905
1313.336
1316.729
1318.695
1329.173
1334.425
1335.893
1337.772
1339.456
1358.773
1363.888
1366.428
1370.903
1374.271
1375.533
1379.795
1381.044
1382.228
1384.793
1408.951
1418.703
1420.53
1427.682
1435.007
1442.117
1442.732
1448.468
1450.695
1451.038
1452.489
1456.869
1458.375

1462.006
1464.496
1465.54
1466.211
1468.338
1474.05
1481.439
1482.838
1484.874
1493.045
1502.614
1506.147
1542.782
1560.426
1578.684
1617.456
1660.256
1951.743
2965.575
2969.807
2993.23
2999.846
3001.202
3008.804
3045.523
3045.826
3046.99
3047.76
3049.011
3050.095
3051.008
3057.326
3064.398
3066.663
3097.802
3098.155

3099.814
3101.817
3104.902
3106.084
3106.9
3109.839
3111.872
3112.241
3112.764
3114.005
3118.238
3122.721
3155.483
3199.556
3203.151
3214.663
3217.412
3228.687
3235.729
3248.67
3364.382
3521.671

(IIIc)

Ground state optimized

Atom	X	Y	Z
C	-0.796324	0.033673	-0.854692
C	-1.174068	-0.511233	-2.056412
C	-1.420119	-1.893421	-2.172464
C	-1.271458	-2.727347	-1.099655
C	-0.898052	-2.199001	0.158967
C	-0.745301	-3.024194	1.301373
C	-0.42826	-2.490747	2.519528
C	-0.262926	-1.095084	2.662215
C	-0.386428	-0.274399	1.575517
C	-0.680787	-0.803815	0.296509

O	-0.575005	1.361955	-0.751799
H	0.314541	1.503916	-0.285847
H	-1.272358	0.145865	-2.909286
H	-1.718013	-2.29452	-3.131962
H	-1.444762	-3.791269	-1.192706
H	-0.89642	-4.090758	1.191675
H	-0.321188	-3.133923	3.382397
H	-0.047668	-0.677396	3.636324
H	-0.271664	0.795626	1.685339
N	1.935326	1.506575	0.124127
C	2.535902	2.221935	-1.003604
C	2.138583	3.691594	-0.95025
C	2.539748	4.310321	0.387544
C	1.980275	3.490572	1.549112
C	2.394474	2.032722	1.409115
H	2.153164	0.505267	0.081305
H	2.178564	1.764393	-1.926988
H	3.632885	2.135178	-0.985817
H	1.055275	3.761592	-1.079294
H	2.602024	4.229071	-1.778075
H	2.19802	5.343772	0.44814
H	3.631841	4.33024	0.460449
H	0.887908	3.547119	1.545
H	2.326661	3.886759	2.504183
H	1.965959	1.419586	2.203112
H	3.489573	1.957688	1.490634
N	-3.548742	1.095064	0.572763
C	-3.907494	-0.312503	0.695664
C	-5.424689	-0.448282	0.701359
C	-6.009306	0.155778	-0.574555
C	-5.523623	1.59253	-0.760014
C	-4.002438	1.650218	-0.695469
H	-2.546196	1.209927	0.645867
H	-3.476886	-0.706434	1.617815
H	-3.503933	-0.91236	-0.138445
H	-5.819794	0.080796	1.571932

H	-5.705449	-1.498863	0.792293
H	-7.099503	0.116915	-0.556619
H	-5.681767	-0.442898	-1.430905
H	-5.928355	2.220147	0.037689
H	-5.873248	1.996368	-1.711663
H	-3.650725	2.678744	-0.772672
H	-3.58602	1.093853	-1.552651
N	2.496139	-1.504782	0.322736
C	2.449992	-2.103674	-1.009285
C	3.519089	-1.469931	-1.890206
C	4.898807	-1.606376	-1.249085
C	4.883966	-1.05782	0.176292
C	3.77772	-1.722395	0.985349
H	1.737088	-1.862864	0.891256
H	1.456074	-1.937592	-1.42768
H	2.61756	-3.191387	-0.966347
H	3.282264	-0.410293	-2.022032
H	3.504738	-1.931161	-2.878229
H	5.653688	-1.097174	-1.849143
H	5.175858	-2.664886	-1.218927
H	4.699459	0.021025	0.151563
H	5.847808	-1.215076	0.66175
H	3.72469	-1.2983	1.988908
H	4.005586	-2.795058	1.087528

Absolute energy
-1216.75394630

Normal-mode frequencies
17.094
18.3
24.544
28.216
35.961
45.848
48.8

50.771
59.653
62.39
69.539
72.543
75.258
80.795
84.708
98.267
117.583
155.425
200.27
202.598
261.515
263.15
267.32
268.891
270.36
278.147
294.129
325.056
416.366
421.907
432.926
440.375
443.998
445.084
455.423
456.088
456.706
458.664
476.59
482.902
489.621
544.548
564.251

568.396
585.633
593.573
600.32
668.367
734.773
762.377
801.937
804.75
808.449
812.269
826.377
829.011
829.845
832.073
838.734
840.681
841.034
864.48
883.254
885.645
896.688
897.472
899.702
900.657
902.124
907.499
925.161
926.616
928.176
978.33
981.36
983.842
993.436
1002.308
1010.484

1012.585
1027.656
1048.896
1060.549
1062.67
1064.29
1073.975
1074.333
1075.268
1076.731
1078.192
1080.315
1112.695
1118.132
1155.867
1158.04
1158.686
1167.142
1171.846
1172.77
1175.524
1176.198
1181.375
1186.784
1189.181
1195.541
1197.97
1200.062
1210.016
1236.933
1271.552
1289.059
1291.197
1296.673
1297.706
1299.179

1301.04
1317.198
1321.844
1323.037
1324.456
1351.202
1352.069
1352.997
1361.34
1365.108
1366.337
1373.289
1381.324
1383.169
1383.441
1384.25
1386.422
1389.269
1421.019
1425.263
1426.785
1427.129
1440.638
1474.602
1476.471
1478.35
1483.829
1485.25
1486.283
1487.693
1488.226
1489.59
1495.167
1496.692
1497.386
1500.074

1500.543
1501.662
1507.11
1512.574
1515.76
1517.846
1531.619
1547.464
1563.539
1652.165
1672.973
1705.011
2810.03
2947.909
2955.365
2966.181
2966.849
2975.932
2980.567
3037.724
3040.807
3041.717
3047.728
3053.897
3056.369
3056.577
3058.17
3061.142
3090.125
3093.637
3095.173
3096.784
3098.839
3101.929
3102.324
3104.567

3105.221
3106.051
3106.387
3106.585
3108.874
3110.5
3113.14
3194.961
3200.507
3204.691
3215.51
3217.374
3225.569
3227.032
3320.266
3551.031
3575.663

(IIIc)
Lb state optimized

Atom	X	Y	Z
C	-0.873355	-0.047622	-0.776505
C	-1.182443	-0.586926	-2.059188
C	-1.111631	-1.987532	-2.285093
C	-0.705643	-2.854429	-1.268377
C	-0.365227	-2.381646	0.032309
C	0.094266	-3.222037	1.066735
C	0.366283	-2.735694	2.343356
C	0.108387	-1.351166	2.640307
C	-0.339854	-0.501455	1.634516
C	-0.521698	-0.950435	0.315036
O	-0.851559	1.219384	-0.571647
H	0.538653	1.42445	0.088497
H	-1.431045	0.116693	-2.85343
H	-1.360869	-2.390461	-3.266984
H	-0.646026	-3.928249	-1.46332

H	0.228827	-4.285903	0.851634
H	0.716956	-3.408182	3.125267
H	0.230248	-0.979747	3.658309
H	-0.56741	0.543067	1.87035
N	1.602107	1.581131	0.21104
C	2.010651	2.352444	-0.986133
C	1.271813	3.685118	-1.012943
C	1.499048	4.464206	0.284051
C	1.119066	3.613353	1.498101
C	1.873735	2.290555	1.479307
H	2.066476	0.60885	0.225732
H	1.760317	1.738797	-1.862814
H	3.103884	2.493478	-0.948812
H	0.199126	3.469302	-1.143222
H	1.604704	4.265357	-1.885087
H	0.915313	5.395337	0.274695
H	2.562337	4.752351	0.360855
H	0.036615	3.401648	1.47889
H	1.333957	4.14305	2.436844
H	1.572139	1.620876	2.296831
H	2.962033	2.454875	1.550059
N	-3.642993	0.874495	0.670349
C	-3.823577	-0.569645	0.780855
C	-5.313794	-0.898098	0.74746
C	-5.942069	-0.370509	-0.543816
C	-5.631745	1.11725	-0.719643
C	-4.128083	1.357873	-0.617983
H	-2.647828	1.089609	0.727978
H	-3.366258	-0.915472	1.72039
H	-3.316995	-1.115298	-0.048171
H	-5.797533	-0.418503	1.614771
H	-5.463584	-1.984943	0.837097
H	-7.028997	-0.546752	-0.551706
H	-5.518892	-0.927026	-1.399154
H	-6.132611	1.693196	0.076426
H	-6.010724	1.482129	-1.687059

H	-3.900036	2.430921	-0.701415
H	-3.620171	0.844842	-1.465885
N	2.676512	-0.988988	0.267116
C	2.702187	-1.519597	-1.103826
C	3.857035	-0.898503	-1.882952
C	5.187145	-1.12288	-1.162485
C	5.100107	-0.627898	0.2819
C	3.918076	-1.277249	0.992299
H	1.90172	-1.433807	0.766577
H	1.732847	-1.295973	-1.576476
H	2.81309	-2.622583	-1.091308
H	3.679006	0.186101	-1.988344
H	3.884315	-1.318897	-2.898819
H	6.008928	-0.623783	-1.696895
H	5.417156	-2.202601	-1.157102
H	4.963041	0.468569	0.288565
H	6.030124	-0.84272	0.828479
H	3.811629	-0.89811	2.01948
H	4.086536	-2.370891	1.058188

Absolute energy
-1216.25206236

Normal-mode frequencies
15.452
20.9
27.151
30.026
32.784
49.185
56.331
61.395
66.739
71.09
72.452
77.704

92.992
98.199
103.12
127.09
145.163
149.857
177.684
207.867
253.695
259.586
260.332
267.439
276.327
285.907
291.266
319.176
348.457
414.799
418.881
422.878
424.469
442.674
450.39
451.654
451.72
452.404
453.807
458.868
467.837
484.92
535.774
559.696
569.876
581.555
584.639
625.948

643.724
689.931
713.723
747.581
770.841
775.52
806.609
814.718
817.151
820.99
826.844
835.927
841.726
848.488
849.269
859.966
885.77
888.925
897.195
902.135
902.459
907.512
908.815
914.638
936.748
940.06
954.482
957.621
965.784
968.766
974.19
996.568
1011.291
1046.062
1060.741
1063.331

1064.729
1075.682
1076.041
1076.966
1083.567
1086.764
1091.92
1123.234
1137.002
1140.403
1147.908
1150.892
1156.1
1158.682
1160.275
1165.485
1165.532
1165.797
1172.211
1198.197
1199.697
1210.86
1221.814
1235.814
1248.166
1280.121
1282.3
1287.03
1287.737
1291.127
1306.278
1313.284
1316.216
1318.119
1325.941
1334.163

1335.212
1336.373
1358.394
1358.675
1370.248
1373.153
1376.78
1380.031
1381.276
1386.309
1391.43
1393.608
1404.59
1419.568
1419.863
1423.945
1442.241
1444.438
1444.959
1450.398
1451.429
1452.449
1456.314
1457.881
1460.552
1463.072
1464.544
1465.299
1466.921
1471.493
1479.063
1480.472
1483.319
1484.926
1488.326
1496.169

1514.569
1535.35
1558.809
1581.178
1597.507
1671.314
2060.554
2444.593
2567.593
2940.499
2944.864
2998.57
3002.292
3038.082
3039.39
3047.838
3049.214
3052.185
3053.837
3055.567
3058.725
3062.04
3064.772
3077.2
3091.078
3093.354
3096.963
3102.608
3103.3
3105.602
3109.994
3110.992
3111.689
3117.709
3119.858
3125.808

3130.126
3131.772
3136.893
3172.982
3181.742
3191.203
3218.586
3225.574
3236.162
3238.376
3523.144
3543.755

(IIIc)

La state optimized

Atom	X	Y	Z
C	-0.951823	0.170836	-0.826085
C	-1.33497	-0.295548	-2.147071
C	-1.304065	-1.640269	-2.446503
C	-0.897476	-2.560385	-1.460373
C	-0.545122	-2.167074	-0.132318
C	-0.109735	-3.115432	0.837974
C	0.150433	-2.67288	2.169054
C	0.013012	-1.343462	2.51701
C	-0.370179	-0.367926	1.545274
C	-0.631184	-0.798738	0.211022
O	-0.855785	1.413867	-0.589816
H	0.679025	1.438031	0.111435
H	-1.614055	0.467962	-2.874058
H	-1.583984	-1.996915	-3.438117
H	-0.863154	-3.624322	-1.70496
H	-0.044262	-4.169746	0.572627
H	0.451468	-3.40061	2.924857
H	0.1927	-1.032506	3.548283
H	-0.558443	0.667781	1.828681
N	1.734019	1.482597	0.167822

C	2.188345	2.195643	-1.048385
C	1.595829	3.59905	-1.075134
C	1.945264	4.36221	0.204067
C	1.510275	3.570512	1.439251
C	2.111602	2.171238	1.421883
H	2.093315	0.453189	0.185115
H	1.860802	1.601681	-1.912876
H	3.290594	2.220052	-1.034355
H	0.502518	3.499245	-1.171127
H	1.963368	4.130112	-1.96461
H	1.466743	5.351546	0.198494
H	3.035463	4.53304	0.245864
H	0.411066	3.478291	1.45301
H	1.808052	4.083258	2.364694
H	1.74508	1.547971	2.248662
H	3.212379	2.208284	1.467576
N	-3.657726	0.782218	0.817305
C	-3.887019	-0.657417	0.779399
C	-5.389262	-0.925795	0.768932
C	-6.036837	-0.236885	-0.434443
C	-5.670105	1.248606	-0.467004
C	-4.154803	1.420786	-0.392465
H	-2.659315	0.965211	0.90993
H	-3.403734	-1.117244	1.654073
H	-3.436148	-1.12712	-0.125188
H	-5.823015	-0.525742	1.70034
H	-5.581937	-2.009414	0.745704
H	-7.130023	-0.368378	-0.421228
H	-5.667055	-0.715527	-1.359246
H	-6.120269	1.756883	0.401765
H	-6.064405	1.726296	-1.377593
H	-3.882676	2.48633	-0.371324
H	-3.700762	0.984028	-1.312124
N	2.586419	-1.139116	0.264265
C	2.743554	-1.751092	-1.061991
C	3.977595	-1.187592	-1.758449

C	5.225656	-1.381678	-0.89565
C	5.002484	-0.806231	0.503834
C	3.744083	-1.400638	1.126307
H	1.761905	-1.556568	0.708331
H	1.827861	-1.54706	-1.637735
H	2.836375	-2.85136	-0.968491
H	3.825989	-0.109473	-1.944337
H	4.10133	-1.667756	-2.740158
H	6.103926	-0.92086	-1.371483
H	5.43812	-2.461322	-0.807786
H	4.886153	0.290924	0.435987
H	5.869997	-1.00011	1.151625
H	3.539461	-0.966884	2.116479
H	3.883548	-2.491064	1.26723

Absolute energy
-1216.27633260

Normal-mode frequencies
18.318
23.104
26.064
27.23
40.096
48.154
53.127
61.132
62.164
67.961
70.635
79.967
86.909
100.937
109.311
119.474
146.761

154.868
193.259
202.318
230.748
255.684
260.608
260.885
274.589
281.85
290.117
308.395
354.386
417.459
420.285
422.906
444.907
450.752
451.736
453.027
453.433
457.746
459.879
471.855
487.733
532.372
542.689
556.483
563.481
567.855
577.6
623.065
647.658
662.459
705.129
723.121
770.243

782.509
812.8
813.813
816.004
821.229
826.728
835.97
840.466
848.101
849.984
857.567
876.974
882.823
886.858
901.43
902.731
906.848
909.585
912.059
937.01
941.131
954.174
958.684
962.681
968.21
974.297
1006.53
1033.431
1058.031
1060.131
1063.697
1063.982
1075.248
1075.953
1076.873
1077.502

1079.709
1089.036
1091.181
1112.484
1131.74
1144.811
1148.965
1154.813
1155.693
1161.737
1164.399
1164.772
1165.87
1174.417
1198.652
1199.68
1212.677
1215.728
1217.236
1230.12
1278.637
1281.681
1286.095
1287.883
1290.234
1304.184
1315.883
1316.135
1329.326
1332.401
1334.922
1335.442
1337.194
1357.032
1359.075
1366.373

1370.55
1371.064
1375.548
1378.594
1380.368
1386.908
1390.355
1398.866
1415.328
1417.072
1418.86
1422.072
1440.734
1443.053
1445.566
1450.797
1451.092
1454.943
1457.559
1458.356
1461.873
1464.088
1465.109
1465.61
1467.982
1474.611
1479.007
1479.961
1482.334
1484.083
1486.179
1510.176
1531.275
1565.831
1596.678
1607.702

1632.641
1667.461
2353.323
2877.999
2935.051
2944.104
3004.509
3005.676
3034.871
3034.935
3045.992
3046.925
3052.544
3053.935
3055.462
3063.446
3066.72
3070.989
3074.88
3094.938
3099.907
3102.322
3104.901
3105.392
3107.003
3109.681
3111.169
3113.895
3115.648
3122.575
3128.997
3131.213
3137.508
3144.766
3187.639
3200.617

3206.863
3218.406
3221.356
3228.91
3234.61
3495.754
3556.61

(IIId)

Ground state optimized

Atom	X	Y	Z
C	0.406077	-1.143118	-0.015486
C	-0.074909	-1.139727	1.272001
C	0.554433	-1.912838	2.269687
C	1.646148	-2.680253	1.980147
C	2.159906	-2.713185	0.660329
C	3.304124	-3.474862	0.320474
C	3.80411	-3.463336	-0.951023
C	3.180334	-2.692148	-1.955206
C	2.067809	-1.952653	-1.663456
C	1.534911	-1.94588	-0.353575
O	-0.137446	-0.381013	-0.988339
H	-0.46065	0.479169	-0.560799
H	-0.937879	-0.529431	1.507478
H	0.160421	-1.889268	3.277075
H	2.131371	-3.269147	2.747204
H	3.781112	-4.064355	1.093379
H	4.682104	-4.046779	-1.193215
H	3.584636	-2.691773	-2.958254
H	1.573428	-1.364059	-2.423883
N	-0.475192	2.04681	0.068927
C	-1.003587	2.353469	1.399315
C	-2.491183	2.033504	1.452452
C	-3.241649	2.795995	0.361619
C	-2.608793	2.533528	-1.003993
C	-1.120486	2.85265	-0.970338

H	0.535538	2.185169	0.044179
H	-0.449208	1.76555	2.131803
H	-0.850449	3.41562	1.64045
H	-2.632392	0.963168	1.281889
H	-2.886608	2.27931	2.439048
H	-4.293747	2.505647	0.354686
H	-3.207206	3.869137	0.576495
H	-2.730813	1.476473	-1.253744
H	-3.098811	3.124506	-1.778927
H	-0.650032	2.616385	-1.925865
H	-0.976278	3.926169	-0.781707
N	-3.115424	-1.036902	-0.281347
C	-3.832044	-1.091805	-1.548622
C	-5.166032	-0.368648	-1.414561
C	-5.985438	-0.973992	-0.276249
C	-5.172375	-0.998211	1.01676
C	-3.841191	-1.704076	0.790122
H	-2.18684	-1.424347	-0.389826
H	-3.211617	-0.625672	-2.315208
H	-4.023411	-2.130233	-1.865142
H	-4.972956	0.686827	-1.204124
H	-5.715356	-0.422985	-2.355489
H	-6.915661	-0.422127	-0.13579
H	-6.260578	-1.999768	-0.542064
H	-4.973208	0.026784	1.342344
H	-5.728523	-1.496312	1.81211
H	-3.230963	-1.675451	1.694625
H	-4.036092	-2.763934	0.558265
N	2.517573	1.389124	-0.482624
C	3.166032	0.774938	0.67716
C	3.935773	1.834931	1.45257
C	4.957023	2.524217	0.549988
C	4.280011	3.063107	-0.708545
C	3.49838	1.956929	-1.404363
H	1.967542	0.688138	-0.967637
H	2.400469	0.31685	1.305165

H	3.857382	-0.025854	0.368571
H	3.225848	2.575035	1.832312
H	4.427241	1.378526	2.312625
H	5.466859	3.325867	1.085631
H	5.722085	1.797501	0.259121
H	3.585899	3.862609	-0.436915
H	5.017306	3.484064	-1.393451
H	2.972438	2.348255	-2.275639
H	4.204165	1.188397	-1.758001

Absolute energy
-1216.75390323

Normal-mode frequencies
13.019
17.69
23.348
26.515
32.919
38.431
46.554
53.308
58.558
62.907
64.715
71.191
78.729
97.073
102.594
103.774
107.395
142.254
185.332
204.11
257.395
259.535

266.093
266.927
271.604
277.736
292.574
325.437
414.955
420.407
428.177
436.631
439.621
446.712
452.163
453.735
454.202
457.032
480.435
486.868
490.218
543.18
561.927
567.485
584.127
591.287
598.661
675.392
736.957
762.406
783.264
803.499
811.14
818.056
825.575
826.262
828.464
830.098

834.153
840.395
841.62
847.979
880.276
888.361
889.36
897.048
898.298
898.862
901.016
905.965
924.274
926.417
928.15
937.2
982.915
983.416
986.301
1002.126
1010.831
1030.956
1045.206
1050.078
1061.036
1062.746
1062.859
1070.137
1074.749
1076.849
1077.939
1079.251
1079.331
1114.897
1127.224
1153.94

1156.619
1160.431
1166.49
1173.624
1173.917
1174.012
1176.416
1179.578
1184.445
1188.819
1198.154
1199.742
1200.571
1202.93
1237.847
1272.461
1291.273
1292.407
1296.993
1299.404
1300.302
1308.943
1315.745
1320.663
1322.36
1325.364
1351.714
1352.294
1352.809
1361.778
1367.473
1368.484
1374.718
1383.45
1384.606
1385.097

1386.771
1388.431
1394.354
1424.068
1425.114
1427.044
1428.231
1440.487
1467.974
1475.13
1477.29
1478.769
1482.682
1486.749
1487.41
1490.031
1493.856
1494.518
1496.758
1499.218
1501.948
1503.677
1504.533
1507.612
1515.603
1517.575
1518.173
1528.137
1548.021
1588.814
1651.644
1670.925
1706.102
2840.932
2954.033
2956.618

2962.947
2963.719
2983.656
2989.599
3038.266
3040.034
3042.757
3052.209
3053.214
3056.582
3058.501
3062.912
3066.141
3087.459
3093.936
3094.566
3096.459
3097.222
3098.989
3099.437
3100.283
3102.786
3104.667
3105.492
3107.907
3108.648
3112.251
3115.897
3194.389
3197.127
3205.417
3209.365
3218.401
3219.55
3227.84
3430.809

3540.396
3575.657

(IIId)
Lb state optimized

Atom	X	Y	Z
C	0.426182	-1.159982	-0.067485
C	-0.1153	-1.183606	1.240551
C	0.472363	-2.000572	2.243683
C	1.608787	-2.765789	1.944893
C	2.185039	-2.764928	0.655278
C	3.360335	-3.484306	0.334692
C	3.9187	-3.439504	-0.94042
C	3.309155	-2.653789	-1.965347
C	2.147509	-1.928913	-1.68852
C	1.562658	-1.951344	-0.409847
O	-0.097428	-0.372535	-1.007796
H	-0.447454	0.50663	-0.554389
H	-1.005219	-0.5861	1.443861
H	0.038503	-2.02927	3.242237
H	2.068352	-3.380617	2.721702
H	3.834906	-4.081687	1.116477
H	4.822944	-4.007856	-1.157219
H	3.743688	-2.629134	-2.964034
H	1.668256	-1.332392	-2.466717
N	-0.46873	1.980801	-0.003684
C	-0.920695	2.255699	1.365866
C	-2.418313	1.99431	1.482436
C	-3.187785	2.845772	0.471156
C	-2.645069	2.598257	-0.937235
C	-1.141201	2.846441	-0.980773
H	0.552282	2.113117	-0.068347
H	-0.348251	1.611923	2.049916
H	-0.705616	3.308999	1.637246
H	-2.616002	0.933628	1.253613
H	-2.754304	2.200043	2.50983

H	-4.263222	2.613911	0.515565
H	-3.079298	3.915352	0.726001
H	-2.831688	1.545806	-1.206234
H	-3.151503	3.237846	-1.675609
H	-0.732934	2.618452	-1.976547
H	-0.93087	3.913532	-0.766608
N	-3.094683	-0.983474	-0.385862
C	-3.897301	-0.940806	-1.604284
C	-5.243207	-0.286037	-1.306621
C	-5.96739	-1.045406	-0.193487
C	-5.064994	-1.188557	1.033571
C	-3.727436	-1.808152	0.638245
H	-2.165718	-1.342078	-0.604476
H	-3.345571	-0.371287	-2.367541
H	-4.077896	-1.957235	-2.018008
H	-5.064622	0.754723	-0.98632
H	-5.857394	-0.252198	-2.219188
H	-6.909972	-0.543364	0.071838
H	-6.233718	-2.052296	-0.561334
H	-4.876833	-0.192696	1.470277
H	-5.552464	-1.802988	1.805541
H	-3.053968	-1.87075	1.506752
H	-3.904356	-2.847875	0.284715
N	2.465616	1.395895	-0.502668
C	3.090121	0.805438	0.685583
C	3.778379	1.897193	1.498176
C	4.809822	2.635889	0.644053
C	4.165832	3.148029	-0.645169
C	3.46604	2.007796	-1.377527
H	1.992749	0.651391	-1.018857
H	2.309485	0.310542	1.283383
H	3.831006	0.025619	0.405766
H	3.013212	2.610972	1.849111
H	4.251621	1.45675	2.38836
H	5.263131	3.464587	1.208506
H	5.626421	1.93914	0.385058

H	3.417114	3.920535	-0.401509
H	4.918203	3.610566	-1.301578
H	2.961687	2.38018	-2.281393
H	4.225912	1.264497	-1.700796

Absolute energy
-1216.24919596

Normal-mode frequencies
18.661
19.865
25.567
28.879
34.183
42.608
46.039
51.753
57.076
68.001
69.359
74.089
81.306
102.447
104.433
108.527
114.036
123.629
178.63
197.691
246.315
258.755
260.585
268.277
270.738
274.231
293.147

327.679
372.893
389.901
419.528
420.353
433.163
439.249
444.853
450.136
450.753
452.012
454.843
471.117
471.369
483.511
536.02
555.53
561.65
575.254
584.263
599.979
663.61
689.226
709.432
725.14
783.495
798.36
800.263
806.345
818.562
818.832
822.908
825.244
837.218
847.209
847.94

855.332
878.913
889.566
892.648
901.296
904.129
905.168
907.345
908.74
932.966
933.555
934.368
939.072
965.163
972.203
973.442
976.123
1005.833
1046.329
1059.801
1061.343
1063.737
1070.948
1075.938
1077.105
1077.52
1079.587
1081.768
1090.58
1153.639
1154.637
1155.183
1158.338
1158.898
1159.661
1164.59

1165.678
1166.86
1168
1171.646
1180.351
1199.5
1201.136
1204.396
1223.059
1241.549
1259.073
1280.116
1282.808
1285.333
1288.049
1288.435
1302.864
1311.147
1311.427
1316.691
1320.15
1334.476
1334.565
1335.018
1359.845
1361.224
1365.991
1374.481
1377.921
1380.083
1382.302
1382.969
1387.038
1402.035
1417.415
1420.263

1421.895
1428.585
1440.383
1442.669
1444.244
1447.794
1452.312
1452.897
1461.228
1462.175
1465.118
1466.619
1467.234
1467.951
1471.343
1475.461
1484.33
1485.284
1487.935
1489.038
1493.241
1519.036
1532.976
1539.865
1584.495
1613.842
1627.728
2194.039
2335.29
2953.401
2957.871
2973.175
2974.796
2993.389
2999.572
3039.063

3041.641
3045.122
3050.338
3052.98
3053.295
3054.48
3062.947
3070.864
3090.788
3097.202
3097.652
3098.232
3101.013
3102.54
3103.381
3104.098
3104.376
3109.185
3111.892
3112.096
3114.355
3121.109
3127.297
3197.291
3201.698
3212.704
3223.354
3235.443
3238.995
3251.482
3340.498
3520.874
3554.77

(IIId)
La state optimized

Atom	X	Y	Z
C	0.229649	-1.600715	1.473317
C	0.926621	-2.156037	2.621658
C	2.058865	-2.921297	2.450269
C	2.54496	-3.153301	1.148462
C	1.891723	-2.655466	-0.021189
C	2.446582	-2.848183	-1.321439
C	1.725987	-2.371446	-2.456699
C	0.517085	-1.720101	-2.309287
C	-0.038545	-1.484514	-1.01384
C	0.683244	-1.938867	0.129899
O	-0.728497	-0.791059	1.648158
H	-0.316398	0.489785	0.407351
H	0.516461	-1.916287	3.603243
H	2.585634	-3.338917	3.308858
H	3.454288	-3.743334	1.014718
H	3.377753	-3.401409	-1.43592
H	2.133293	-2.535253	-3.456181
H	-0.029142	-1.386762	-3.194695
H	-1.01939	-1.02395	-0.895883
N	0.228025	1.352112	0.174697
C	0.273605	2.172046	1.406376
C	-1.142047	2.567039	1.803388
C	-1.840804	3.309715	0.662134
C	-1.815869	2.478225	-0.622695
C	-0.397118	2.051637	-0.97274
H	1.219608	1.010357	-0.126455
H	0.7572	1.563472	2.182215
H	0.899949	3.055545	1.199845
H	-1.686205	1.639638	2.049035
H	-1.106468	3.181634	2.714152
H	-2.87982	3.540133	0.940505
H	-1.333333	4.276271	0.493173
H	-2.422319	1.564496	-0.496774
H	-2.236965	3.045506	-1.465712
H	-0.373337	1.350185	-1.818237

H	0.243777	2.916614	-1.2119
N	-3.312816	-0.49141	0.173004
C	-3.882545	-1.583409	-0.609322
C	-4.927509	-1.02978	-1.573631
C	-6.014898	-0.27751	-0.803853
C	-5.394168	0.783848	0.106587
C	-4.324282	0.157573	0.997987
H	-2.546572	-0.83399	0.758232
H	-3.069016	-2.084107	-1.154245
H	-4.365594	-2.346209	0.040383
H	-4.427097	-0.340381	-2.274353
H	-5.366197	-1.846367	-2.166754
H	-6.740322	0.178502	-1.494634
H	-6.575326	-0.997397	-0.18115
H	-4.924966	1.568926	-0.511591
H	-6.166733	1.266609	0.724581
H	-3.837614	0.929612	1.615471
H	-4.813725	-0.556884	1.696098
N	2.674144	0.462318	-0.716924
C	3.663102	0.244706	0.346998
C	4.133976	1.582396	0.907353
C	4.690204	2.473482	-0.20435
C	3.670156	2.615272	-1.33525
C	3.230691	1.241014	-1.828384
H	2.393604	-0.454636	-1.081775
H	3.191006	-0.371658	1.126678
H	4.530141	-0.323898	-0.044547
H	3.280296	2.089688	1.391185
H	4.889573	1.412224	1.688232
H	4.973476	3.460069	0.191309
H	5.609083	2.01382	-0.608051
H	2.785241	3.163989	-0.964202
H	4.086105	3.198778	-2.16971
H	2.461237	1.319759	-2.610855
H	4.099318	0.715214	-2.272829

Absolute energy
-1216.28111842

Normal-mode frequencies
19.148
26.505
29.577
36.338
41.663
47.252
52.924
58.939
63.735
69.304
75.464
85.716
96.256
107.911
108.963
124.99
145.181
156.368
175.3
199.315
223.726
253.519
258.82
264.92
271.608
285.442
289.975
303.746
351.954
414.463
419.955
420.916

446.555
449.992
451.475
452.691
454.033
457.534
459.148
472.397
487.842
532.049
542.316
557.724
565.988
570.318
580.135
613.511
649.028
690.936
701.946
722.724
772.238
782.183
810.508
813.57
817.544
820.542
834.088
836.088
839.046
848.744
849.246
857.1
876.955
880.758
891.969
902.342

903.16
906.595
909.755
910.386
941.083
941.769
949.018
956.261
959.598
968.32
973.26
1002.448
1035.797
1058.232
1060.784
1061.933
1064.65
1075.176
1075.393
1076.647
1078.127
1081.377
1086.692
1088.765
1102.001
1129.722
1143.37
1147.205
1153.954
1154.854
1159.064
1165.318
1165.473
1170.616
1174.073
1200.47

1204.919
1206.955
1215.764
1217.999
1229.33
1278.845
1281.94
1284.954
1286.065
1289.992
1307.905
1312.586
1315.678
1328.843
1331.507
1333.021
1334.916
1339.213
1356.673
1360.381
1364.918
1368.645
1374.965
1375.123
1379.576
1379.981
1385.343
1397.778
1402.547
1415.752
1416.958
1420.13
1422.153
1426.315
1443.609
1443.746

1451.009
1451.094
1453.588
1456.605
1460.833
1463.014
1464.436
1465.499
1466.932
1468.021
1472.354
1483.794
1484.916
1486.232
1486.66
1505.715
1515.536
1532.475
1569.748
1595.656
1610.228
1634.693
1663.518
2351.225
2950.745
2958.099
3000.736
3003.487
3035.134
3038.959
3041.523
3045.07
3045.679
3051.142
3052.283
3056.083

3063.506
3065.284
3069.805
3078.468
3101.218
3104.164
3105.098
3106.421
3107.522
3108.793
3109.223
3112.047
3112.452
3114.218
3119.268
3127.437
3132.131
3141.361
3142.514
3183.95
3200.247
3204.846
3217.073
3224.655
3227.682
3233.612
3478.963
3487.897

(IIIe)

Ground state optimized

Atom	X	Y	Z
C	-0.874133	0.25817	0
C	-0.371488	1.536534	0
C	-1.241618	2.643846	0
C	-2.597668	2.475596	0

C	-3.147474	1.170234	0
C	-4.545708	0.945312	0
C	-5.053567	-0.322761	0
C	-4.187852	-1.43757	0
C	-2.832767	-1.256685	0
C	-2.284064	0.046642	0
O	-0.101927	-0.839955	0
H	0.874191	-0.638874	0
H	0.700989	1.684739	0
H	-0.819654	3.640145	0
H	-3.264297	3.327654	0
H	-5.206835	1.802865	0
H	-6.124252	-0.477141	0
H	-4.601882	-2.436653	0
H	-2.157071	-2.100221	0
N	2.606953	-0.938942	0
C	3.353376	-0.607414	1.220089
C	3.648577	0.885187	1.255133
C	4.405591	1.315388	0
C	3.648577	0.885187	-1.255133
C	3.353376	-0.607414	-1.220089
H	2.411067	-1.934745	0
H	2.754854	-0.917224	2.078297
H	4.305419	-1.15748	1.250623
H	2.705273	1.433906	1.323425
H	4.22359	1.121114	2.15182
H	4.567103	2.393699	0
H	5.393612	0.844391	0
H	2.705273	1.433906	-1.323425
H	4.22359	1.121114	-2.15182
H	2.754854	-0.917224	-2.078297
H	4.305419	-1.15748	-1.250623
N	1.22879	-1.299754	-4.130818
C	1.403483	0.145231	-4.243599
C	0.525848	0.838226	-3.211103
C	-0.938672	0.459262	-3.411183

C	-1.087184	-1.06011	-3.378935
C	-0.151755	-1.703114	-4.395278
H	1.851256	-1.773065	-4.772912
H	2.455599	0.384033	-4.073587
H	1.13789	0.515157	-5.247286
H	0.841698	0.508701	-2.218254
H	0.662295	1.920078	-3.26188
H	-1.562652	0.926011	-2.647392
H	-1.278244	0.836824	-4.381596
H	-0.832135	-1.425553	-2.381431
H	-2.117495	-1.352233	-3.587053
H	-0.210679	-2.789954	-4.33569
H	-0.471105	-1.40658	-5.40799
N	1.22879	-1.299754	4.130818
C	1.403483	0.145231	4.243599
C	0.525848	0.838226	3.211103
C	-0.938672	0.459262	3.411183
C	-1.087184	-1.06011	3.378935
C	-0.151755	-1.703114	4.395278
H	1.851256	-1.773065	4.772912
H	2.455599	0.384033	4.073587
H	1.13789	0.515157	5.247286
H	0.841698	0.508701	2.218254
H	0.662295	1.920078	3.26188
H	-1.562652	0.926011	2.647392
H	-1.278244	0.836824	4.381596
H	-0.832135	-1.425553	2.381431
H	-2.117495	-1.352233	3.587053
H	-0.210679	-2.789954	4.33569
H	-0.471105	-1.40658	5.40799

Absolute energy
-1216.74809538

Normal-mode frequencies
16.177

21.918
35.375
37.775
40.105
49.191
56.691
57.41
59.123
71.877
75.433
80.188
88.54
95.312
100.427
106.042
124.439
147.47
158.865
196.3
261.983
264.726
273.636
279.445
281.427
284.25
292.496
321.12
416.967
418.006
429.525
436.578
443.011
444.344
451.423
455.263
457.452

458.23
483.845
484.39
493.146
546.153
562.067
562.37
577.537
596.675
598.288
672.113
738.936
761.035
787.537
788.137
803.659
806.486
826.432
830.395
830.509
831.168
834.072
839.704
839.712
847.584
885.877
886.132
896.29
896.403
897.118
897.896
898.807
902.217
913.67
922.698
922.732

926.832
943.842
984.349
987.661
992.121
1000.547
1009.587
1030.061
1051.219
1061.216
1061.434
1063.953
1073.701
1073.826
1075.657
1075.747
1078.03
1081.059
1084.989
1117.234
1156.49
1156.76
1158.197
1167.876
1173.641
1175.178
1176.276
1176.377
1178.275
1180.543
1183.712
1195.798
1195.899
1198.583
1208.138
1238.466

1275.625
1290.438
1295.866
1297.488
1298.107
1301.272
1309.181
1319.309
1319.463
1325.99
1333.928
1349.584
1349.697
1350.418
1359.079
1365.76
1366.345
1367.72
1381.307
1383.323
1387.356
1387.953
1388.103
1391.463
1419.456
1425.425
1426.443
1435.262
1443.826
1453.653
1473.336
1473.734
1476.895
1484.945
1485.549
1485.848

1486.405
1487.669
1488.297
1495.484
1495.633
1498.977
1501.907
1503.617
1504.022
1515.51
1516.868
1518.206
1525.358
1531.224
1580.028
1654.364
1670.204
1706.594
2952.886
2952.981
2955.912
2956.105
2979.862
2980.816
3036.68
3036.769
3044.01
3060.5
3061.156
3066.615
3066.639
3067.338
3067.43
3080.658
3080.679
3099.7

3099.849
3101.786
3101.933
3102.222
3103.49
3103.558
3105.334
3109.315
3113.635
3113.68
3117.702
3117.91
3119.46
3191.623
3194.319
3204.346
3205.294
3217.225
3217.915
3230.879
3525.69
3555.856
3555.86

(IIIe)

Lb state optimized

Atom	X	Y	Z
C	-0.851118	0.294641	0
C	-0.311864	1.602037	0
C	-1.176131	2.728451	0
C	-2.566562	2.545172	0
C	-3.144843	1.256016	0
C	-4.542055	1.036625	0
C	-5.078974	-0.248128	0
C	-4.216053	-1.386054	0
C	-2.830552	-1.211791	0

C	-2.260061	0.073038	0
O	-0.073176	-0.782271	0
H	0.924839	-0.57871	0
H	0.771762	1.722874	0
H	-0.755639	3.733034	0
H	-3.227731	3.414457	0
H	-5.205251	1.904791	0
H	-6.160138	-0.385204	0
H	-4.639174	-2.390037	0
H	-2.164782	-2.075873	0
N	2.566044	-0.869875	0
C	3.31054	-0.526326	1.22214
C	3.574111	0.975148	1.258932
C	4.31767	1.426434	0
C	3.574111	0.975148	-1.258932
C	3.31054	-0.526326	-1.22214
H	2.399478	-1.878505	0
H	2.716613	-0.859547	2.087232
H	4.281913	-1.061337	1.24234
H	2.610809	1.507752	1.337238
H	4.152267	1.224179	2.161823
H	4.453042	2.517988	0
H	5.327133	0.978511	0
H	2.610809	1.507752	-1.337238
H	4.152267	1.224179	-2.161823
H	2.716613	-0.859547	-2.087232
H	4.281913	-1.061337	-1.24234
N	1.314051	-1.319758	-4.064349
C	1.357222	0.125069	-4.281411
C	0.44097	0.809818	-3.273183
C	-0.9912	0.295231	-3.412536
C	-1.005828	-1.228686	-3.286168
C	-0.031858	-1.853071	-4.281378
H	1.960873	-1.775134	-4.70732
H	2.396562	0.468133	-4.153743
H	1.039279	0.404598	-5.310211

H	0.803598	0.571315	-2.259313
H	0.484741	1.903343	-3.39444
H	-1.643637	0.754704	-2.654298
H	-1.38695	0.586304	-4.402515
H	-0.698206	-1.507576	-2.26541
H	-2.019033	-1.625577	-3.450984
H	0.002363	-2.944965	-4.154022
H	-0.391888	-1.648328	-5.313857
N	1.314051	-1.319758	4.064349
C	1.357222	0.125069	4.281411
C	0.44097	0.809818	3.273183
C	-0.9912	0.295231	3.412536
C	-1.005828	-1.228686	3.286168
C	-0.031858	-1.853071	4.281378
H	1.960873	-1.775134	4.70732
H	2.396562	0.468133	4.153743
H	1.039279	0.404598	5.310211
H	0.803598	0.571315	2.259313
H	0.484741	1.903343	3.39444
H	-1.643637	0.754704	2.654298
H	-1.38695	0.586304	4.402515
H	-0.698206	-1.507576	2.26541
H	-2.019033	-1.625577	3.450984
H	0.002363	-2.944965	4.154022
H	-0.391888	-1.648328	5.313857

Absolute energy
-1216.24308668

Normal-mode frequencies
13.506
21.309
33.418
38.139
38.99
48.07

54.36
56.032
62.104
72.719
79.42
82.208
89.526
93.519
96.819
102.699
106.474
148.418
155.113
184.742
241.319
261.255
262.612
278.233
280.233
284.783
288.035
316.735
363.271
389.593
416.227
416.975
431.626
441.244
441.369
450.243
454.055
454.573
455.006
470.371
474.368
488.216

535.999
554.989
555.537
570.522
586.428
588.841
650.779
689.157
710.985
722.748
783.697
783.826
799.492
801.247
801.731
819.958
822.056
822.428
837.482
845.858
845.863
849.49
883.401
883.505
888.685
900.939
901.002
904.235
905.813
910.788
929.209
929.328
933.177
933.92
947.941
974.346

977.64
980.384
1008.745
1030.81
1051.134
1060.966
1061.28
1063.396
1074.627
1074.847
1076.444
1076.842
1078.659
1086.546
1092.35
1154.192
1157.243
1157.294
1157.578
1162.134
1162.933
1165.048
1165.168
1167.758
1168.108
1174.271
1176.229
1197.024
1197.211
1209.528
1242.668
1263.73
1278.569
1282.877
1285.139
1287.573

1290.47
1301.225
1309.948
1310.454
1318.31
1330.764
1331.846
1332.051
1343.277
1357.195
1357.236
1361.949
1373.873
1373.991
1381.822
1382.161
1383.162
1385.171
1388.713
1419.223
1419.782
1428.814
1435.881
1437.277
1437.871
1445.879
1445.948
1449.987
1450.408
1456.207
1462.656
1463.297
1464.031
1464.45
1469.873
1475.186

1480.907
1481.333
1483.761
1484.474
1485.281
1489.411
1500.574
1516.382
1532.957
1555.682
1602.484
1619.458
2302.66
2799.57
2949.254
2949.349
2952.332
2952.61
2983.491
2986.323
3034.66
3034.701
3046.163
3059.977
3060.502
3062.463
3062.732
3071.389
3071.665
3080.29
3080.539
3101.501
3101.685
3105.435
3105.66
3106.884

3106.988
3108.476
3110.148
3113.697
3115.219
3116.579
3125.039
3125.165
3195.734
3200.9
3217.387
3224.929
3235.668
3238.592
3258.289
3504.341
3529.779
3529.816

(IIIe)

La state optimized

Atom	X	Y	Z
C	-0.857377	0.280332	0
C	-0.291536	1.607603	0
C	-1.131556	2.690694	0
C	-2.540441	2.485519	0
C	-3.130843	1.198056	0
C	-4.528174	1.003356	0
C	-5.0685	-0.315714	0
C	-4.233737	-1.409743	0
C	-2.813279	-1.243326	0
C	-2.268233	0.053193	0
O	-0.077068	-0.781453	0
H	0.93759	-0.593713	0
H	0.794351	1.710466	0
H	-0.732336	3.704538	0

H	-3.200193	3.355809	0
H	-5.186822	1.872096	0
H	-6.150682	-0.451054	0
H	-4.649941	-2.418079	0
H	-2.148325	-2.104625	0
N	2.526039	-0.916718	0
C	3.281579	-0.594756	1.223452
C	3.598011	0.89636	1.258277
C	4.358199	1.320126	0
C	3.598011	0.89636	-1.258277
C	3.281579	-0.594756	-1.223452
H	2.337269	-1.921895	0
H	2.677142	-0.907478	2.088985
H	4.232884	-1.163512	1.241892
H	2.655096	1.464509	1.336426
H	4.183508	1.124598	2.161791
H	4.533438	2.405878	0
H	5.350346	0.835437	0
H	2.655096	1.464509	-1.336426
H	4.183508	1.124598	-2.161791
H	2.677142	-0.907478	-2.088985
H	4.232884	-1.163512	-1.241892
N	1.286144	-1.28248	-4.072726
C	1.369461	0.16478	-4.258412
C	0.469569	0.850749	-3.236355
C	-0.976299	0.380865	-3.392734
C	-1.035842	-1.144507	-3.302232
C	-0.073795	-1.773698	-4.305614
H	1.921897	-1.741252	-4.724342
H	2.417486	0.476881	-4.121847
H	1.060848	0.47637	-5.28059
H	0.825459	0.572964	-2.230043
H	0.546622	1.945389	-3.328234
H	-1.621064	0.841865	-2.628999
H	-1.357194	0.706458	-4.377781
H	-0.749161	-1.459368	-2.285544

H	-2.059067	-1.506497	-3.481657
H	-0.070111	-2.868438	-4.201283
H	-0.422229	-1.537282	-5.335121
N	1.286144	-1.28248	4.072726
C	1.369461	0.16478	4.258412
C	0.469569	0.850749	3.236355
C	-0.976299	0.380865	3.392734
C	-1.035842	-1.144507	3.302232
C	-0.073795	-1.773698	4.305614
H	1.921897	-1.741252	4.724342
H	2.417486	0.476881	4.121847
H	1.060848	0.47637	5.28059
H	0.825459	0.572964	2.230043
H	0.546622	1.945389	3.328234
H	-1.621064	0.841865	2.628999
H	-1.357194	0.706458	4.377781
H	-0.749161	-1.459368	2.285544
H	-2.059067	-1.506497	3.481657
H	-0.070111	-2.868438	4.201283
H	-0.422229	-1.537282	5.335121

Absolute energy
-1216.25488363

Normal-mode frequencies
23.108
26.031
39.782
47.492
48.739
54.253
62.654
63.601
70.26
79.78
85.417

86.772
94.879
100.834
104.297
108.134
124.227
157.876
162.9
187.309
221.374
263.622
265.422
283.684
284.014
287.432
292.211
322.816
332.699
418.184
419.385
433.068
443.143
443.674
450.185
454.175
454.791
456.495
458.082
464.004
473.721
502.844
525.976
551.64
557.215
557.69
581.719

612.413
692.51
700.067
719.406
720.12
786.17
790.284
802.084
802.584
808.209
819.563
821.476
822.294
837.283
845.762
845.77
849.376
859.928
869.014
885.259
885.419
902.456
902.463
904.307
908.732
929.303
929.417
929.698
949.588
952.45
974.105
977.134
981.136
1029.531
1047.272
1060.033

1060.308
1062.965
1071.956
1073.25
1074.553
1074.7
1077.325
1077.355
1088.716
1089.936
1091.332
1154.152
1157.598
1157.8
1161.975
1162.141
1165.143
1165.575
1169.955
1170.013
1177.507
1179.437
1197.806
1198.007
1212.04
1226.333
1252.139
1278.695
1283.438
1285.614
1288.848
1291.28
1301.897
1310.617
1311.053
1322.976

1331.767
1331.921
1335.79
1344.142
1358.533
1358.612
1361.713
1362.477
1375.117
1375.285
1382.884
1383.526
1385.744
1385.937
1419.226
1420.016
1420.315
1434.701
1435.623
1436.139
1440.365
1443.248
1446.444
1449.829
1450.568
1459.685
1463.291
1464.019
1464.494
1464.721
1468.9
1474.752
1477.744
1481.941
1482.121
1484.878

1485.671
1490.868
1491.855
1500.161
1505.469
1526.755
1612.983
1661.102
2592.18
2950.605
2950.726
2954.391
2954.612
2990.304
2991.965
3037.347
3037.354
3047.152
3060.368
3060.669
3062.96
3063.062
3074.581
3074.584
3079.125
3079.392
3103.85
3103.984
3104.462
3104.714
3107.456
3109.559
3109.74
3110.992
3113.885
3116.754

3117.498
3126.997
3127.211
3199.292
3202.384
3212.701
3216.325
3227.258
3236.266
3247.181
3498.515
3530.147
3530.186

(IIIf)
Ground state optimized

Atom	X	Y	Z
C	-3.834902	-0.121513	-0.643501
C	-3.462145	1.118063	-1.103726
C	-4.314484	2.22832	-0.93561
C	-5.524847	2.10164	-0.318164
C	-5.94133	0.836086	0.163567
C	-7.188665	0.653624	0.808033
C	-7.571513	-0.575756	1.265118
C	-6.724285	-1.691971	1.101074
C	-5.512385	-1.550803	0.484088
C	-5.095384	-0.288969	0.003473
O	-3.063942	-1.215814	-0.769477
H	-2.180927	-0.990617	-1.172903
H	-2.509497	1.233656	-1.603508
H	-3.994183	3.192837	-1.306951
H	-6.177835	2.954688	-0.190208
H	-7.836484	1.512478	0.931902
H	-8.528236	-0.697585	1.755201
H	-7.038275	-2.660496	1.46589
H	-4.852824	-2.395826	0.348939

N	-0.511295	-0.869369	-1.720163
C	0.097549	-2.064892	-1.120493
C	-0.002727	-1.986482	0.397804
C	0.662323	-0.709509	0.906805
C	0.07203	0.514037	0.209686
C	0.185659	0.354554	-1.298335
H	-0.479755	-0.947255	-2.729703
H	-0.427672	-2.94306	-1.496383
H	1.156047	-2.146904	-1.409378
H	-1.056935	-1.992627	0.682222
H	0.460538	-2.871132	0.837397
H	0.555009	-0.627029	1.989177
H	1.735634	-0.753228	0.687282
H	-0.981886	0.624961	0.481803
H	0.602028	1.417972	0.507602
H	-0.261265	1.20501	-1.813771
H	1.248398	0.320096	-1.570507
N	3.235631	1.493222	-0.086251
C	3.379306	1.795772	1.329527
C	3.042302	3.260184	1.582187
C	3.919894	4.1652	0.719917
C	3.822283	3.764062	-0.750574
C	4.137462	2.282289	-0.911149
H	3.379178	0.503663	-0.264376
H	2.70676	1.147104	1.894753
H	4.405212	1.600885	1.69077
H	1.991402	3.424215	1.330478
H	3.169252	3.494576	2.63986
H	3.640817	5.210953	0.852948
H	4.960489	4.069127	1.04673
H	2.807375	3.94425	-1.112907
H	4.504304	4.359872	-1.35877
H	4.016479	1.974515	-1.950922
H	5.196087	2.121576	-0.638215
N	4.51644	-1.284823	-0.950246
C	5.464257	-1.03681	0.136233

C	4.893945	-1.574794	1.440943
C	4.587561	-3.065171	1.311633
C	3.684847	-3.32093	0.106807
C	4.287602	-2.714373	-1.152639
H	4.862795	-0.868669	-1.805944
H	5.637292	0.03793	0.208903
H	6.435257	-1.518905	-0.055963
H	3.974724	-1.029187	1.673698
H	5.597068	-1.392326	2.254418
H	4.124717	-3.442966	2.223583
H	5.526214	-3.612511	1.179546
H	2.708578	-2.862482	0.28093
H	3.526446	-4.390325	-0.038032
H	3.613258	-2.84226	-1.9998
H	5.224403	-3.242827	-1.389596

Absolute energy
-1216.74506616

Normal-mode frequencies
7.376
10.1095
19.058
21.5401
28.0759
41.6238
45.431
47.1388
58.7184
63.7646
67.9767
73.5422
75.9706
87.2201
99.071
113.0344

126.5826
145.9141
150.4933
178.1533
258.3561
262.3145
269.2742
270.5671
275.6425
278.7425
292.4992
327.2716
415.2142
418.1248
426.2347
432.8042
441.382
445.9561
447.9687
454.0427
455.5984
456.0224
480.6309
483.8662
490.7469
547.6776
559.9267
568.2805
575.9788
591.527
596.5918
665.3064
737.9118
754.8199
801.6216
802.9455

803.6752
811.5
824.7841
825.3406
828.1212
829.4976
834.7213
838.1157
839.8512
847.0753
883.6688
887.2219
888.7272
892.0106
898.0303
898.2656
899.2378
902.1531
908.1963
916.4847
922.8053
940.9865
982.4309
983.719
986.574
993.1842
1002.4218
1010.1308
1024.5708
1049.7628
1060.8189
1062.0799
1063.5166
1074.1843
1075.308
1077.511

1078.3835
1078.3928
1079.8517
1082.9275
1116.3298
1146.6251
1157.2246
1161.8989
1165.9227
1171.9034
1173.3461
1174.5387
1175.5483
1176.5011
1178.6844
1184.3914
1189.4447
1195.1899
1198.2143
1209.0354
1236.9206
1274.1815
1290.8538
1291.9203
1297.4361
1299.4199
1300.6569
1303.2899
1321.3088
1321.8597
1322.0193
1324.5161
1349.0658
1351.3859
1354.3857
1355.1285

1366.5962
1367.5807
1372.2497
1383.0903
1384.2698
1385.6024
1386.5101
1388.2498
1393.0878
1420.6506
1425.4845
1426.1795
1427.9606
1441.1616
1457.0183
1471.872
1474.8234
1477.7127
1480.733
1484.8119
1486.826
1487.1449
1490.0494
1495.9167
1496.7465
1498.0184
1499.3504
1502.3845
1503.7093
1506.4785
1513.104
1517.4425
1521.0514
1527.5991
1534.9377
1583.697

1654.2935
1673.039
1708.2226
2925.7467
2930.701
2966.3263
2971.0825
2984.3105
3016.9023
3037.177
3039.6549
3043.5624
3057.5143
3057.9538
3058.2616
3059.6197
3068.652
3070.7854
3084.4283
3088.1066
3097.8836
3099.9788
3101.3678
3101.7715
3102.1527
3103.5875
3105.3745
3107.4719
3109.6981
3110.56
3113.0056
3115.6916
3117.4503
3127.2699
3192.079
3196.075

3204.7999
3211.4793
3218.1845
3221.3813
3234.6938
3505.3101
3546.6897
3551.2154

(IIIf)
Lb state optimized

Atom	X	Y	Z
C	-3.818592	-0.090416	-0.618927
C	-3.45942	1.205686	-1.056508
C	-4.356647	2.29275	-0.883593
C	-5.601534	2.083365	-0.273606
C	-5.999088	0.804998	0.176248
C	-7.24644	0.558661	0.795402
C	-7.609055	-0.715399	1.225596
C	-6.715299	-1.814621	1.047466
C	-5.473337	-1.611382	0.441649
C	-5.0802	-0.338206	-0.002018
O	-2.996754	-1.126327	-0.769591
H	-2.114703	-0.845373	-1.183312
H	-2.496587	1.347215	-1.547545
H	-4.074307	3.286958	-1.226871
H	-6.288397	2.921863	-0.140214
H	-7.933506	1.396788	0.933434
H	-8.578202	-0.873195	1.698681
H	-7.003016	-2.810332	1.383182
H	-4.783957	-2.444171	0.300263
N	-0.52078	-0.684878	-1.712745
C	0.105633	-1.910467	-1.188585
C	-0.004921	-1.927982	0.333449
C	0.654265	-0.681192	0.924314
C	0.064983	0.583821	0.299093

C	0.174374	0.51637	-1.218435
H	-0.478553	-0.700751	-2.732333
H	-0.409632	-2.776858	-1.62794
H	1.1751	-1.95737	-1.481062
H	-1.070837	-1.954982	0.60921
H	0.460148	-2.846	0.723891
H	0.539893	-0.664511	2.018663
H	1.738208	-0.709257	0.706637
H	-0.99799	0.683469	0.579676
H	0.602886	1.475109	0.650663
H	-0.282955	1.402176	-1.68383
H	1.244624	0.504316	-1.49672
N	3.238537	1.422363	-0.050369
C	3.446624	1.73071	1.358313
C	3.108846	3.195393	1.625794
C	3.940228	4.108796	0.723745
C	3.781625	3.700632	-0.741632
C	4.103587	2.218713	-0.910588
H	3.4135	0.430388	-0.231997
H	2.799983	1.073088	1.961429
H	4.498117	1.54408	1.679216
H	2.037193	3.353335	1.418606
H	3.279744	3.433747	2.68631
H	3.655925	5.1618	0.868347
H	5.004559	4.022923	1.007212
H	2.73946	3.868455	-1.060021
H	4.432568	4.307367	-1.389085
H	3.94438	1.90612	-1.95415
H	5.184123	2.066214	-0.678739
N	4.552436	-1.259961	-0.952122
C	5.507262	-1.081433	0.143687
C	4.915326	-1.647586	1.43023
C	4.557225	-3.123236	1.249332
C	3.650344	-3.304074	0.031427
C	4.284606	-2.675889	-1.204853
H	4.931299	-0.832797	-1.797407

H	5.711986	-0.005347	0.255158
H	6.474252	-1.587476	-0.064685
H	4.005377	-1.075214	1.680975
H	5.625899	-1.513938	2.259487
H	4.074495	-3.519694	2.154591
H	5.484516	-3.704148	1.099606
H	2.684168	-2.806634	0.218032
H	3.446898	-4.369798	-0.151909
H	3.609393	-2.756614	-2.069467
H	5.214255	-3.231102	-1.454616

Absolute energy
-1216.23747982

Normal-mode frequencies
9.809
11.88
20.601
23.266
28.698
37.968
44.336
49.039
57.068
65.645
68.744
73.517
79.176
87.816
102.729
111.928
125.84
133.987
157.477
169.034
227.47

257.971
261.521
269.166
276.307
278.479
293.512
325.751
366.833
386.158
414.106
416.477
425.568
440.642
444.402
449.17
451.35
453.401
453.902
468.685
472.67
487.954
541.626
554.481
560.935
573.005
577.292
578.221
645.424
685.227
710.176
719.056
772.704
785.209
796.579
813.827
817.51

818.896
821.065
823.16
841.031
844.181
846.361
853.28
882.495
885.932
896.906
899.669
902.865
903.322
907.8
913.196
923.336
929.092
929.225
934.647
954.624
972.259
974.918
976.446
1008.242
1051.272
1060.496
1061.488
1063.904
1069.052
1075.206
1076.239
1078.297
1079.039
1089.529
1091.222
1093.755

1150.037
1155.191
1156.199
1157.99
1159.438
1163
1163.646
1165.924
1166.448
1168.649
1172.279
1176.62
1186.735
1196.632
1211.889
1242.267
1268.349
1280.259
1280.465
1285.92
1287.565
1289.344
1291.133
1310.853
1312.349
1312.953
1320.39
1333.01
1334.864
1336.689
1356.082
1359.52
1366.796
1375.991
1376.885
1378.388

1380.949
1381.501
1383.428
1396.644
1417.861
1420.275
1421.459
1430.829
1437.058
1440.104
1442.858
1449.411
1452.185
1453.875
1455.947
1460.62
1462.587
1463.502
1464.927
1466.299
1468.103
1475.426
1481.31
1482.657
1483.022
1485.474
1487.387
1522.117
1524.624
1539.504
1573.809
1610.569
1620.169
2531.546
2873.759
2916.383

2923.2
2965.006
2966.321
2989.154
3031.992
3037.801
3042.261
3044.871
3056.032
3056.393
3056.841
3057.089
3067.455
3071.702
3085.492
3086.741
3096.545
3098.035
3104.68
3105.992
3108.827
3109.032
3109.768
3112.28
3114.71
3115.075
3120.698
3122.461
3135.15
3195.073
3201.111
3222.452
3228.311
3240.749
3242.741
3289.602

3478.994
3524.97
3532.728

(IIIf)
La state optimized

Atom	X	Y	Z
C	-3.799579	-0.096129	-0.667495
C	-3.444866	1.202151	-1.187219
C	-4.317978	2.246712	-1.027034
C	-5.552225	2.031221	-0.351768
C	-5.936542	0.770422	0.164274
C	-7.163497	0.567322	0.832297
C	-7.498691	-0.724391	1.336138
C	-6.63002	-1.77967	1.176245
C	-5.380183	-1.602987	0.505253
C	-5.038581	-0.334035	0.002954
O	-2.96867	-1.112718	-0.800914
H	-2.074657	-0.840098	-1.227687
H	-2.496516	1.313037	-1.713458
H	-4.078754	3.237112	-1.41331
H	-6.238601	2.871371	-0.226876
H	-7.846154	1.407554	0.959849
H	-8.449828	-0.869256	1.849763
H	-6.889778	-2.766568	1.562083
H	-4.692121	-2.434756	0.373818
N	-0.526223	-0.690259	-1.724781
C	0.098106	-1.917629	-1.195807
C	-0.025439	-1.939543	0.325045
C	0.624088	-0.69246	0.92569
C	0.035744	0.572876	0.300207
C	0.160292	0.512177	-1.216316
H	-0.467269	-0.70324	-2.743912
H	-0.41134	-2.783207	-1.643101
H	1.169108	-1.958061	-1.480574
H	-1.093066	-1.973697	0.593916

H	0.440808	-2.856981	0.714971
H	0.499881	-0.680011	2.01878
H	1.709787	-0.714989	0.717026
H	-1.028701	0.668886	0.575761
H	0.568447	1.464406	0.658387
H	-0.292877	1.39906	-1.683643
H	1.232688	0.501642	-1.483779
N	3.195826	1.428525	-0.024411
C	3.409304	1.725117	1.386442
C	3.05947	3.183682	1.670884
C	3.876578	4.11407	0.773259
C	3.712655	3.719429	-0.695181
C	4.048034	2.242576	-0.881508
H	3.381433	0.440331	-0.216275
H	2.772677	1.055391	1.986905
H	4.464298	1.545023	1.698871
H	1.985027	3.334067	1.472391
H	3.234749	3.412585	2.732711
H	3.583336	5.162753	0.930473
H	4.943356	4.035371	1.049273
H	2.66688	3.880516	-1.00535
H	4.353476	4.339026	-1.340476
H	3.88589	1.93918	-1.927388
H	5.131116	2.09805	-0.657467
N	4.516934	-1.239083	-0.963804
C	5.479243	-1.061736	0.126146
C	4.901983	-1.642216	1.412947
C	4.553672	-3.119154	1.223807
C	3.638617	-3.297748	0.011711
C	4.258686	-2.65559	-1.224596
H	4.887597	-0.803996	-1.808752
H	5.677036	0.014958	0.244266
H	6.44808	-1.558826	-0.094118
H	3.989768	-1.078783	1.675661
H	5.618138	-1.509361	2.23746
H	4.081208	-3.526132	2.129751

H	5.484004	-3.69187	1.062276
H	2.670206	-2.808988	0.210048
H	3.441558	-4.363516	-0.178007
H	3.578529	-2.736054	-2.085433
H	5.190963	-3.201261	-1.484782

Absolute energy
-1216.24824364

Normal-mode frequencies
8.055
13.632
19.63
21.393
28.498
38.845
44.435
48.188
55.717
66.228
67.768
72.673
79.598
88.489
104.685
121.019
134.216
137.839
159.739
170.603
209.651
258.74
260.805
269.299
277.717
280.646

293.902
324.773
334.074
414.066
416.434
426.27
440.807
444.198
449.085
450.161
451.392
453.332
453.82
455.484
472.486
500.005
525.561
554.552
554.905
563.087
573.411
603.021
682.625
689.247
701.353
718.961
773.318
785.51
800.003
814.257
817.098
818.706
820.952
828.068
841.114
844.736

846.375
853.251
856.241
862.931
886.336
898.801
901.106
902.803
904.002
907.652
918.981
927.467
929.352
945.748
955.602
972.473
974.38
975.715
1028.312
1043.31
1060.278
1061.399
1063.913
1070.131
1074.924
1076.309
1077.922
1078.455
1079.148
1090.317
1090.732
1145.937
1150.163
1156.977
1157.998
1159.227

1159.519
1163.635
1165.252
1166.438
1168.746
1172.257
1178.94
1185.694
1196.286
1211.227
1224.341
1249.718
1280.415
1280.678
1286.019
1287.85
1289.344
1291.348
1311.347
1312.471
1313.234
1328.642
1333.39
1334.935
1336.678
1354.835
1359.543
1366.453
1367.32
1376.131
1377.058
1378.735
1381.241
1381.726
1384.28
1416.018

1418.831
1420.21
1421.521
1433.875
1438.209
1440.104
1443.133
1449.306
1451.104
1452.285
1453.906
1460.135
1462.528
1463.107
1464.667
1466.292
1467.283
1472.741
1476.256
1481.213
1482.68
1485.511
1486.953
1497.047
1502.678
1524.595
1568.91
1619.465
1664.147
2657.822
2918.566
2925.079
2967.859
2968.948
2996.954
3038.786

3040.124
3043.169
3044.994
3055.868
3056.501
3057.989
3058.837
3067.039
3072.133
3084.464
3085.909
3096.15
3097.49
3105.373
3108.907
3110.423
3111.111
3112.819
3113.087
3115.367
3115.781
3120.74
3122.749
3137.102
3198.845
3201.642
3214.323
3220.435
3227.886
3239.019
3255.164
3479.438
3520.88
3532.652

(IIIg)

Ground state optimized

Atom	X	Y	Z
C	3.803051	-0.203615	-0.560465
C	3.704034	-1.571261	-0.648515
C	4.815157	-2.388296	-0.356304
C	6.010931	-1.846776	0.016735
C	6.147901	-0.439941	0.113186
C	7.368115	0.169378	0.492988
C	7.478967	1.528423	0.580124
C	6.371317	2.35317	0.29103
C	5.177967	1.797529	-0.07839
C	5.040008	0.394492	-0.17548
O	2.779492	0.626832	-0.82245
H	1.941499	0.118955	-1.012437
H	2.766275	-2.016105	-0.954066
H	4.707807	-3.462213	-0.433904
H	6.862827	-2.475412	0.239328
H	8.216235	-0.46676	0.713654
H	8.419019	1.97765	0.871414
H	6.470859	3.427711	0.362938
H	4.320835	2.415054	-0.304967
N	0.31866	-0.505016	-1.228967
C	-0.514881	0.662993	-0.896943
C	-0.256729	1.08279	0.54453
C	-0.526538	-0.081637	1.495497
C	0.288325	-1.304628	1.078565
C	-0.012576	-1.653103	-0.371766
H	0.165781	-0.755923	-2.198645
H	-0.256944	1.470619	-1.583177
H	-1.579754	0.42368	-1.017989
H	0.781961	1.405982	0.641601
H	-0.891717	1.936343	0.787787
H	-0.297973	0.202257	2.523023
H	-1.589361	-0.341178	1.450658
H	1.357445	-1.098168	1.184806
H	0.054055	-2.159741	1.714309

H	0.576017	-2.511386	-0.697233
H	-1.076018	-1.905751	-0.464448
N	-3.780387	-1.089079	-0.227211
C	-4.203695	-1.474812	1.111538
C	-3.650774	-2.854547	1.444228
C	-4.129528	-3.873909	0.412054
C	-3.794761	-3.407341	-1.003626
C	-4.314161	-1.993978	-1.237845
H	-4.06624	-0.136952	-0.439422
H	-3.840968	-0.733802	1.82636
H	-5.303826	-1.506739	1.201628
H	-2.557983	-2.801498	1.433213
H	-3.957949	-3.150552	2.448118
H	-3.693327	-4.854348	0.60627
H	-5.214869	-3.985025	0.503025
H	-2.711014	-3.411951	-1.142191
H	-4.22213	-4.087098	-1.742179
H	-4.012599	-1.63288	-2.221687
H	-5.417278	-2.017886	-1.219228
N	-5.060049	1.824856	-0.743662
C	-5.213112	1.917793	0.707475
C	-3.861461	2.223924	1.33908
C	-3.298772	3.524699	0.771223
C	-3.233446	3.446935	-0.752228
C	-4.597251	3.083966	-1.324625
H	-5.939925	1.555804	-1.165444
H	-5.604977	0.96898	1.077065
H	-5.92689	2.706194	0.992588
H	-3.173799	1.402311	1.112343
H	-3.962124	2.281556	2.423609
H	-2.31379	3.735687	1.189056
H	-3.950498	4.354537	1.062299
H	-2.514425	2.678038	-1.046725
H	-2.897025	4.394283	-1.174734
H	-4.539695	2.966318	-2.406388
H	-5.299537	3.905937	-1.114156

Absolute energy
-1216.74502641

Normal-mode frequencies
8.9772
13.3958
19.0458
22.1663
30.2772
37.7168
45.327
51.6553
52.6578
55.3794
64.5883
72.1322
82.5091
85.4284
91.8663
120.1826
122.4089
146.0709
148.5018
178.8069
259.846
267.7001
269.9257
270.7052
275.3946
278.6907
287.4219
327.1067
418.5539
421.0075
427.8651

433.4043
441.9158
442.1682
448.0783
454.3356
455.1664
457.9788
481.285
484.3319
491.0889
548.2223
560.105
568.9955
577.1357
591.9456
597.1509
666.0904
738.3581
756.772
794.5233
802.8392
803.9172
816.7267
826.1279
828.3777
828.9166
832.2045
835.0549
838.174
839.5966
849.0366
885.9687
888.3038
891.4648
894.7925
896.4337

897.7138
899.5998
901.0595
909.7427
917.9656
921.1735
945.1814
982.6685
985.4895
989.8951
994.4073
1004.3516
1020.8597
1025.3809
1050.8955
1060.9526
1061.7192
1063.3996
1072.9728
1074.337
1076.6182
1078.5176
1079.3265
1081.1596
1083.6204
1116.8451
1146.9103
1156.7
1160.0192
1166.6908
1172.9694
1174.5769
1174.7872
1175.9563
1178.4004
1180.4039

1189.9228
1191.9503
1196.711
1198.9036
1207.1089
1236.8099
1275.0072
1288.5309
1294.0141
1297.1575
1300.5956
1301.6539
1307.8955
1320.4938
1322.5113
1322.7993
1333.2743
1351.9341
1352.5551
1353.4997
1357.329
1368.5149
1369.2594
1371.1169
1382.1398
1384.5118
1385.5844
1389.2709
1389.4603
1393.6237
1422.6401
1427.0684
1429.1051
1432.7548
1442.7807
1458.9656

1475.1073
1475.5187
1479.7776
1485.0279
1486.3437
1487.3619
1488.5472
1489.7326
1497.27
1498.0584
1499.0828
1500.2372
1502.2586
1505.2209
1506.8024
1515.4664
1518.3181
1521.1729
1535.2516
1536.995
1585.115
1655.2283
1673.6639
1708.7597
2933.8094
2942.2486
2966.2305
2970.4053
3009.9905
3025.2929
3040.8071
3042.3596
3050.4834
3052.4656
3053.1593
3056.4807

3061.7117
3064.7666
3070.0063
3085.0809
3087.5263
3095.1092
3096.135
3099.7848
3100.9794
3101.9574
3102.4082
3104.5786
3105.9588
3107.1891
3108.1396
3108.3601
3109.7541
3114.0419
3116.9452
3190.876
3196.3792
3205.2678
3211.0827
3218.4686
3222.0472
3234.4797
3489.74
3545.9571
3555.7914

(IIIg)
Lb state optimized

Atom	X	Y	Z
C	-3.775785	0.20575	-0.53726
C	-3.671313	1.616127	-0.58059
C	-4.796765	2.426225	-0.274883

C	-6.015681	1.828801	0.075885
C	-6.162867	0.425159	0.130066
C	-7.376666	-0.209809	0.481273
C	-7.489223	-1.597234	0.523917
C	-6.363943	-2.418335	0.209637
C	-5.14721	-1.82868	-0.140007
C	-5.003816	-0.432578	-0.192073
O	-2.736916	-0.575037	-0.81936
H	-1.898177	-0.029145	-1.001294
H	-2.723935	2.064091	-0.880383
H	-4.709625	3.511042	-0.315942
H	-6.87877	2.454863	0.31223
H	-8.239947	0.414902	0.722406
H	-8.438979	-2.056825	0.797211
H	-6.455881	-3.503468	0.241836
H	-4.282205	-2.446767	-0.382007
N	-0.352594	0.579757	-1.194291
C	0.49426	-0.602536	-0.93817
C	0.239655	-1.112667	0.477495
C	0.514485	-0.007866	1.499036
C	-0.297889	1.242632	1.158231
C	-0.000895	1.67547	-0.272663
H	-0.195483	0.892011	-2.153405
H	0.240985	-1.373802	-1.680802
H	1.563239	-0.335984	-1.042977
H	-0.808274	-1.443571	0.556735
H	0.879657	-1.988581	0.66598
H	0.286143	-0.356031	2.517126
H	1.587256	0.253079	1.465361
H	-1.37764	1.034819	1.253943
H	-0.058333	2.065418	1.848779
H	-0.586061	2.566202	-0.545635
H	1.074816	1.915661	-0.362373
N	3.682672	1.064064	-0.258181
C	4.162511	1.438684	1.067837
C	3.648226	2.827591	1.434305

C	4.105015	3.849373	0.391844
C	3.711608	3.396315	-1.015206
C	4.200807	1.973844	-1.275842
H	4.012745	0.116408	-0.470728
H	3.809278	0.692629	1.79761
H	5.275865	1.448251	1.119299
H	2.545329	2.795158	1.467223
H	4.00119	3.110796	2.43734
H	3.689744	4.844506	0.610752
H	5.204415	3.943571	0.443538
H	2.613714	3.419945	-1.116035
H	4.124502	4.080089	-1.772431
H	3.862757	1.625891	-2.263602
H	5.314559	1.981454	-1.29332
N	5.168567	-1.69079	-0.545055
C	5.207483	-1.989625	0.887619
C	3.80725	-2.364031	1.363504
C	3.286223	-3.56647	0.575405
C	3.350696	-3.279536	-0.925176
C	4.76146	-2.859365	-1.326299
H	6.09239	-1.386158	-0.850872
H	5.573671	-1.099658	1.420434
H	5.902294	-2.826443	1.115639
H	3.13696	-1.500949	1.200756
H	3.820806	-2.575728	2.443123
H	2.260045	-3.821104	0.880605
H	3.912159	-4.447082	0.803888
H	2.65626	-2.458441	-1.171509
H	3.043583	-4.160952	-1.507442
H	4.79801	-2.597384	-2.393326
H	5.449995	-3.717061	-1.167476

Absolute energy
-1216.23826813

Normal-mode frequencies

13.081
14.685
19.775
25.337
32.628
34.599
42.191
49.39
52.893
55.234
66.194
67.207
80.448
84.776
93.799
116.306
129.281
134.689
155.018
168.913
227.838
257.681
263.528
267.747
275.564
281.746
293.196
326.178
366.467
387.151
416.14
420.377
431.888
440.388
443.375
448.556

451.452
453.206
455.38
469.16
473.076
487.106
541.189
554.329
563.419
568.97
577.24
578.225
644.051
684.946
710.295
719.382
770.516
785.176
796.56
810.977
819.405
820.429
824.198
826.656
840.313
844.617
845.745
853.718
883.618
886.866
901.225
902.057
902.632
904.377
907.709
912.409

925.761
928.528
930.357
936.229
971.399
973.405
976.66
981.19
1008.366
1051.144
1061.588
1062.076
1064.423
1072.16
1073.887
1076.516
1078.64
1078.948
1091.234
1105.213
1109.135
1154.154
1154.736
1157.036
1157.743
1158.702
1162.827
1166.311
1167.154
1168.577
1170.357
1172.172
1184.259
1185.876
1197.237
1212.791

1242.059
1268.221
1277.55
1283.68
1286.462
1289.749
1292.277
1297.498
1310.223
1314.509
1318.896
1329.754
1334.715
1335.732
1338.623
1360.349
1360.712
1365.359
1374.86
1377.449
1378.565
1380.05
1385.851
1388.471
1398.804
1422.413
1423.483
1426.195
1430.887
1439.621
1442.99
1447.434
1450.023
1451.294
1451.865
1458.101

1460.288
1462.443
1466.153
1466.617
1467.781
1469.91
1475.313
1481.385
1483.197
1483.862
1486.406
1489.385
1523.157
1539.626
1545.555
1576.348
1612.196
1619.756
2517.016
2820.933
2927.31
2936.272
2967.186
2968.2
3027.579
3033.618
3040.957
3046.095
3048.958
3051.949
3053.048
3054.406
3058.926
3060.886
3071.66
3083.641

3093.915
3103.028
3104.373
3105.594
3107.512
3108.154
3109.035
3109.907
3110.333
3112.296
3112.919
3113.863
3118.389
3124.331
3194.617
3200.753
3221.611
3228.334
3239.507
3242.181
3284.945
3438.076
3524.969
3536.601

(IIIg)

La state optimized

Atom	X	Y	Z
C	-3.754562	0.24249	-0.572589
C	-3.647647	1.680809	-0.622915
C	-4.739245	2.443705	-0.297542
C	-5.952091	1.804551	0.084029
C	-6.096547	0.397316	0.136632
C	-7.304807	-0.226454	0.516634
C	-7.393271	-1.649524	0.556279
C	-6.303945	-2.423293	0.226591

C	-5.06749	-1.819033	-0.15982
C	-4.968019	-0.416304	-0.203972
O	-2.71291	-0.509691	-0.868707
H	-1.858284	0.042242	-1.039197
H	-2.703684	2.123322	-0.942029
H	-4.689124	3.531671	-0.332245
H	-6.814246	2.42221	0.344428
H	-8.163215	0.3912	0.781048
H	-8.332056	-2.120392	0.850402
H	-6.3757	-3.511551	0.257132
H	-4.20483	-2.426204	-0.42373
N	-0.35316	0.612896	-1.193468
C	0.474336	-0.58479	-0.932185
C	0.198783	-1.097358	0.478457
C	0.477392	-0.001324	1.508231
C	-0.316798	1.260517	1.166572
C	0.000304	1.698736	-0.258364
H	-0.173739	0.928977	-2.147759
H	0.216939	-1.348066	-1.681403
H	1.546283	-0.329456	-1.026361
H	-0.853286	-1.41787	0.546703
H	0.826564	-1.981668	0.667787
H	0.234677	-0.351755	2.521957
H	1.553258	0.247481	1.486732
H	-1.399087	1.064018	1.255585
H	-0.074124	2.076991	1.863254
H	-0.569311	2.599045	-0.533175
H	1.079638	1.923629	-0.336185
N	3.657101	1.054024	-0.252965
C	4.140162	1.416978	1.075623
C	3.64268	2.810177	1.448638
C	4.112406	3.831465	0.411512
C	3.714911	3.390149	-0.998067
C	4.187259	1.96321	-1.265522
H	3.978987	0.104171	-0.469375
H	3.778085	0.671465	1.801566

H	5.253339	1.412997	1.127474
H	2.53938	2.791516	1.481736
H	3.998705	3.08395	2.453152
H	3.709157	4.830475	0.635
H	5.212752	3.912049	0.464453
H	2.617398	3.428042	-1.100057
H	4.13667	4.072625	-1.7515
H	3.846706	1.624317	-2.255581
H	5.300857	1.957453	-1.281431
N	5.116042	-1.712943	-0.550301
C	5.15452	-2.01667	0.88153
C	3.752299	-2.383311	1.357497
C	3.222816	-3.580239	0.566616
C	3.288649	-3.290458	-0.933363
C	4.701491	-2.877309	-1.334345
H	6.041878	-1.41401	-0.855841
H	5.52738	-1.131056	1.416939
H	5.843845	-2.858833	1.10596
H	3.087788	-1.515163	1.197433
H	3.765054	-2.597867	2.436532
H	2.195193	-3.829221	0.871678
H	3.84292	-4.465458	0.792825
H	2.598841	-2.464922	-1.177928
H	2.976111	-4.168723	-1.517402
H	4.738979	-2.612996	-2.400749
H	5.385193	-3.73916	-1.177985

Absolute energy
-1216.24914685

Normal-mode frequencies
11.921
14.327
19.236
23.346
32.318

35.011
41.565
49.903
53.226
56.332
65.977
66.201
81.528
85.386
95.688
127.42
130.012
141.992
160.786
170.471
210.003
257.511
263.819
267.718
277.604
281.646
294.388
325.511
335.024
416.223
420.458
431.552
440.489
442.805
448.68
450.234
451.345
453.033
455.4
457.225
472.962

500.479
526.266
554.421
555.661
564.402
569.189
604
682.228
689.105
700.661
719.421
773.577
785.725
798.977
812.025
819.257
820.069
822.674
829.153
840.32
844.951
845.669
853.805
856.528
863.113
887.365
900.855
902.218
903.626
905.368
907.988
918.694
928.573
929.93
945.649
972.448

973.427
976.87
981.476
1028.853
1043.414
1061.521
1061.658
1064.266
1070.443
1073.167
1076.604
1077.006
1079.07
1080.159
1090.867
1107.206
1154.195
1155.986
1157.686
1158.487
1158.617
1166.252
1167.138
1168.487
1169.526
1171.087
1174.359
1185.516
1188.061
1196.928
1212.362
1224.574
1250.07
1277.809
1283.727
1286.53

1289.762
1292.083
1298.037
1310.195
1314.648
1327.457
1332.513
1334.778
1335.776
1339.047
1358.55
1360.395
1365.253
1368.144
1375.017
1377.705
1378.566
1380.319
1385.922
1389.254
1417.56
1422.598
1423.536
1426.296
1434.276
1439.495
1442.75
1447.385
1450.004
1451.138
1451.734
1453.235
1459.917
1462.654
1465.955
1466.49

1467.29
1468.469
1473.843
1476.706
1481.467
1483.645
1486.336
1489.236
1498.57
1503.602
1545.753
1574.681
1620.22
1663.363
2595.183
2929.863
2938.708
2968.885
2970.404
3035.061
3038.383
3041.165
3046.723
3048.727
3051.924
3053.445
3056.69
3057.699
3061.176
3071.31
3083.371
3093.937
3103.162
3104.628
3105.577
3108.54

3109.02
3110.167
3111.735
3111.936
3112.803
3113.241
3116.255
3118.803
3124.859
3198.282
3201.205
3213.878
3220.749
3227.632
3239.364
3255.372
3434.43
3520.706
3536.534

(IIIh)
Ground state optimized

Atom	X	Y	Z
C	-3.695856	0.184976	-0.619667
C	-3.276622	-1.026972	-1.113317
C	-4.143207	-2.139009	-1.107911
C	-5.413402	-2.041846	-0.618546
C	-5.878819	-0.805245	-0.107077
C	-7.188847	-0.653176	0.407784
C	-7.617911	0.548546	0.896366
C	-6.75651	1.665966	0.89585
C	-5.4848	1.553732	0.406522
C	-5.019387	0.320931	-0.103928
O	-2.916092	1.278803	-0.592936
H	-1.989211	1.071262	-0.899833
H	-2.276372	-1.117676	-1.515701

H	-3.785752	-3.08098	-1.50267
H	-6.077285	-2.896089	-0.61629
H	-7.847417	-1.512802	0.406114
H	-8.622469	0.647434	1.285513
H	-7.107191	2.61242	1.284387
H	-4.813415	2.40019	0.397197
N	-0.2742	0.958675	-1.237388
C	0.359427	-0.287843	-0.783505
C	0.048574	-0.501577	0.690694
C	0.561573	0.682189	1.508697
C	-0.023921	1.987435	0.974057
C	0.266237	2.123559	-0.515094
H	-0.106344	1.078154	-2.229432
H	-0.025376	-1.112389	-1.385395
H	1.448387	-0.241099	-0.918609
H	-1.033316	-0.603385	0.817934
H	0.506767	-1.433156	1.026799
H	0.317774	0.555342	2.563741
H	1.652219	0.72527	1.421963
H	-1.104461	2.00233	1.13173
H	0.399451	2.843708	1.501318
H	-0.203424	3.020922	-0.918383
H	1.350839	2.193661	-0.662615
N	3.901722	0.853327	-0.333715
C	4.419486	1.306428	0.949631
C	4.13599	2.79345	1.11785
C	4.769558	3.580585	-0.027813
C	4.322267	3.023639	-1.37808
C	4.568371	1.521219	-1.444925
H	4.003152	-0.153287	-0.432578
H	3.943975	0.732691	1.747369
H	5.508686	1.145193	1.033621
H	3.051931	2.941499	1.114004
H	4.514778	3.142005	2.079545
H	4.524941	4.640448	0.050136
H	5.858675	3.498972	0.04791

H	3.25485	3.212233	-1.51469
H	4.849704	3.522835	-2.192196
H	4.182972	1.110761	-2.378858
H	5.657368	1.343115	-1.43099
N	4.599491	-2.288468	-0.501815
C	4.762089	-2.24407	0.950594
C	3.390356	-2.208648	1.611544
C	2.575608	-3.431328	1.196549
C	2.493557	-3.513526	-0.325813
C	3.88927	-3.490521	-0.934779
H	5.505687	-2.245348	-0.950554
H	5.337094	-1.353496	1.208783
H	5.316307	-3.118363	1.325789
H	2.869268	-1.300433	1.290603
H	3.50085	-2.161451	2.695603
H	1.577893	-3.399635	1.635619
H	3.061805	-4.333619	1.580652
H	1.931807	-2.656292	-0.706369
H	1.970316	-4.418027	-0.637756
H	3.832598	-3.486778	-2.022981
H	4.4231	-4.40467	-0.630612

Absolute energy
-1216.74503168

Normal-mode frequencies
9.985
15.2556
18.0825
24.3647
32.1275
39.7697
47.3452
51.5343
55.2236
55.8216

68.3807
71.7555
81.7494
85.5109
100.5464
114.731
122.6006
147.3443
150.1581
178.5095
260.3486
269.2555
270.1942
270.7591
274.8679
281.0322
287.4545
328.3558
419.4621
421.4736
429.1201
433.5317
441.9647
442.2139
448.509
454.1573
455.1271
457.4431
481.3809
484.5752
491.1889
548.5004
561.6514
567.7062
576.4236
592.1345

597.482
665.796
738.4675
756.9345
797.2857
802.7131
804.1791
814.7814
826.4152
828.0916
829.2123
832.9261
834.7378
838.2559
839.8132
848.445
885.9853
887.0755
891.1951
894.2995
896.7205
897.4334
899.8835
901.3734
910.1194
917.5691
922.3294
944.7145
982.7517
985.7709
990.1974
994.1031
1004.9203
1017.6723
1026.2197
1051.5012

1060.9041
1061.5845
1063.2676
1073.1678
1074.3409
1076.931
1078.6707
1079.4202
1080.9706
1083.8642
1116.8362
1147.3288
1156.5376
1160.1667
1166.6044
1172.6275
1174.5656
1174.6221
1176.257
1178.856
1180.7262
1189.6383
1192.6391
1196.4055
1198.9515
1207.311
1237.1741
1275.3954
1288.1181
1293.9217
1297.1659
1300.5034
1301.5145
1308.1206
1320.7064
1322.5245

1322.7731
1333.7033
1351.8848
1352.5308
1353.3449
1357.1011
1367.784
1369.0135
1370.9012
1382.3155
1384.4632
1385.217
1389.247
1390.7789
1393.1586
1423.2248
1426.9987
1428.5551
1432.9863
1443.3102
1459.1113
1474.7006
1475.4419
1479.027
1484.4056
1485.803
1486.6268
1487.7005
1490.458
1496.7624
1498.6844
1499.4215
1501.3812
1502.6449
1505.7685
1506.9129

1515.6702
1519.2706
1521.0413
1534.9568
1537.192
1585.241
1655.5489
1673.3703
1708.585
2934.71
2940.9234
2967.3105
2969.3263
3011.2604
3024.4644
3040.6669
3042.9048
3050.4482
3052.878
3053.8989
3058.8738
3062.0109
3062.7651
3067.0187
3084.6638
3088.2224
3095.5024
3095.8961
3096.4871
3101.772
3102.5821
3104.9245
3105.8493
3106.4959
3107.095
3108.4573

3109.4358
3111.3922
3112.7505
3115.7021
3190.6814
3194.6566
3203.9369
3210.4055
3218.2288
3221.4897
3233.7317
3490.4014
3544.8548
3556.3864

(IIIh)
Lb state optimized

Atom	X	Y	Z
C	3.633664	-0.303068	-0.631216
C	3.254609	0.723305	-1.52912
C	4.168666	1.75847	-1.861234
C	5.452669	1.765855	-1.297718
C	5.871729	0.759776	-0.399729
C	7.158014	0.738943	0.188953
C	7.53879	-0.265208	1.075002
C	6.625274	-1.308823	1.413922
C	5.345535	-1.32219	0.853907
C	4.934185	-0.324827	-0.044511
O	2.796509	-1.283403	-0.304107
H	1.866868	-1.116445	-0.688541
H	2.267199	0.683768	-1.989003
H	3.871104	2.540164	-2.558738
H	6.154024	2.562359	-1.555356
H	7.860107	1.536248	-0.065924
H	8.537994	-0.254151	1.51043
H	6.927165	-2.093645	2.106553

H	4.640203	-2.114718	1.105156
N	0.267579	-0.866287	-1.03288
C	-0.168688	0.310224	-0.257115
C	0.128306	0.079967	1.221452
C	-0.581946	-1.18227	1.712656
C	-0.195699	-2.377183	0.839422
C	-0.487554	-2.067361	-0.625232
H	0.088188	-0.691096	-2.022635
H	0.376094	1.191125	-0.630066
H	-1.254958	0.472309	-0.396242
H	1.216872	-0.03022	1.353994
H	-0.189079	0.959866	1.80133
H	-0.341158	-1.377285	2.767911
H	-1.674728	-1.030447	1.644762
H	0.878369	-2.594698	0.95858
H	-0.751071	-3.278951	1.139759
H	-0.182344	-2.902108	-1.272646
H	-1.571959	-1.888897	-0.749403
N	-3.912504	-0.572507	-0.429564
C	-4.467299	-1.161019	0.786796
C	-4.242781	-2.669969	0.793082
C	-4.877767	-3.304096	-0.445229
C	-4.380059	-2.612926	-1.715466
C	-4.582537	-1.103448	-1.615249
H	-4.092372	0.436243	-0.386513
H	-3.977386	-0.696764	1.658063
H	-5.559237	-0.962332	0.880795
H	-3.156196	-2.864082	0.793932
H	-4.657336	-3.110327	1.712461
H	-4.670288	-4.384037	-0.481852
H	-5.97469	-3.190897	-0.381676
H	-3.306306	-2.822897	-1.852911
H	-4.905017	-3.002838	-2.600746
H	-4.172893	-0.600797	-2.504357
H	-5.67625	-0.896121	-1.594943
N	-4.779268	2.381354	0.23828

C	-4.285749	2.424716	1.615577
C	-2.784252	2.152129	1.620661
C	-2.053929	3.164869	0.736115
C	-2.670925	3.206954	-0.663242
C	-4.176462	3.43664	-0.57588
H	-5.792928	2.486252	0.23693
H	-4.819452	1.662931	2.20282
H	-4.478486	3.410803	2.090644
H	-2.611252	1.132351	1.235351
H	-2.399707	2.18593	2.651673
H	-0.980061	2.928888	0.679612
H	-2.133922	4.16656	1.194023
H	-2.492595	2.246946	-1.176914
H	-2.205018	3.997895	-1.269812
H	-4.630072	3.411104	-1.57707
H	-4.364912	4.444547	-0.147064

Absolute energy
-1216.23935248

Normal-mode frequencies
10.529
13.749
21.304
26.291
35.141
48.149
49.313
55.633
57.383
59.669
69.515
74.68
84.559
89.767
95.379

109.834
126.832
132.852
151.697
172.292
228.76
255.082
262.986
269.638
276.398
278.633
281.734
332.219
367.086
386.841
415.694
418.955
427.921
437.513
443.132
446.54
451.67
453.222
455.991
468.446
473.859
486.892
540.357
553.187
561.225
563.017
577.491
582.253
645.604
685.602
710.034

719.413
772.415
785.282
796.962
805.137
818.273
820.814
822.345
830.813
838.709
844.744
844.86
852.641
881.302
883.557
901.003
902.595
904.086
906.557
907.751
912.548
926.896
929.98
930.889
934.348
972.034
973.132
975.254
981.087
1008.066
1050.768
1061.042
1063.305
1064.874
1072.431
1074.882

1076.542
1078.649
1080.434
1091.244
1107.275
1108.578
1154.778
1155.747
1156.884
1157.964
1159.651
1162.631
1166.171
1167.339
1170.045
1171.17
1172.565
1183.218
1191.84
1195.458
1212.698
1241.438
1265.793
1277.855
1281.87
1287.507
1289.368
1291.081
1296.969
1309.451
1314.069
1317.201
1330.242
1334.804
1335.836
1339.416

1358.628
1360.919
1363.969
1374.937
1377.674
1379.35
1380.738
1383.932
1386.412
1398.949
1422.369
1424.178
1428.017
1430.738
1440.874
1441.653
1445.436
1448.794
1451.054
1451.981
1455.099
1459.654
1463.685
1464.852
1466.006
1468.401
1469.537
1474.378
1481.782
1483.14
1483.914
1486.976
1489.163
1523.743
1541.067
1541.44

1578.052
1615.31
1620.625
2508.159
2765.268
2934.254
2942.26
2966.104
2969.059
3025.758
3032.543
3042.358
3043.711
3044.77
3053.68
3054.741
3058.985
3063.358
3064.044
3069.437
3083.2
3090.808
3102.573
3103.619
3103.815
3105.115
3107.726
3109.55
3111.12
3112.048
3112.521
3113.021
3116.027
3117.575
3122.459
3196.783

3202.772
3222.198
3227.494
3240.411
3241.4
3281.425
3439.8
3519.465
3542.43

(IIIh)
La state optimized

Atom	X	Y	Z
C	-3.550032	-0.65864	0.641345
C	-3.18582	0.006218	1.870754
C	-4.045932	0.925596	2.413579
C	-5.275616	1.209556	1.756979
C	-5.670567	0.572238	0.55604
C	-6.890663	0.864768	-0.08992
C	-7.236315	0.198448	-1.302932
C	-6.381309	-0.729213	-1.853156
C	-5.136702	-1.04121	-1.224093
C	-4.786856	-0.394833	-0.024014
O	-2.729992	-1.534917	0.094378
H	-1.794146	-1.51968	0.537452
H	-2.249496	-0.267153	2.357434
H	-3.801717	1.43358	3.346286
H	-5.950784	1.946575	2.196917
H	-7.559712	1.606745	0.34624
H	-8.183604	0.429837	-1.791267
H	-6.648856	-1.238489	-2.780262
H	-4.459229	-1.774555	-1.65506
N	-0.250722	-1.386991	0.936181
C	0.173187	-0.027447	0.539402
C	-0.090905	0.177112	-0.949029
C	0.649206	-0.881599	-1.7678

C	0.257319	-2.281149	-1.291482
C	0.520784	-2.413695	0.204614
H	-0.075183	-1.504339	1.935529
H	-0.396871	0.69924	1.138562
H	1.252751	0.103542	0.739738
H	-1.173705	0.105658	-1.142128
H	0.229217	1.190965	-1.233738
H	0.436344	-0.761315	-2.839995
H	1.736834	-0.752142	-1.624192
H	-0.81209	-2.459063	-1.491937
H	0.828369	-3.05294	-1.829354
H	0.211996	-3.40187	0.574538
H	1.600427	-2.274561	0.395555
N	3.752632	-0.578103	0.41634
C	4.500342	-0.915789	-0.790595
C	4.534551	-2.429809	-0.976449
C	5.163759	-3.096473	0.247912
C	4.458613	-2.64673	1.528628
C	4.405941	-1.122883	1.603349
H	3.715259	0.443255	0.506693
H	4.017577	-0.432445	-1.654987
H	5.549032	-0.541231	-0.747355
H	3.499724	-2.790826	-1.108138
H	5.092676	-2.687224	-1.889167
H	5.138093	-4.192351	0.153414
H	6.227878	-2.805618	0.304082
H	3.428644	-3.040929	1.539716
H	4.971782	-3.048651	2.415449
H	3.84459	-0.800188	2.493169
H	5.445662	-0.739223	1.713966
N	4.158163	2.541119	0.4231
C	4.309298	2.647727	-1.02944
C	2.95001	2.451405	-1.693544
C	1.956722	3.493891	-1.178873
C	1.887364	3.444554	0.347777
C	3.281944	3.588971	0.949441

H	5.074944	2.617217	0.863123
H	5.020367	1.878053	-1.364298
H	4.718866	3.635912	-1.330318
H	2.580383	1.439573	-1.447035
H	3.053252	2.510422	-2.787329
H	0.96054	3.3398	-1.620256
H	2.29057	4.497794	-1.495101
H	1.467075	2.474958	0.664206
H	1.22867	4.23495	0.736985
H	3.242375	3.495113	2.044045
H	3.670982	4.602695	0.713492

Absolute energy
-1216.24925027

Normal-mode frequencies
6.915
17.688
18.736
26.789
29.625
38.959
45.111
49.973
54.237
56.088
59.637
70.91
78.814
85.575
100.837
116.834
128.073
142.368
160.851
175.904

211.631
256.675
263.801
265.892
278.006
278.537
284.849
324.647
340.043
416.057
418.816
427.443
440.244
442.819
447.912
449.295
451.163
452.372
454.16
456.766
474.656
500.736
525.373
551.552
552.903
566.156
568.933
605.076
683.179
689.654
702.109
718.329
776.103
786.321
800.12
810.287

818.839
819.845
821.371
832.828
839.829
845.364
845.73
854.144
856.273
863.428
886.362
901.803
902.522
903.647
906.071
907.748
920.198
928.256
935.041
945.949
971.012
973.233
975.889
981.104
1027.189
1044.525
1061.497
1061.998
1064.209
1070.087
1073.031
1076.173
1077.898
1079.443
1081.976
1091.006

1104.198
1147.096
1155.449
1157.874
1158.155
1158.818
1161.365
1166.236
1167.452
1168.669
1171.312
1176.933
1186.561
1197.168
1202.931
1211.906
1225.145
1250.726
1278.555
1283.353
1286.188
1289.751
1293.584
1298.498
1310.239
1314.124
1325.74
1331.974
1334.824
1335.806
1339.491
1358.082
1360.581
1364.949
1368.264
1375.842

1378.157
1380.513
1381.349
1385.171
1388.879
1418.627
1421.695
1422.36
1425.84
1434.154
1438.963
1443.045
1446.312
1448.157
1450.84
1451.581
1452.521
1459.753
1463.217
1465.807
1466.326
1466.798
1467.717
1472.472
1476.05
1481.976
1483.673
1486.117
1487.853
1497.62
1504.47
1543.47
1582.488
1621.834
1661.566
2533.075

2928.09
2936.168
2965.697
2967.085
3033.678
3040.455
3043.438
3044.798
3048.939
3050.207
3051.929
3059.058
3062.234
3063.862
3069.657
3086.693
3093.429
3104.222
3104.943
3105.46
3105.931
3108.393
3109.575
3112.501
3112.57
3114.098
3115.886
3119.885
3120.293
3124.442
3198.695
3202.307
3214.109
3220.062
3228.901
3238.874

3254.98
3431.019
3515.153
3537.486

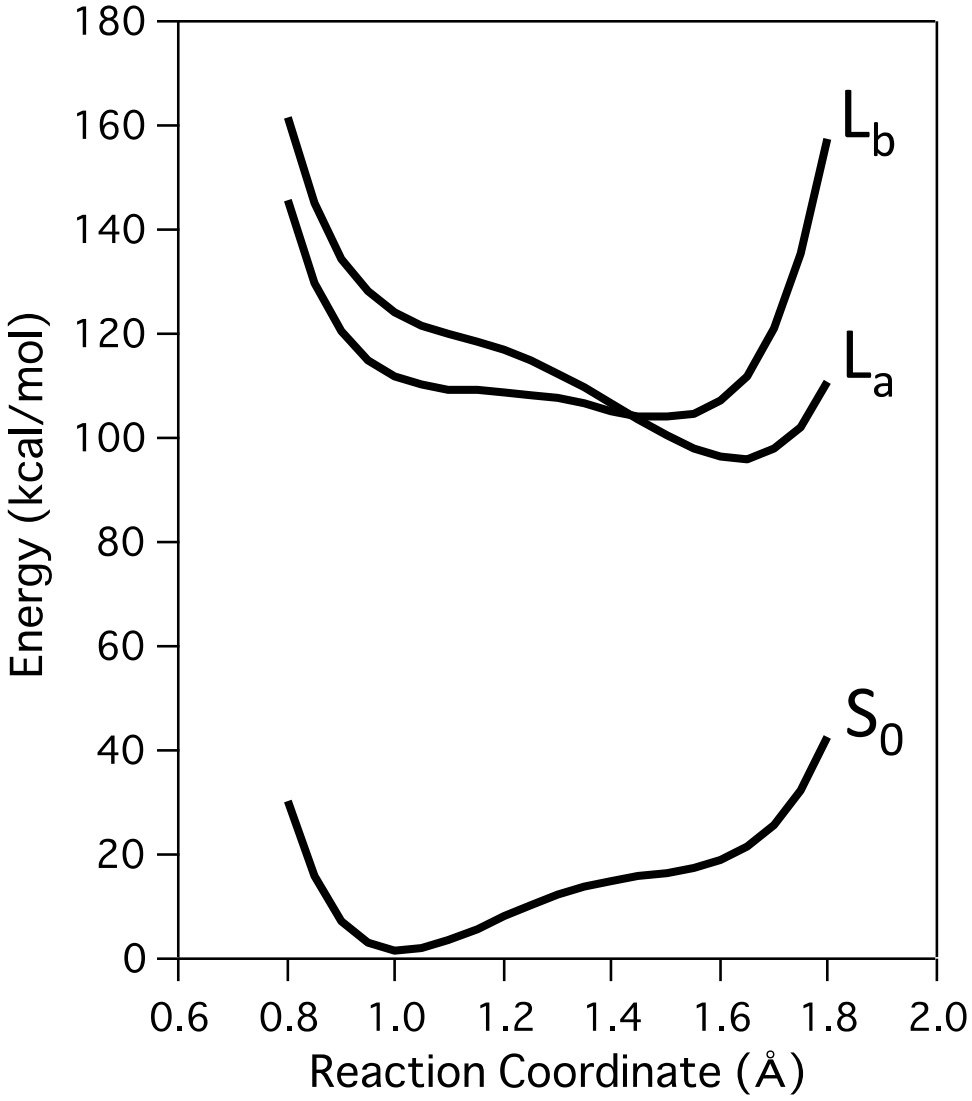

Fig. S1 Potential energy curves along OH distance in IIa at the CISD/Lan2DZ level. Other geometric parameters were fixed at those in IIa.