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Supporting Information

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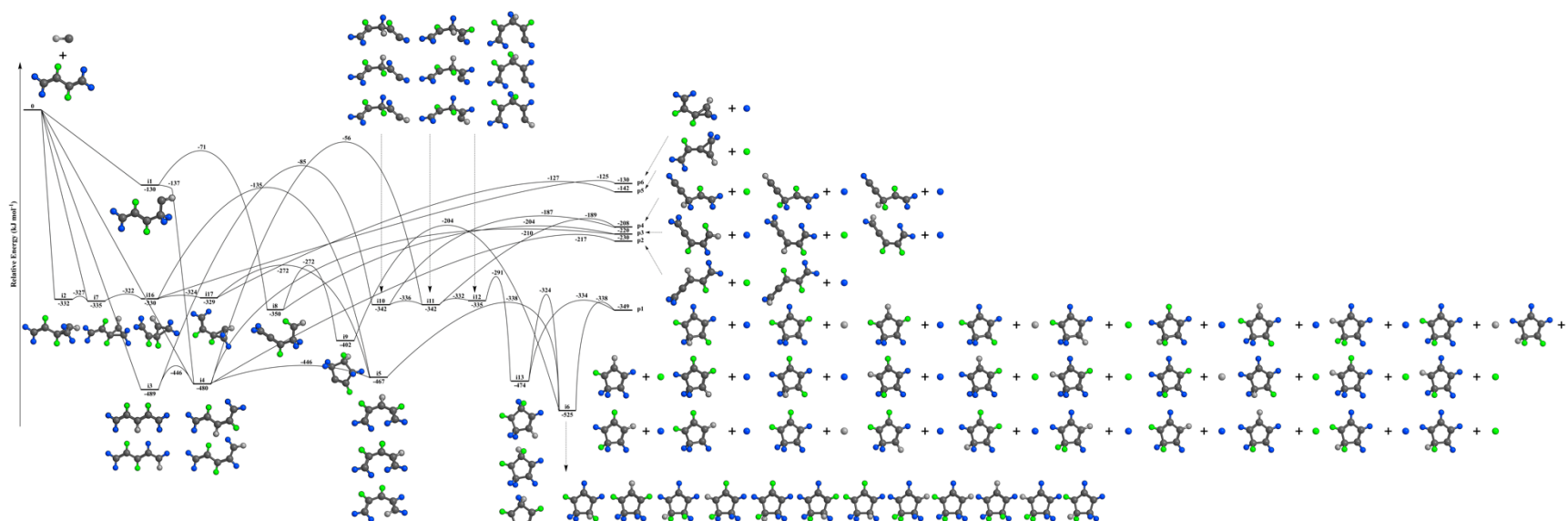


Figure S1. Portion of the C₅H₇ potential energy surface (PES) leading to **p1-p6**. H atoms from methylidyne radical, CH moiety and CH₂ moiety of 1,3-butadiene reactant are highlighted in grey, green and blue, respectively.

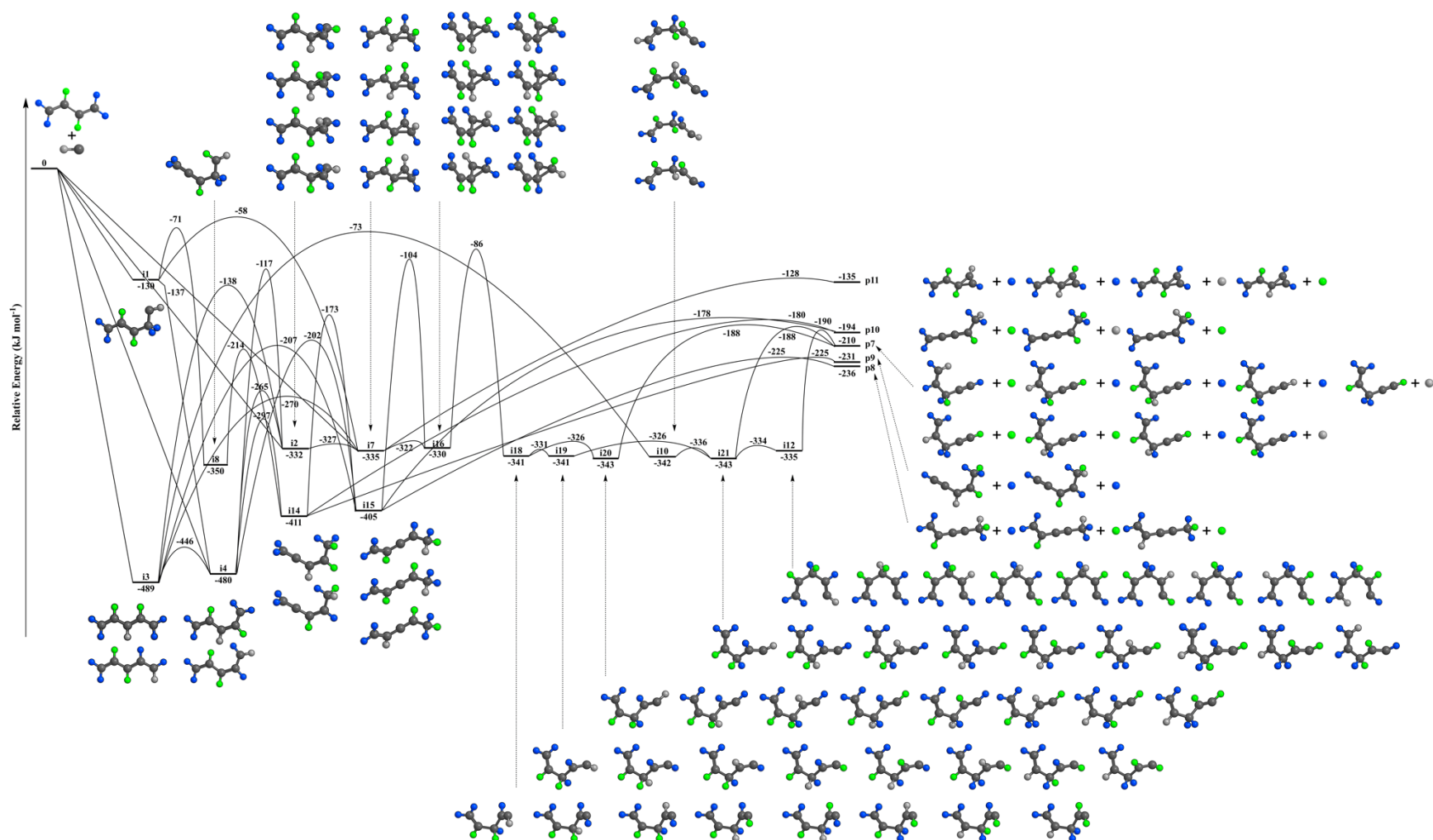


Figure S2. Portion of the C_5H_7 PES leading to **p7-p11**. H atoms from methylidyne radical, CH moiety and CH_2 moiety of 1,3-butadiene reactant are highlighted in grey, green and blue, respectively.

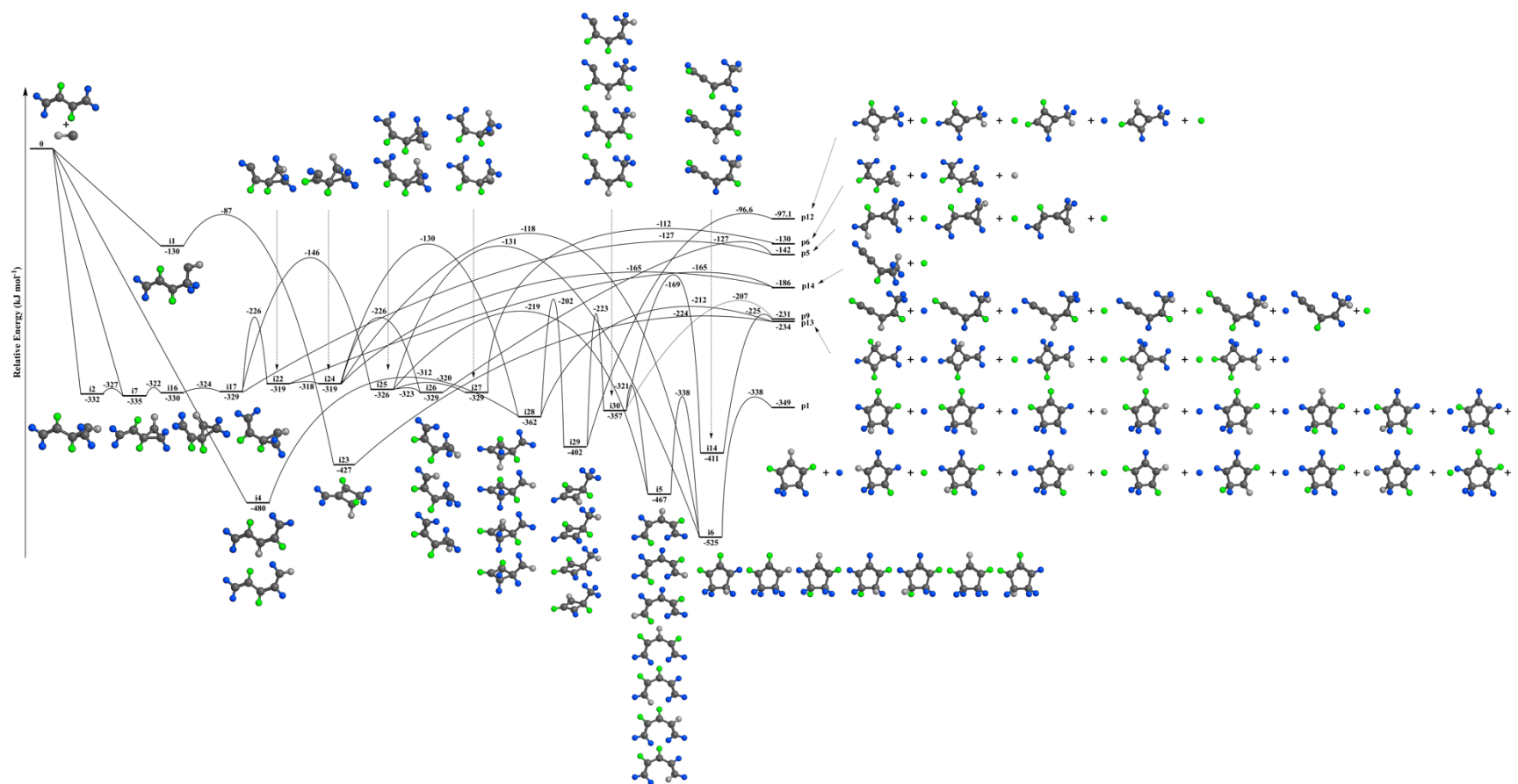


Figure S3. Portion of the C_5H_7 PES leading to **p1**, **p5**, **p6**, **p9**, **p12**-**p14**. H atoms from methylidyne radical, CH moiety and CH_2 moiety of 1,3-butadiene reactant are highlighted in grey, green and blue, respectively.

Table S1. Rate constants (k , in s^{-1}) for all unimolecular reactions in the CH + 1,3-butadiene system calculated using RRKM theory at $E_{\text{col}} = 20.6 \text{ kJ mol}^{-1}$.

Reaction	k	Reaction	k	Reaction	k	Reaction	k
i3-i4	5.63E+12	i25-i26	2.65E+12	i17-i16	1.18E+13	i30-p9	8.04E+10
i4-i3	3.63E+12	i26-i25	2.59E+12	i4-i15	2.55E+07	i31-i32	5.94E+07
i4-i5	2.53E+12	i16-i18	6.44E+05	i15-i4	4.31E+08	i32-i31	3.43E+07
i5-i4	5.26E+12	i18-i16	1.81E+05	i15-p10	2.40E+08	i32-p2	6.36E+09
i5-i6	2.39E+10	i24-i28	2.40E+07	i23-p13	5.07E+09	i32-p15	3.42E+10
i6-i5	2.97E+10	i28-i24	2.74E+06	i1-i23	1.19E+10	i32-i33	2.92E+08
i6-p1	1.07E+11	i8-i9	3.93E+09	i23-i1	9.38E+03	i33-i32	2.99E+09
i1-i4	1.56E+13	i9-i8	1.98E+11	i4-i14	2.81E+09	i31-i33	2.37E+07
i4-i1	2.25E+05	i18-i19	3.16E+12	i14-i4	2.06E+10	i33-i31	2.80E+08
i4-p2	4.52E+08	i19-i18	3.16E+12	i3-i7	2.91E+08	i33-i34	9.70E+12
i6-i13	9.77E+09	i17-i25	3.06E+08	i7-i3	4.65E+11	i34-i33	8.92E+12
i13-i6	5.89E+10	i25-i17	3.13E+08	i24-p14	7.16E+09	i34-p15	2.10E+10
i3-i10	1.08E+03	i24-i26	1.52E+10	i22-p14	7.16E+09	i33-i35	4.00E+12
i10-i3	2.26E+05	i26-i24	8.83E+09	i10-p4	7.91E+09	i35-i33	4.89E+12
i4-p3	4.63E+08	i15-i16	6.22E+04	i14-i15	2.06E+07	i35-i36	1.80E+14
i10-i11	2.25E+12	i16-i15	3.03E+06	i15-i14	4.76E+07	i36-i35	6.15E+13
i11-i10	2.50E+12	i28-p13	2.89E+09	i14-p10	1.13E+08	i36-p15	1.86E+10
i11-i12	1.99E+12	i17-p5	2.03E+08	i8-i14	1.52E+09	i11-i36	1.49E+02
i12-i11	2.40E+12	i15-i31	5.19E+11	i14-i8	4.25E+08	i36-i11	3.49E+01
i12-i13	7.56E+10	i31-i15	5.20E+11	i14-p9	2.29E+10	i36-i37	4.48E+10
i13-i12	5.41E+09	i1-i7	1.28E+09	i25-i27	1.14E+13	i37-i36	6.00E+11
i13-p1	5.26E+11	i7-i1	2.30E+04	i27-i25	6.77E+12	i37-p11	1.31E+08
i19-i21	9.00E+12	i3-i15	2.55E+07	i27-p6	7.62E+07	i37-p16	1.76E+06
i21-i19	8.95E+12	i15-i3	5.56E+08	i12-p7	1.17E+10	i37-i38	6.91E+11
i17-i22	8.84E+09	i16-p6	7.52E+08	i11-p4	1.25E+10	i38-i37	1.07E+12
i22-i17	1.52E+10	i22-i24	2.83E+12	i21-p7	8.78E+09	i38-p6	1.22E+07
i1-i8	5.63E+09	i24-i22	2.83E+12	i29-p12	7.60E+05	i17-i38	7.58E+06
i8-i1	2.13E+03	i7-i16	3.84E+12	i20-p7	8.74E+09	i38-i17	8.31E+06
i8-p3	4.10E+09	i16-i7	2.55E+12	i28-i29	3.68E+08	i5-i17	1.20E+09
i6-i24	6.34E+04	i2-i4	3.63E+11	i29-i28	3.87E+08	i17-i5	4.55E+11
i24-i6	6.70E+07	i4-i2	2.86E+08	i18-i20	9.14E+12	i4-i28	2.62E+09
i10-i21	2.08E+12	i26-p5	2.03E+08	i20-i18	9.02E+12	i28-i4	8.14E+11
i21-i10	2.96E+12	i4-i11	1.54E+01	i29-i30	1.77E+09	i5-i25	8.71E+07
i12-i21	2.27E+12	i11-i4	5.54E+03	i30-i29	1.07E+09	i25-i5	3.39E+10
i21-i12	2.41E+12	i17-p11	6.93E+08	i5-i30	1.13E+10	i6-i25	2.25E+04
i15-p8	2.03E+10	i2-i7	1.05E+13	i30-i5	1.08E+12	i25-i6	1.41E+07
i6-i9	6.34E+06	i7-i2	1.02E+13	i14-i30	2.08E+07	i5-i16	1.61E+05
i9-i6	1.62E+09	i16-i17	6.17E+12	i30-i14	2.82E+08	i16-i5	6.40E+07

Optimized Cartesian coordinates (in Å) and calculated vibrational frequencies (in cm⁻¹) of the reactants, products, intermediates, and transition states in the methylidyne radical plus 1,3-butadiene reaction.

1 INTERMEDIATES

i1

C	-1.431922	-0.488095	-0.007296
C	0.057343	-0.682429	-0.005239
C	2.357183	0.167268	0.008162
C	0.987717	0.344332	-0.010681
C	-1.968941	0.881753	0.009705
H	-1.892286	-1.036973	-0.855551
H	-1.882486	-1.009850	0.863371
H	0.408649	-1.711646	0.007131
H	3.034381	1.011496	-0.014439
H	2.797603	-0.823471	0.046782
H	0.595709	1.358266	-0.035101
H	-3.069847	0.875204	0.019901

Frequencies

91.9596	185.3773	207.3731
237.5956	386.6491	539.5833
600.7926	610.2978	760.3025
806.2752	861.1748	928.6508
1015.2724	1021.3408	1099.6852
1113.4335	1203.4761	1283.6949
1314.1196	1329.1194	1367.7955
1495.4967	1518.4179	2875.8803
2885.5093	3007.8304	3130.9815
3136.4137	3144.7171	3230.1367

i16

C	-1.468386	-0.100005	-0.632913
C	-0.399019	-0.519769	0.418283
C	1.844680	0.447881	-0.183508
C	1.045465	-0.586859	0.072653
C	-1.150865	0.736964	0.523043
H	-1.124827	0.210658	-1.617409
H	-2.383958	-0.686739	-0.642314
H	-0.737941	-1.339963	1.049604
H	2.884231	0.301674	-0.452067
H	1.493033	1.473492	-0.138929
H	1.459173	-1.592333	0.023292
H	-0.820958	1.763938	0.592479

Frequencies

59.4840	259.1047	292.0546
530.8460	595.2431	655.0260
782.5876	848.1068	873.9948
929.1111	935.1382	1021.0059
1026.9511	1055.8851	1065.3708
1104.5092	1113.0272	1245.5841
1330.2440	1385.4396	1447.4681
1463.6993	1693.2646	3075.6131
3088.9529	3124.4751	3136.0802
3152.0012	3204.7384	3215.9474

i3

C	-1.247024	0.391393	-0.000118
C	-0.000038	-0.271576	-0.000085
C	2.460638	-0.227013	0.000079
C	1.246943	0.391212	0.000097
C	-2.460578	-0.227030	0.000058
H	-1.223363	1.479937	-0.000192
H	-2.541681	-1.308868	0.000196
H	-0.000216	-1.359604	-0.000161
H	3.384036	0.338074	-0.000014
H	2.542215	-1.308836	-0.000267
H	1.223518	1.479793	-0.000012
H	-3.384157	0.337591	0.000271

Frequencies

157.1994	203.8249	255.7876
454.5763	492.6832	586.2926
627.0054	834.6782	854.7655
873.5676	921.8113	984.7204
1011.0370	1030.4246	1168.0496
1255.0541	1279.8851	1301.6895
1303.0369	1443.5366	1487.9647
1521.9903	1589.8185	3121.0417
3122.1092	3136.3543	3136.6552
3139.3291	3229.3588	3229.9683

i4

C	1.005914	-0.354273	-0.000157
C	0.047131	0.690515	-0.000119
C	-2.074819	-0.623449	0.000073
C	-1.361544	0.539533	0.000030
C	2.349610	-0.158664	0.000123
H	0.640397	-1.378079	-0.000450
H	0.433395	1.706226	-0.000118
H	-3.157338	-0.608923	0.000101
H	-1.601364	-1.598232	0.000157
H	-1.930321	1.466511	0.000087
H	2.773650	0.840159	0.000401
H	3.043818	-0.989641	0.000121

Frequencies

141.4443	219.4607	236.5522
395.5770	577.3508	611.4989
623.1879	817.2661	847.8632
877.3821	919.7505	1000.0811
1011.8468	1038.5197	1096.2510
1195.0101	1270.3874	1312.2925
1379.8274	1444.8444	1479.5751
1545.7774	1591.4766	3128.2620
3134.3882	3139.9179	3148.3089
3152.7473	3227.4932	3232.3218

i5

C	-1.284170	0.436808	0.102503
C	-1.642337	-0.858283	-0.111563
H	-2.087675	1.128344	0.349229
H	-0.941946	-1.610939	-0.447292
H	-2.674727	-1.166436	0.000497
C	0.000024	1.038614	0.000035
C	1.642236	-0.858304	0.111604
C	1.284268	0.436790	-0.102496
H	0.000051	2.124816	0.000013
H	2.674541	-1.166740	-0.000716
H	0.941847	-1.610968	0.447297
H	2.087780	1.128179	-0.349528

Frequencies

133.3319	243.5107	277.4382
376.8691	572.8968	590.7022
697.0076	806.5978	871.0013
877.1310	901.3722	989.1513
1004.7381	1009.0864	1122.1980
1179.3454	1269.0199	1314.8904
1416.2983	1448.8253	1471.7295
1556.7040	1599.7454	3117.7415
3122.3881	3149.4651	3151.3626
3158.6275	3235.6491	3246.0282

i6

C	0.490839	1.145867	0.000023
C	-0.971546	0.779126	-0.000127
C	1.273704	0.000770	-0.000020
C	-0.970585	-0.780285	0.000131
C	0.492293	-1.145294	-0.000041
H	0.858065	2.163533	0.000594
H	-1.491679	1.186472	-0.875740
H	-1.492080	1.186978	0.875002
H	2.357468	0.001438	-0.000101
H	-1.490527	-1.188659	-0.875080
H	-1.490191	-1.188336	0.875703
H	0.860723	-2.162533	-0.000175

Frequencies

124.1706	449.7200	597.3540
641.9963	727.0993	804.5544
810.3011	905.6072	911.5470
948.8191	992.3520	1026.8690
1072.8327	1105.5569	1141.8848
1221.9749	1274.2185	1300.4541
1317.9040	1400.3031	1469.5809
1478.6199	1493.4128	2997.5239
3008.7137	3010.3043	3030.6200
3179.9963	3201.9144	3213.6407

i17

C	1.438924	-0.314582	0.603299
C	0.377951	-0.356237	-0.529231
C	-1.880385	0.423882	0.226397
C	-1.054445	-0.542858	-0.166925
C	1.122608	0.867404	-0.201877
H	1.042216	-0.378001	1.613612
H	2.390145	-0.824490	0.464071
H	0.679223	-0.890761	-1.430962
H	-2.906851	0.211931	0.502944
H	-1.551949	1.456350	0.284311
H	-1.418395	-1.567042	-0.225927
H	1.737694	1.526358	-0.798021

Frequencies

113.8659	242.9815	296.9006
530.3711	604.6858	672.9709
744.4772	815.4055	873.9716
946.6027	981.6462	1019.8260
1038.0048	1051.0050	1070.4353
1087.0405	1133.7476	1231.3626
1325.4103	1383.6367	1442.0719
1464.0371	1695.4426	3074.2559
3075.5481	3122.6136	3134.8822
3151.2159	3205.7892	3216.7946

i8

C	1.421799	-0.425527	-0.003749
C	0.006268	-0.966709	0.009869
C	-2.188586	0.441728	-0.011727
C	-1.089153	-0.259466	-0.001887
C	1.561004	1.054664	-0.000995
H	1.955369	-0.858986	0.861010
H	1.945611	-0.852589	-0.873610
H	-0.086189	-2.051478	0.032087
H	-2.670439	0.727962	-0.942236
H	-2.665099	0.763019	0.910097
H	0.715817	1.699871	0.196868
H	2.536943	1.504067	-0.133280

Frequencies

48.0610	123.7414	158.3975
332.7267	372.9261	445.6960
521.9754	634.9379	852.3884
866.6696	877.0373	917.2361
991.8621	1022.8197	1093.9303
1161.7132	1191.9762	1337.6804
1374.2673	1449.5290	1457.0912
1484.3295	2054.4234	2920.8677
2961.7728	3109.8446	3115.9325
3147.3555	3180.6674	3253.4171

i9

C	0.924445	0.813963	0.100282
C	1.121523	-0.692477	-0.051689
C	-1.259491	-0.401937	0.088694
C	-0.058512	-1.279671	-0.056460
C	-0.606656	1.005526	-0.118024
H	1.236459	1.136438	1.101396
H	1.515848	1.390020	-0.617806
H	2.093096	-1.167495	-0.102557
H	-2.044673	-0.608500	-0.642720
H	-1.706404	-0.511217	1.083562
H	-1.034561	1.758524	0.546483
H	-0.787627	1.329806	-1.145176

Frequencies

137.8487	372.4520	616.0320
749.2827	761.8559	808.4100
875.2964	889.0067	925.7360
969.8328	1011.5062	1049.2511
1134.5725	1190.1821	1212.2763
1230.9241	1291.4342	1301.7532
1332.2806	1481.3545	1489.4207
1505.0061	1673.9001	3007.3907
3020.8662	3045.6754	3056.6234
3067.9338	3099.5600	3193.5100

i10

C	1.326863	0.291790	-0.209654
C	0.056468	0.417589	0.611613
C	-2.165982	-0.525141	-0.096645
C	-1.186047	0.360742	-0.239281
C	2.246159	-0.622941	-0.053598
H	1.455537	1.045450	-0.996671
H	0.085295	1.383172	1.135876
H	0.032061	-0.364332	1.373462
H	-3.040290	-0.513367	-0.737668
H	-2.129854	-1.295664	0.667557
H	-1.259700	1.112645	-1.023693
H	3.192189	-0.900137	-0.493478

Frequencies

82.1052	118.3216	280.2196
411.3211	426.5275	609.0954
657.6236	778.1648	816.7800
932.9595	939.8652	950.4471
1018.6188	1032.5169	1131.1391
1225.5485	1265.7175	1315.1775
1329.2043	1452.6645	1474.6240
1675.2704	1709.5570	2991.1517
3009.1034	3081.6843	3118.1128
3129.4259	3209.8456	3242.5333

i11

C	-1.448669	0.345727	-0.097814
C	-1.805419	-0.912208	-0.093739
H	-2.221997	1.109653	-0.248003
H	-2.709458	-1.491253	-0.204641
C	-0.045682	0.888268	0.088910
C	2.112232	-0.345443	-0.271796
C	0.988839	-0.152961	0.410974
H	-0.081703	1.631580	0.898517
H	0.245008	1.443276	-0.811048
H	2.828546	-1.106462	0.016589
H	2.357523	0.249556	-1.146698
H	0.774268	-0.776650	1.276077

Frequencies

82.9464	153.6152	222.2027
404.9440	496.9100	590.4492
655.8084	804.4486	828.5739
881.5703	935.5281	947.9609
1010.2379	1032.0638	1132.7986
1235.7651	1256.8996	1318.6905
1340.6837	1448.4456	1469.6633
1676.5341	1711.4397	2986.4246
3008.2868	3031.6780	3122.8401
3134.7502	3208.0731	3244.9096

i12

C	1.333055	-0.307040	0.000129
C	1.530823	0.985185	-0.000008
C	0.041024	-1.089405	-0.000177
H	2.222998	-0.951380	0.000486
H	2.381982	1.649875	0.000002
H	0.063616	-1.768771	0.864873
H	0.063589	-1.767935	-0.865905
C	-1.515654	0.935037	-0.000051
C	-1.281653	-0.372530	0.000140
H	-2.530866	1.317033	0.000193
H	-0.712131	1.663640	-0.000372
H	-2.134760	-1.049948	0.000526

Frequencies

67.3766	166.4240	226.4881
369.8941	516.8935	616.8735
630.2011	808.9787	821.0974
854.2551	943.9462	967.0059
1017.5074	1028.9874	1084.5895
1245.6107	1258.1739	1334.2598
1387.3866	1442.0943	1453.7389
1685.3034	1713.5386	2979.8521
2991.5512	2993.7626	3111.4752
3122.4734	3206.9262	3235.0516

i13

C	0.666058	1.033790	-0.000266
C	-0.666259	1.033670	0.000464
C	1.235890	-0.368801	-0.000036
C	-1.235878	-0.368968	-0.000346
C	0.000105	-1.218883	0.000066
H	1.290483	1.919476	-0.000374
H	-1.290603	1.919432	0.000635
H	1.881997	-0.550442	0.874899
H	1.882178	-0.550803	-0.874560
H	-1.881734	-0.550894	-0.875242
H	-1.882221	-0.551164	0.874252
H	0.000401	-2.300454	0.001099

Frequencies

205.8843	331.1613	390.0321
681.6008	742.8666	791.9530
896.0363	913.6082	924.0704
944.1522	961.7924	969.4016
1033.8085	1128.6138	1128.6583
1132.3383	1274.4514	1299.3070
1324.5548	1386.7380	1456.4985
1462.4737	1675.4155	2942.8478
2943.1634	2944.2467	2947.7481
3172.7613	3197.0995	3206.3454

i14

C	-1.303497	0.536837	0.000031
C	-1.721634	-0.896372	0.000001
C	1.132021	0.222467	0.000009
C	2.214328	-0.497245	0.000000
C	0.020091	0.986249	-0.000010
H	-2.084580	1.289814	0.000000
H	-2.336204	-1.130960	-0.878262
H	-0.861963	-1.569068	0.000438
H	2.695701	-0.817090	0.924321
H	2.695656	-0.817157	-0.924320
H	0.180542	2.063623	-0.000091
H	-2.337015	-1.130776	0.877728:

Frequencies

70.3364	151.4621	180.9024
308.0255	370.4207	512.3105
645.1933	669.4543	883.5710
890.4053	916.4078	977.2019
985.6518	1018.6738	1103.7325
1203.0405	1375.6538	1409.5858
1431.6184	1454.5882	1478.2240
1503.2426	1904.5102	2997.3465
3030.4160	3061.7642	3100.8593
3112.8507	3117.8171	3166.0048

i15

C	-2.289889	0.405967	-0.249140
C	0.073503	-0.367629	0.058738
C	2.360332	0.485399	0.138234
C	1.371392	-0.385570	-0.314003
C	-1.174763	-0.363253	0.424775
H	-2.759342	1.100086	0.455628
H	-3.070958	-0.276787	-0.599612
H	-1.920197	0.976070	-1.102208
H	3.378056	0.396045	-0.217752
H	2.134634	1.267229	0.852118
H	1.661583	-1.151982	-1.032667
H	-1.467221	-0.960151	1.292874

Frequencies

113.2298	151.5780	195.8528
274.9207	452.4188	541.3825
565.5378	739.3898	758.0670
816.5849	940.2293	998.1411
1053.8636	1071.2590	1114.6937
1193.7736	1315.9930	1401.7285
1412.2987	1485.2192	1491.5257
1493.9670	1918.8997	3018.1820
3052.6996	3066.8635	3103.8565
3115.9414	3149.5801	3249.3998

i2

C	1.517604	0.675501	0.190322
C	0.273568	-0.239258	0.329318
C	-2.202756	-0.027377	0.123351
C	-0.976928	0.144313	-0.366963
C	1.476792	-0.648250	-0.424976
H	2.141435	0.847298	1.064910
H	1.392450	1.555068	-0.437582
H	0.119229	-0.706690	1.301125
H	-3.081998	0.274050	-0.433548
H	-2.369248	-0.477507	1.097137
H	-0.848984	0.593474	-1.349931
H	2.117433	-1.515263	-0.348426

Frequencies

118.0305	273.0979	294.2721
448.0776	567.7686	697.1501
751.9138	806.2611	885.3880
923.9223	981.7379	995.0602
1019.4108	1044.9056	1072.7772
1107.4139	1190.4920	1235.1918
1311.6951	1349.1868	1455.0111
1467.6397	1696.4096	3074.7158
3092.1112	3125.0798	3132.5633
3146.3414	3206.2158	3213.9205

i7

C	1.574923	-0.550538	0.346576
C	1.453984	0.722061	-0.358017
H	1.577254	-0.564068	1.434834
H	2.141144	-1.361595	-0.104280
H	1.545239	1.738810	-0.000401
C	0.271918	-0.163933	-0.404176
C	-2.197690	-0.086284	-0.062919
C	-0.955699	0.180579	0.341417
H	0.108129	-0.724372	-1.322962
H	-3.059415	0.198355	0.529019
H	-2.393351	-0.599641	-0.999160
H	-0.803607	0.701201	1.285663

Frequencies

121.4659	268.8449	304.8282
439.3987	601.2843	681.0078
800.1308	843.3700	878.9650
924.0993	936.9277	999.5934
1014.1200	1041.0249	1086.5402
1095.2915	1206.0471	1242.6278
1314.0351	1343.5287	1456.6187
1467.5263	1688.7066	3077.5298
3097.5420	3121.0806	3131.9076
3150.8845	3198.0434	3215.2320

i18

C	2.132012	-0.523211	-0.250014
C	0.097464	0.929855	0.009233
C	-1.715267	-0.841233	-0.059234
C	-1.322820	0.427945	-0.099630
C	1.109872	-0.110557	0.453188
H	0.402251	1.362370	-0.951099
H	2.572013	-0.336100	-1.219439
H	0.118398	1.760773	0.727666
H	-2.761856	-1.107460	-0.153007
H	-1.009491	-1.656279	0.059507
H	-2.070678	1.207863	-0.232524
H	0.941799	-0.527965	1.447637

Frequencies

86.9842	147.8613	255.9346
376.1901	517.7699	573.0398
695.1390	819.6048	844.8054
919.1844	941.4633	954.7174
1023.7112	1037.7269	1099.2726
1205.4838	1278.0016	1323.5969
1341.0004	1443.8538	1466.9191
1668.6320	1705.7811	2997.4240
3031.4760	3085.0132	3120.1108
3137.4910	3217.0687	3226.0096

i19

C	-2.132338	-0.522837	-0.249886
C	-0.097449	0.929769	0.009114
C	1.715349	-0.841196	-0.059331
C	1.322891	0.427986	-0.099545
C	-1.109869	-0.110754	0.453227
H	-2.571265	-0.336691	-1.219940
H	-0.118535	1.760672	0.727649
H	-0.402264	1.362052	-0.951216
H	2.761994	-1.107312	-0.152791
H	1.009547	-1.656261	0.059165
H	2.070794	1.207945	-0.231979
H	-0.941772	-0.528211	1.447634

Frequencies

87.0507	147.8915	255.9097
376.1470	517.7557	573.0463
694.9477	819.4933	844.7109
919.1126	941.4550	954.7030
1023.6847	1037.7222	1099.2428
1205.4387	1277.9366	1323.5789
1340.9216	1443.8352	1466.8631
1668.4569	1705.7727	2997.0729
3032.0978	3085.1956	3120.0715
3137.4529	3217.0675	3226.3434

i20

C	2.140803	-0.395697	-0.347759
C	0.048616	0.950261	-0.013087
C	-1.698685	-0.886889	-0.039828
C	-1.354992	0.396481	-0.078595
C	1.111619	-0.047954	0.379435
H	2.996256	-1.049976	-0.269774
H	0.306992	1.399618	-0.978526
H	0.059346	1.775618	0.712140
H	-2.737154	-1.191580	-0.101035
H	-0.959364	-1.676152	0.043513
H	-2.135559	1.148714	-0.176735
H	0.985313	-0.503457	1.369426

Frequencies

94.7970	149.4630	261.2267
397.3439	512.3916	572.9886
670.2357	780.1933	828.2189
907.5910	938.4603	953.0041
1030.9780	1045.8444	1109.2640
1207.2044	1275.5152	1326.0330
1348.6470	1444.7620	1467.6632
1678.2815	1706.3576	2996.9276
3011.7788	3040.6403	3122.3936
3137.4958	3216.5011	3239.1941

i21

C	-1.111490	-0.048219	0.379400
C	-0.048599	0.950234	-0.013156
C	-2.140848	-0.395618	-0.347669
H	-0.985285	-0.502962	1.369743
H	-0.059468	1.775670	0.712019
H	-0.307062	1.399688	-0.978547
H	-2.996474	-1.049703	-0.269904
C	1.698679	-0.886840	-0.039884
C	1.354944	0.396513	-0.078546
H	2.737138	-1.191629	-0.100969
H	0.959427	-1.676223	0.043248
H	2.135609	1.148741	-0.176466

Frequencies

94.8587	149.5862	261.2462
397.3912	512.4101	573.096
670.2748	780.0799	828.2312
907.622	938.5341	953.0874
1031.0532	1045.8603	1109.2076
1207.1294	1275.4922	1326.1066
1348.6986	1444.8478	1467.7263
1678.2893	1706.4365	2996.7222
3011.8479	3040.4544	3122.0202
3137.3159	3216.2996	3239.1734

i22

C	1.336455	-0.355961	0.636487
C	0.311977	-0.425490	-0.486002
C	-1.908347	0.499057	0.224683
C	-1.140987	-0.490253	-0.160496
C	1.110832	0.830500	-0.262083
H	0.951742	-0.303419	1.647716
H	2.251441	-0.926018	0.525144
H	0.600240	-1.039025	-1.333989
H	-2.934507	0.648357	0.523789
H	0.584012	1.683360	0.148270
H	-1.588739	-1.489286	-0.239068
H	1.876228	1.078914	-0.987392

Frequencies

92.6985	242.7430	323.2898
525.6375	650.4598	743.8581
797.8933	818.8015	829.9495
841.1088	920.5924	1009.3020
1049.7506	1077.8724	1112.0640
1124.5858	1198.4259	1222.2150
1265.8935	1393.8636	1466.1920
1503.7041	1668.2416	3004.8465
3121.6576	3126.5814	3134.7561
3202.2830	3216.7254	3245.2640

i23

C	1.550758	0.118469	-0.000486
C	0.371340	1.060097	0.000232
C	-1.954277	-0.010840	-0.000290
C	-0.582552	0.038366	0.000186
C	0.499469	-1.046702	0.000327
H	2.195459	0.160439	0.884733
H	2.193646	0.160323	-0.887058
H	0.295412	2.141529	0.001259
H	-2.485320	-0.954887	-0.000495
H	-2.545354	0.898072	-0.000275
H	0.519105	-1.680006	0.890582
H	0.518626	-1.681806	-0.888563

Frequencies

179.5691	345.9480	420.7349
533.0104	657.8923	700.3821
775.5666	797.5977	875.0004
905.7070	952.3699	1010.2825
1014.4139	1081.4720	1179.7007
1203.9554	1219.5346	1261.0163
1331.9510	1400.8433	1461.9129
1485.5103	1511.8018	3009.9223
3039.5217	3046.1562	3093.8373
3136.2727	3178.4730	3227.4796

i24

C	1.336472	0.355924	0.636519
C	0.311979	0.425528	-0.485950
C	-1.908380	-0.499071	0.224696
C	-1.140971	0.490198	-0.160523
C	1.110856	-0.830480	-0.262143
H	2.251442	0.925999	0.525156
H	0.951801	0.303296	1.647755
H	0.600284	1.039146	-1.333859
H	-2.934586	-0.648072	0.523834
H	-1.588857	1.489160	-0.239208
H	1.876215	-1.078837	-0.987496
H	0.583967	-1.683289	0.148216

Frequencies

92.6324	242.7369	323.2755
525.6770	650.4783	743.9106
797.9130	818.8009	830.0046
841.1409	920.5921	1009.3319
1049.7183	1077.8342	1112.0740
1124.5896	1198.4295	1222.2253
1265.9260	1393.8969	1466.1732
1503.6870	1668.2514	3004.8616
3121.6812	3126.6229	3134.7760
3202.3435	3216.7876	3245.1535

i25

C	1.179520	-0.847644	0.116318
C	0.390600	0.423803	0.444193
C	-1.912903	-0.407707	-0.145697
C	-1.046579	0.577911	0.065444
C	1.457720	0.415621	-0.577371
H	1.891319	-1.228172	0.845614
H	0.654269	-1.628548	-0.427711
H	0.644408	0.923407	1.381171
H	-2.939924	-0.203813	-0.426563
H	-1.381487	1.609057	-0.035559
H	2.353022	1.007046	-0.707472
H	-1.631759	-1.450875	-0.046805

Frequencies

96.3616	254.3334	299.2148
502.3383	608.2618	665.6659
752.6420	805.7899	896.8598
944.8706	982.1541	1019.4094
1039.3028	1057.8536	1068.2674
1096.4508	1119.1540	1231.4726
1323.1990	1375.5653	1446.0191
1464.4523	1702.0672	3062.2757
3080.4521	3118.8070	3135.4443
3150.1235	3205.2408	3213.9973

i26

C	-1.438712	-0.313902	0.603992
C	-0.377932	-0.356849	-0.528905
C	1.880263	0.424212	0.226344
C	1.054564	-0.542803	-0.166897
C	-1.122942	0.866963	-0.202994
H	-2.389752	-0.82439	0.465879
H	-1.041180	-0.375592	1.614085
H	-0.679369	-0.892696	-1.429797
H	2.906860	0.212490	0.502528
H	1.418929	-1.566838	-0.226173
H	-1.738336	1.524773	-0.800096
H	1.551408	1.456528	0.284332

Frequencies

113.8917	242.9473	296.8604
530.4155	604.7011	672.9546
744.3354	815.4016	873.8646
946.4432	981.7125	1019.8039
1037.9070	1051.0169	1070.4545
1087.0438	1133.7702	1231.3677
1325.4614	1383.6689	1442.0321
1463.9656	1695.3747	3074.2367
3075.6571	3122.5451	3134.9126
3151.4402	3205.6942	3216.9563

i27

C	1.280192	0.716438	-0.291233
C	0.403846	-0.543806	-0.402583
C	-1.819824	0.510883	0.135201
C	-1.058077	-0.548650	-0.129732
C	1.366543	-0.352398	0.707842
H	2.062120	0.802855	-1.041596
H	0.834636	1.668680	-0.015656
H	0.713984	-1.230814	-1.189004
H	-2.876431	0.401651	0.350361
H	-1.424716	1.521059	0.142331
H	-1.518013	-1.535326	-0.134996
H	1.172341	-0.322905	1.771582

Frequencies

59.1873	262.3946	297.6659
513.2219	637.6806	679.3850
774.8206	863.0745	865.9204
933.1560	942.0023	1021.0154
1032.6119	1069.9715	1075.1921
1090.7147	1114.8817	1240.0032
1327.3609	1379.4499	1446.6856
1469.7611	1696.0300	3085.1527
3087.0581	3123.0842	3138.4290
3156.6004	3199.0182	3216.4689

i28

C	1.808174	-0.061399	-0.303683
C	0.545291	-0.019001	0.460592
C	-1.451510	-0.124396	-0.248694
C	-0.542621	-1.035845	0.106647
C	-0.551695	1.064405	0.015783
H	2.753494	0.218030	0.144935
H	1.794481	-0.290235	-1.363637
H	0.743984	0.045146	1.535529
H	-2.475779	-0.192126	-0.597068
H	-0.538925	-2.119817	0.140620
H	-0.860160	1.745260	0.815811
H	-0.262928	1.651156	-0.860057

Frequencies

141.9281	212.1489	325.5504
466.0559	541.8427	713.9026
776.4586	824.8006	876.5501
932.0887	950.2149	968.8744
1043.6901	1076.4835	1130.8679
1162.6058	1175.9279	1217.1798
1302.3213	1344.5048	1460.4785
1472.8788	1637.6483	3027.4139
3034.3316	3078.8355	3129.7267
3162.7911	3195.1434	3233.3387

i29

C	0.458121	-0.000427	0.482151
C	1.769283	-0.000052	-0.299987
H	0.660823	-0.001104	1.560400
H	2.368914	-0.883734	-0.059870
H	2.369080	0.883105	-0.058199
H	1.579550	0.001010	-1.376742
C	-1.513798	0.000417	-0.256105
C	-0.619164	-1.018769	0.073302
C	-0.618665	1.018803	0.074358
H	-2.533199	0.000827	-0.623668
H	-0.651151	-2.099889	0.058493
H	-0.648677	2.099953	0.057268

Frequencies

232.5566	246.6619	320.2812
490.4976	560.5013	613.1872
792.5362	852.2987	911.1609
920.1846	955.3202	1032.4706
1055.9319	1097.5747	1174.2706
1196.0453	1215.5323	1327.0221
1350.3275	1405.5866	1449.1246
1495.6991	1497.1321	3010.7731
3017.9294	3075.9892	3090.5345
3178.7816	3205.8943	3220.0358

i30

C	1.146570	0.582552	0.033202
C	1.540784	-0.859226	-0.043539
H	1.960483	1.300334	0.101531
H	1.684542	-1.280898	0.959258
H	2.485446	-0.979948	-0.581317
H	0.771026	-1.461959	-0.533686
C	-1.360207	0.326936	-0.062985
C	-1.564356	-0.966584	0.080962
C	-0.101055	1.076043	0.026421
H	-2.243075	0.945176	-0.268967
H	-2.411149	-1.635836	0.045636
H	-0.217680	2.154806	0.073173

Frequencies

86.9692	127.9951	221.1698
375.2709	417.3283	611.1505
671.9381	715.8242	850.1903
860.2409	904.4331	993.7330
1017.3344	1054.4650	1102.8729
1274.1613	1279.9476	1399.7284
1440.2382	1476.0818	1481.2348
1627.8176	1691.0090	3005.5056
3006.5915	3052.8281	3084.4790
3131.1913	3157.1139	3236.4052

i31

C	1.175705	0.367631	-0.422443
C	2.287962	-0.409344	0.247443
C	-1.370293	0.382643	0.317119
C	-2.360098	-0.484220	-0.141029
C	-0.073561	0.369686	-0.059828
H	1.471335	0.971992	-1.284243
H	3.068939	0.269061	0.606462
H	2.758465	-1.097497	-0.462462
H	1.915081	-0.986845	1.094117
H	-2.136131	-1.258903	-0.863202
H	-3.376983	-0.398492	0.218245
H	-1.658994	1.142305	1.043520

Frequencies

113.0927	151.6166	195.8693
274.9519	452.4700	541.5382
565.5395	739.2666	758.1003
816.7037	940.1577	998.0028
1053.8257	1071.4021	1114.5420
1193.8424	1316.1179	1401.5889
1412.3087	1485.1683	1491.6165
1493.9500	1918.9168	3018.1755
3053.0849	3066.8695	3103.7667
3115.9859	3149.5356	3249.3211

i32

C	1.024310	-0.421703	-0.000677
C	2.457769	-0.002958	0.000675
C	-1.353504	0.150751	-0.001751
C	-2.614685	-0.161797	0.001019
C	-0.044921	0.476037	-0.000340
H	0.804726	-1.484960	-0.001908
H	2.992012	-0.391150	-0.876137
H	2.990177	-0.390415	0.878960
H	2.560673	1.085133	0.000389
H	-3.173466	-0.301180	0.926609
H	-3.177709	-0.300654	-0.922056
H	0.189772	1.541240	0.000586

Frequencies

122.7135	138.9963	164.2493
254.5519	385.0601	498.9586
558.5767	714.7595	885.4856
909.2392	917.9279	985.0945
1018.5625	1034.0588	1120.2006
1220.5110	1304.5315	1412.4072
1432.4236	1472.4871	1473.0112
1509.5998	1909.0803	2991.4082
3022.6769	3061.9007	3085.7404
3097.5196	3117.6402	3157.0138

i33

C	-1.027152	0.410653	-0.000018
C	-2.383089	-0.225427	0.000018
C	1.446585	0.402173	-0.000011
C	2.610501	-0.213235	0.000091
C	0.135388	-0.253080	-0.000019
H	-1.003490	1.499530	-0.000014
H	-2.962828	0.080837	-0.878318
H	-2.962902	0.080977	0.878254
H	-2.316729	-1.315798	0.000100
H	2.989110	-1.225170	-0.000314
H	1.431036	1.493975	-0.000094
H	0.132415	-1.340858	0.000021

Frequencies

133.9140	199.8399	211.6736
259.9399	429.2444	476.9773
660.1698	807.8214	830.8818
903.4510	945.1982	1003.1417
1063.5808	1082.6900	1148.4579
1242.4210	1321.1578	1333.8217
1413.5942	1478.8346	1490.2499
1629.6692	1697.9359	3009.6350
3050.5299	3080.3232	3092.8714
3121.3589	3135.8587	3231.8899

i34

C	1.032328	0.409124	0.000085
C	2.406904	-0.185114	0.000046
C	-1.436133	0.319277	-0.000257
C	-2.582595	-0.327961	0.000178
C	-0.109372	-0.290020	-0.000123
H	0.975897	1.496931	0.000224
H	2.976462	0.136695	0.879548
H	2.978090	0.140636	-0.876898
H	2.373257	-1.276926	-0.002383
H	-1.458769	1.416229	-0.000236
H	-3.634933	-0.088648	0.000583
H	-0.076797	-1.376753	-0.000416

Frequencies

138.3780	201.7049	210.1470
273.8147	447.2995	484.8493
632.7807	795.7072	802.7677
870.9385	945.3706	1004.0172
1064.2119	1090.7687	1164.8747
1235.8922	1320.7271	1332.1359
1413.1532	1479.0186	1490.1138
1637.5562	1705.8239	3009.3657
3012.0567	3049.9437	3092.9555
3120.0973	3142.7536	3245.6288

i35

C	-0.826487	-0.305964	0.149752
C	-2.300292	-0.124265	-0.049049
C	0.097418	0.633179	-0.074935
H	-0.503498	-1.278526	0.516559
H	-2.850503	-0.302077	0.881867
H	-2.688952	-0.840568	-0.782223
H	-2.539289	0.882189	-0.400424
H	-0.224042	1.623392	-0.394705
C	1.557071	0.467778	0.095756
C	2.244814	-0.637425	-0.087653
H	2.100214	1.372200	0.377104
H	2.070926	-1.656426	-0.401407

Frequencies

111.4483	182.5921	213.2341
254.2674	372.0021	557.1466
673.2122	793.7308	871.1942
888.5661	917.0059	991.2075
1040.5619	1065.9968	1121.6244
1260.7197	1320.2649	1334.6255
1414.4809	1479.2524	1490.8016
1632.1927	1707.0455	3009.8695
3051.1646	3077.3419	3092.4578
3118.2940	3130.3235	3233.0919

i36

C	-0.850749	-0.343592	-0.042172
C	-2.331890	-0.134598	0.016506
C	1.522085	0.450244	-0.029372
C	2.202317	-0.673077	0.046772
C	0.062885	0.631650	0.016703
H	-0.507384	-1.371696	-0.141823
H	-2.770821	-0.666663	0.868637
H	-2.822802	-0.528300	-0.881030
H	-2.587934	0.923613	0.108787
H	2.100270	1.376576	-0.133971
H	3.236942	-0.979235	0.030159
H	-0.276152	1.661940	0.098620

Frequencies

44.5428	193.4510	203.7967
249.1474	382.6177	581.2466
613.6789	781.2283	849.6687
861.9355	900.9192	1001.3408
1048.9201	1066.3437	1126.9943
1269.2228	1326.8148	1343.6494
1413.6469	1478.6082	1490.2469
1637.4804	1707.4298	3008.0451
3011.0249	3048.5295	3090.2716
3127.1937	3136.5485	3245.5932

i37

C	0.817960	-0.000275	-0.438991
C	2.214883	0.000075	0.082971
C	-1.671435	-0.644306	-0.036732
C	-1.671300	0.644440	-0.036913
C	-0.361568	-0.000016	0.420141
H	0.660265	-0.000356	-1.514034
H	2.782721	0.878070	-0.256236
H	2.783804	-0.876461	-0.258097
H	2.234755	-0.001022	1.176473
H	-2.143006	-1.579796	-0.290539
H	-2.142700	1.579954	-0.290952
H	-0.147077	0.000102	1.490531

Frequencies

18.3018	102.6961	272.9922
366.8879	433.4145	536.3686
605.0484	693.5886	845.9332
885.5172	914.0848	989.3568
998.1689	1052.0604	1086.9968
1121.8492	1160.8360	1319.8225
1405.7425	1425.2541	1471.6684
1495.9930	1723.7304	2972.8125
2996.2957	3057.4437	3074.9289
3147.4142	3222.6808	3271.5788

C	-0.955780	0.681612	0.000006
C	-1.759813	-0.575201	-0.000012
H	-1.489000	1.627225	0.000008
H	-2.418806	-0.637708	-0.877217
H	-2.418712	-0.637794	0.877260
H	-1.127078	-1.465889	-0.000079
C	1.373722	-0.343404	-0.644376
C	1.373669	-0.343492	0.644355
C	0.507044	0.741167	0.000029
H	1.657570	-0.802914	-1.577453
H	1.657681	-0.802999	1.577383
H	0.905288	1.755983	0.000087

Frequencies

28.4045	99.7659	240.1831
361.1152	481.5860	522.2101
653.0636	695.3257	842.7339
854.1990	904.0103	987.9355
1000.8728	1021.4944	1057.7397
1121.1556	1172.4787	1375.0048
1394.9871	1415.7573	1476.5927
1497.2426	1723.7179	2976.8596
3000.2606	3071.0632	3086.7062
3156.4886	3220.1208	3268.8715

2 TRANSITION STATES

i3 — i4

C	1.121039	-0.310577	0.233124
C	0.048767	0.519301	-0.069556
C	-2.278054	-0.338251	-0.330591
C	-1.337231	0.277237	0.382286
C	2.427196	-0.091610	-0.156662
H	0.907471	-1.203990	0.816958
H	0.240063	1.424628	-0.643776
H	-3.280227	-0.477691	0.060002
H	-2.077648	-0.723611	-1.325039
H	-1.597123	0.647211	1.376390
H	2.699650	0.779581	-0.742458
H	3.217504	-0.782728	0.106318

Frequencies

-215.5315	152.7076	242.3701
403.1961	485.9003	541.6318
664.3832	736.3868	802.1330
908.8416	958.5548	994.8227
1013.1578	1024.6439	1116.8707
1201.7816	1275.0303	1310.9043
1318.2832	1441.1722	1485.3075
1516.4523	1688.6661	3076.2654
3115.0551	3128.8164	3130.1695
3138.0784	3212.4288	3234.1540

i4 — i5

C	-1.108108	0.148733	0.460526
C	-1.983087	-0.461918	-0.335500
H	-1.252715	0.084189	1.540928
H	-1.886691	-0.431055	-1.415888
H	-2.825072	-1.012948	0.069249
C	0.054765	0.937196	0.001442
C	1.726847	-0.879583	0.053348
C	1.341961	0.430494	-0.149671
H	-0.105966	1.996635	-0.181277
H	2.755998	-1.186129	-0.083249
H	1.011415	-1.638404	0.346316
H	2.108760	1.138187	-0.456944

Frequencies

-168.8161	209.4259	242.2804
438.2514	502.2537	522.7862
678.4002	723.0430	810.1290
913.8033	958.2159	993.6987
1013.2995	1030.8765	1078.6176
1165.0680	1232.8215	1314.8892
1405.4693	1439.7497	1461.3403
1520.6434	1688.8658	3078.9838
3125.7685	3129.2176	3142.5224
3149.4894	3212.7053	3240.0962

i5 — i6

C	-1.167622	0.481019	0.169240
C	-1.183028	-0.837252	-0.229641
C	0.064421	1.202773	-0.084161
C	1.060133	-1.007791	0.197523
C	1.179266	0.438662	-0.086275
H	-1.895098	0.870746	0.875350
H	-0.777404	-1.121089	-1.192265
H	-1.894266	-1.541685	0.193136
H	0.102930	2.283397	-0.174876
H	1.504767	-1.722064	-0.489823
H	1.080877	-1.316618	1.241709
H	2.159169	0.882847	-0.253347

Frequencies

-664.8297	211.4786	406.5081
451.7594	511.2242	642.6582
715.5318	736.0026	771.6530
862.3547	938.2213	963.8755
985.2993	1008.9120	1041.0700
1066.9963	1162.3060	1241.3689
1371.3908	1421.8352	1444.0492
1531.5551	1591.7899	3086.7849
3115.9201	3123.3195	3147.3168
3171.0700	3173.0264	3204.0590

i6 — p1

C	-0.404699	1.140896	-0.107060
C	-1.157814	0.018479	-0.144619
C	0.999725	0.773475	0.041140
C	-0.251133	-1.178523	-0.089469
C	1.108447	-0.565776	0.061649
H	-0.775708	2.155720	-0.165819
H	-2.221139	-0.036776	-0.330408
H	-1.783971	0.028188	1.928027
H	1.813958	1.481812	0.121433
H	-0.322855	-1.760574	-1.017829
H	-0.498232	-1.862741	0.728921
H	2.020792	-1.136934	0.165832

Frequencies

-510.9544	227.5863	295.3875
372.6181	527.7159	697.0797
771.0298	818.3538	821.0934
916.7738	937.7575	969.1519
975.5928	983.5410	1030.0797
1110.1445	1132.4776	1135.5312
1278.0666	1327.1608	1406.0964
1423.3075	1546.1322	1648.7277
3048.7226	3097.1466	3220.7962
3231.2664	3248.9549	3255.6982

i4 — p2

C	1.218351	-0.154595	-0.032392
C	-0.055765	-0.477623	-0.199913
C	-2.456295	0.047634	-0.020956
C	-1.171859	0.397218	0.120685
C	2.447548	0.276137	-0.090768
H	1.360215	-1.167070	1.827137
H	-0.290807	-1.480334	-0.553206
H	-3.258207	0.735095	0.218007
H	-2.741245	-0.935354	-0.381856
H	-0.917998	1.387140	0.488649
H	2.817382	0.749776	-0.996938
H	3.138780	0.178118	0.738269

Frequencies

-523.5479	108.2534	131.4287
179.3323	390.8831	403.1913
426.4583	528.0483	576.2278
727.5600	892.6035	900.1640
921.9303	931.6999	1006.6568
1031.2966	1104.7109	1188.6852
1308.5873	1336.0701	1440.1971
1477.3985	1662.9099	1981.8487
3113.0260	3120.0418	3136.2964
3155.1950	3195.1425	3225.6707

i6 — i13

C	0.441477	1.146362	-0.004430
C	-0.886014	0.889392	-0.019736
C	1.262304	-0.128955	-0.013311
C	-1.138293	-0.538598	-0.020134
C	0.202511	-1.209030	-0.004442
H	0.888385	2.130920	0.045933
H	-1.669877	1.635373	0.001899
H	1.955355	-0.187370	0.841336
H	1.911154	-0.198870	-0.905991
H	-2.045711	-1.025311	-0.352008
H	-0.678718	-1.067679	1.026481
H	0.347506	-2.242083	-0.285326

Frequencies

-1913.1968	271.2348	489.8277
557.9211	682.7480	729.0915
800.3762	826.8239	905.6700
923.7509	930.6590	946.3861
1006.3674	1054.8270	1121.8295
1132.0939	1239.0837	1268.2900
1291.6132	1318.5104	1389.2401
1465.2804	1566.9432	2162.2918
2884.2925	2936.8821	3186.7835
3194.3595	3210.1078	3217.1003

i3 — i10

C	1.328219	0.302107	0.015350
C	0.004203	-0.334339	-0.003566
C	-2.451221	-0.180987	-0.013722
C	-1.224607	0.386938	-0.030026
C	2.581284	-0.314146	-0.176279
H	1.288348	1.397330	-0.067070
H	0.933057	0.039778	1.128356
H	-0.008752	-1.418907	0.043062
H	-3.349323	0.418344	-0.089378
H	-2.577985	-1.255862	0.057023
H	-1.152156	1.471098	-0.099467
H	3.439548	0.190787	0.276925

Frequencies

-1804.4583	157.2180	194.3388
239.3880	455.7313	478.1224
548.1709	607.9375	695.3405
853.4002	871.6119	887.9366
951.5751	1013.3197	1076.8048
1135.6617	1212.1384	1232.2755
1275.7706	1310.7425	1438.1902
1500.4265	1607.5918	2240.7070
2996.1095	3075.8101	3123.2203
3140.9032	3166.8994	3231.9698

i4 — p3

C	1.056017	-0.221015	0.001088
C	-0.060473	-0.926592	-0.074292
C	-1.769408	0.896287	0.052118
C	-1.422813	-0.387275	-0.089148
C	2.135426	0.492546	-0.154390
H	1.168155	-0.455699	2.146966
H	0.035255	-2.010203	-0.090236
H	-2.808148	1.200673	0.016833
H	-1.029744	1.673712	0.210182
H	-2.203857	-1.129757	-0.226956
H	2.485240	0.744068	-1.152927
H	2.720602	0.853491	0.683880

Frequencies

-483.8623	72.1796	126.8183
160.5868	369.0305	397.8297
399.6451	521.7341	654.1081
713.2274	888.7928	901.5570
918.6759	938.2064	1006.2892
1022.6595	1045.5673	1148.9757
1334.6659	1373.7855	1444.2901
1465.5516	1665.5181	1983.7722
3110.7616	3126.2324	3138.1783
3151.6894	3191.5059	3227.1422

i10 — i11

C	-1.435753	0.309415	0.094120
C	-1.868069	-0.907998	-0.105130
H	-2.113199	1.028442	0.569793
H	-2.765738	-1.482210	0.066953
C	-0.050684	0.833678	-0.277379
C	2.080437	-0.495867	-0.149371
C	1.067205	0.126228	0.444111
H	-0.014180	1.902724	-0.040404
H	0.097988	0.745059	-1.357675
H	2.859657	-0.985892	0.423457
H	2.166406	-0.540248	-1.230929
H	1.010244	0.139391	1.530695

Frequencies

-135.5551	94.6226	265.3135
405.1794	438.7726	613.9719
660.6589	781.1289	822.7180
909.0093	929.0481	944.2393
1018.2198	1034.0934	1126.9790
1236.0201	1269.0822	1314.0107
1329.8559	1450.2408	1481.2083
1666.9836	1706.1964	3009.9425
3025.7801	3063.5432	3123.5472
3132.9652	3209.4924	3243.7197

i11 — i12

C	-1.356180	-0.245245	0.111867
C	-1.505924	1.006753	-0.233416
C	-0.080153	-1.065340	0.111492
H	-2.244659	-0.802489	0.435799
H	-2.310717	1.723343	-0.296863
H	-0.240810	-1.928266	-0.544666
H	0.046689	-1.494878	1.114923
C	1.640091	0.784230	0.225439
C	1.187422	-0.349031	-0.301027
H	2.565220	1.232703	-0.119032
H	1.104593	1.309535	1.009190
H	1.768147	-0.828151	-1.085475

Frequencies

-118.2302	129.3353	192.3379
380.6861	523.2744	593.4586
654.4073	808.6139	834.5660
861.0010	937.4241	953.4838
1008.2454	1022.6493	1111.0572
1237.8664	1252.8410	1336.7017
1362.2889	1447.8932	1475.4955
1679.6509	1706.4089	2993.4057
3005.9183	3033.2423	3128.4732
3138.3984	3213.4760	3242.2073

i12 — i13

C	-1.290607	0.068300	-0.000148
C	-0.868071	-1.166239	-0.170515
C	-0.253600	1.180725	0.152977
C	1.326502	-0.695719	0.224507
C	1.050738	0.549784	-0.260185
H	-2.349719	0.325062	0.044756
H	-1.349504	-2.128870	-0.276159
H	-0.242822	1.539252	1.192102
H	-0.504689	2.045205	-0.468443
H	2.095241	-1.311945	-0.230653
H	1.025731	-0.991621	1.223272
H	1.535997	0.901817	-1.164689

Frequencies

-518.3952	235.2388	315.8765
465.9473	603.2208	637.9660
695.1974	815.9137	871.6497
894.0825	907.1708	927.6301
945.9227	984.1812	1087.4920
1193.5268	1212.3706	1270.6601
1311.2295	1421.4046	1479.4873
1561.9783	1644.2632	2988.8245
3057.5818	3093.1520	3125.2523
3159.0753	3204.3096	3217.7943

i13 — p1

C	0.936518	0.823015	0.029571
C	-0.357120	1.165408	-0.087956
C	1.058869	-0.677608	0.054114
C	-1.181745	-0.054768	-0.141811
C	-0.361747	-1.139357	-0.100231
H	1.778498	1.497116	0.108247
H	-0.755321	2.170919	-0.120346
H	1.506022	-1.035708	0.992942
H	1.704159	-1.057373	-0.749677
H	-2.241007	-0.069603	-0.359233
H	-1.897564	-0.029093	1.752107
H	-0.663434	-2.176402	-0.146159

Frequencies

-554.6787	263.1678	295.1440
377.0117	547.6056	691.7145
709.0503	811.0909	817.7765
919.7062	925.1422	955.3196
966.1770	970.5989	1006.5221
1106.3207	1124.5800	1128.7552
1271.0188	1313.1121	1393.2486
1414.6786	1516.4608	1620.5193
3001.3791	3024.8371	3195.7479
3204.1742	3219.1359	3226.2726

i19 — i21

C	-2.136336	-0.453604	-0.263228
C	-0.060472	0.945629	-0.021266
C	1.705251	-0.873648	-0.042366
C	1.346993	0.405088	-0.101306
C	-1.107424	-0.063108	0.423770
H	-2.980467	-0.773923	-0.826833
H	-0.069026	1.785707	0.687191
H	-0.344484	1.368654	-0.991151
H	2.745776	-1.168468	-0.116647
H	0.976543	-1.668706	0.072978
H	2.118386	1.162596	-0.229457
H	-0.934803	-0.467997	1.430300

Frequencies

-705.8802	88.0391	146.4879
261.6810	414.9871	525.3378
578.4253	661.8957	767.0784
899.3558	933.5385	952.2215
1001.9702	1035.2839	1096.4156
1195.9426	1283.0326	1323.8392
1340.3844	1444.3064	1465.6202
1669.9883	1705.5031	2981.9282
2995.6793	3041.2368	3119.3695
3137.0459	3216.3191	3437.4904

i17 — i22

C	1.323368	-0.100348	0.650706
C	0.369455	-0.641726	-0.420197
C	-1.565168	0.569416	0.166581
C	-1.081745	-0.647355	-0.046696
C	0.808806	0.788114	-0.424497
H	0.932909	-0.001691	1.658754
H	2.368279	-0.395992	0.599264
H	0.747299	-1.365519	-1.133491
H	-2.517342	0.940671	0.522298
H	-0.418157	1.284232	-0.104411
H	-1.645142	-1.569301	0.072586
H	1.403865	1.298993	-1.170383

Frequencies

-1906.2505	289.7678	396.3892
585.2056	679.8688	715.8092
784.7283	808.5444	823.9182
895.6020	923.6511	930.1711
1021.8374	1046.0411	1057.6026
1071.8130	1124.1338	1154.7526
1204.2356	1263.5345	1346.9456
1463.8561	1615.0449	1699.3251
3090.4809	3139.1769	3156.2097
3171.2138	3187.4908	3209.6766

i1 — i8

C	1.495910	0.433192	0.001585
C	0.066024	0.907323	0.046643
C	-2.204170	-0.225923	-0.037204
C	-0.849172	-0.102248	0.104271
C	1.427979	-1.048655	-0.176074
H	2.020898	0.836703	-0.882383
H	2.065094	0.800054	0.870010
H	-0.191817	1.959252	0.119942
H	-2.750559	-1.020520	0.458561
H	-2.765966	0.406890	-0.717799
H	-0.136457	-1.095839	0.133615
H	2.139383	-1.668676	0.382731

Frequencies

-1397.8656	181.7018	226.8556
303.1781	384.6311	492.6278
634.7766	668.3747	796.1061
812.3700	860.9730	910.8053
945.1902	1020.0154	1023.2097
1082.5029	1117.5855	1191.8151
1281.2799	1317.3927	1433.7157
1477.4031	1576.5640	1871.5710
2949.1116	2959.8582	3050.7420
3118.5542	3164.1147	3204.2638

i8 — p3

C	-1.350739	0.325793	-0.154349
C	0.001846	0.913297	-0.066326
C	2.239403	-0.428813	0.033418
C	1.124186	0.240041	-0.012221
C	-1.651971	-0.981946	-0.011797
H	-1.999958	1.073271	1.603293
H	-2.118781	1.001112	-0.518743
H	0.057971	1.999384	-0.055340
H	2.775047	-0.702837	-0.871490
H	2.677656	-0.735694	0.979310
H	-0.906192	-1.705834	0.296614
H	-2.662089	-1.339638	-0.165994

Frequencies

-617.0583	79.6360	152.6539
322.1569	338.0889	364.8367
392.9542	519.2149	653.7761
692.3778	877.8116	902.1759
908.4682	913.3575	1011.2822
1023.0494	1047.3486	1149.5089
1313.2804	1369.9709	1438.2204
1474.0232	1609.1206	2036.1091
3106.6447	3129.6280	3142.1099
3154.7616	3176.7848	3234.1875

i6 — i24

C	-1.170679	-0.340110	0.482264
C	0.047304	-0.996050	-0.130175
C	1.605757	0.876194	0.214559
C	1.303526	-0.385451	-0.175445
C	-1.535350	0.851105	-0.340619
H	-1.991992	-1.064284	0.508377
H	-0.954895	-0.042515	1.514020
H	-0.067072	-1.972914	-0.588570
H	2.494526	1.488873	0.234407
H	2.125081	-0.996181	-0.565595
H	-1.894134	0.708817	-1.353595
H	-1.214862	1.844069	-0.052546

Frequencies

-222.8517	184.0532	238.0153
293.3984	362.3899	539.7726
566.1057	604.8798	667.4395
781.5373	850.7062	865.9681
912.7585	1054.7049	1089.4083
1166.4146	1227.4985	1266.3448
1295.3873	1411.2702	1432.5298
1460.6199	1468.5727	3011.9041
3033.7670	3053.9269	3135.3921
3164.2077	3237.4109	3242.8250

i10 — i21

C	-1.186528	0.136889	0.380571
C	-0.054702	0.847362	-0.336621
C	-2.125647	-0.569466	-0.192174
H	-1.183850	0.232970	1.472773
H	-0.155209	1.924593	-0.166986
H	-0.161920	0.685759	-1.412380
H	-2.993742	-1.141517	0.099269
C	1.805126	-0.830281	-0.046482
C	1.318731	0.394084	0.129017
H	2.794346	-1.102314	0.303891
H	1.230332	-1.606093	-0.543562
H	1.928159	1.135074	0.641135

Frequencies

-124.2126	99.5868	274.1960
392.5895	440.3212	619.9942
669.2438	782.4248	813.7086
906.2549	933.2151	955.4424
1022.0629	1053.4126	1105.9459
1217.0209	1278.6105	1322.1638
1335.0922	1444.3757	1483.6955
1670.5860	1701.9296	3018.2245
3029.4765	3073.2973	3125.1637
3135.7769	3211.3153	3238.6917

i12 — i21

C	-1.279274	-0.279755	-0.239402
C	-1.643621	0.862994	0.281311
H	-1.955248	-0.745544	-0.966999
H	-2.475127	1.546375	0.193372
C	-0.027175	-1.075950	0.076418
C	1.516476	0.946592	-0.130602
C	1.293635	-0.343018	0.094481
H	0.052618	-1.902038	-0.640027
H	-0.159773	-1.564599	1.051687
H	2.521812	1.350733	-0.091701
H	0.712844	1.637671	-0.356506
H	2.142628	-0.987776	0.316936

Frequencies

-111.8208	128.2582	223.1372
386.5574	533.8016	578.8678
655.5355	792.1702	836.3145
857.0331	944.7111	962.0470
1020.4479	1034.0929	1090.5951
1240.4556	1259.9804	1329.9726
1369.3455	1440.6318	1473.3350
1673.1192	1711.4109	2995.9901
3004.0111	3031.2607	3116.2311
3138.5439	3219.4603	3237.4768

i15 — p8

C	2.530947	-0.162348	-0.148495
C	-0.100842	0.234053	-0.045865
C	-2.438689	-0.470742	-0.022493
C	-1.496078	0.481032	-0.053744
C	1.098050	0.059201	0.029038
H	2.845626	-1.101179	0.314035
H	3.113684	0.644444	0.303249
H	2.777536	-0.206448	-1.213770
H	-3.490312	-0.211394	-0.031384
H	-2.181715	-1.522664	0.014229
H	-1.795917	1.526046	-0.089005
H	1.170769	0.024021	2.151997

Frequencies

-436.0516	61.5021	130.8792
148.5378	195.6990	333.7757
368.4147	432.8640	540.7011
697.4115	725.7330	943.8399
1005.9474	1040.2267	1051.2835
1061.3021	1192.7389	1319.5467
1414.2879	1446.5029	1475.7629
1480.8282	1655.4117	2275.0336
3026.1372	3084.9310	3092.3495
3130.2766	3145.9753	3235.7614

i6 — i9

C	1.212542	0.275436	-0.101696
C	0.602816	-1.104640	0.058299
C	-1.192572	0.263512	-0.057997
C	-0.789793	-1.093123	-0.140405
C	-0.009311	1.219058	0.107525
H	2.011834	0.439876	0.627846
H	1.666660	0.430938	-1.090295
H	1.181349	-1.970147	0.359060
H	-2.166821	0.608408	-0.396559
H	-1.575998	-0.590252	0.841934
H	0.008668	1.694843	1.093136
H	-0.067788	2.024866	-0.629468

Frequencies

-1516.1606	143.5922	464.5835
555.8428	607.4803	710.2109
787.2740	824.4365	891.3462
909.4491	971.3288	1008.3211
1066.0199	1125.2844	1176.2052
1221.3591	1240.1472	1261.6980
1305.8774	1325.3017	1385.0737
1463.7448	1482.5262	2025.7793
2985.5999	3034.2023	3049.6289
3074.5505	3140.0833	3182.1346

i25 — i26

C	-1.251950	-0.663286	-0.441381
C	-0.402116	0.609400	-0.272222
C	1.823814	-0.504500	0.184470
C	1.086074	0.551151	-0.150624
C	-1.293438	0.106482	0.798782
H	-2.099744	-0.631475	-1.123179
H	-0.712945	-1.607784	-0.461348
H	-0.755659	1.487425	-0.810101
H	2.902346	-0.430444	0.256170
H	1.389757	-1.473516	0.407295
H	1.589881	1.493849	-0.352363
H	-2.087931	0.566461	1.369370

Frequencies

-97.2371	252.3522	284.5180
528.7049	576.7181	682.7805
737.2349	801.4212	890.8806
923.7030	975.8889	1019.6598
1026.0976	1048.7435	1060.7695
1097.7003	1112.4271	1239.6417
1335.2742	1389.0881	1443.9598
1469.8706	1698.7765	3073.2018
3094.5473	3129.6843	3139.2539
3144.1238	3203.9052	3215.7903

i16 — i18

C	1.626828	0.283624	0.680846
C	0.336720	-0.688767	-0.259484
C	-1.792997	0.578740	0.167046
C	-1.134628	-0.562623	-0.014825
C	1.159143	0.511052	-0.633074
H	0.717403	-0.778967	0.917355
H	2.521573	-0.361217	0.754794
H	0.637069	-1.614321	-0.752113
H	-2.860070	0.581618	0.354943
H	-1.290039	1.538613	0.151493
H	-1.670795	-1.507779	0.026872
H	0.774466	1.409898	-1.096391

Frequencies

-924.9097	83.9911	240.7043
317.2774	508.8080	580.8587
626.7445	749.1264	858.8866
898.9090	915.8016	953.5965
1006.4003	1016.9135	1072.7731
1098.8407	1190.3845	1256.6787
1321.0238	1333.8316	1392.2257
1444.3297	1695.8492	2113.8794
2919.2800	3080.2103	3134.8780
3148.0638	3181.4551	3229.1851

i24 — i28

C	-1.641418	-0.375879	0.321505
C	-0.392677	-0.347595	-0.444510
C	1.674262	0.305200	0.138055
C	0.969018	-0.807496	-0.004751
C	-0.318740	1.114024	-0.081401
H	-2.594107	-0.289375	-0.183534
H	-1.633290	-0.508178	1.395095
H	-0.554034	-0.493672	-1.514913
H	2.694363	0.538778	0.427162
H	1.302142	-1.838968	0.096215
H	-0.706571	1.873721	-0.753208
H	-0.251176	1.388179	0.959794

Frequencies

-899.8671	248.6806	271.2401
427.1433	560.8317	635.2642
694.5711	710.5852	778.1310
826.4468	846.8378	908.6437
929.6012	944.0492	1053.3747
1090.3026	1183.7314	1220.5019
1234.1978	1370.1596	1447.0187
1475.5868	1615.4302	3061.7147
3114.6698	3138.8919	3150.3074
3170.4583	3256.7041	3261.3684

i6 — i25

C	1.285197	-0.267483	-0.187473
C	0.082566	-1.138288	0.084450
C	-1.310392	0.812886	-0.148838
C	-1.166668	-0.542697	0.066946
C	1.097927	1.188568	0.129919
H	2.134420	-0.592095	0.439845
H	1.606520	-0.411636	-1.230738
H	0.200577	-2.209763	0.201310
H	-2.239856	1.360579	-0.058037
H	-2.050089	-1.152999	0.234354
H	0.834225	1.249044	1.202412
H	-0.417574	1.438957	-0.459168

Frequencies

-262.1176	171.0617	363.1208
480.2163	516.4456	634.0393
664.3475	727.0398	802.4413
881.9847	935.7809	970.4585
978.3819	1020.9022	1075.3109
1121.5776	1194.9894	1206.1649
1296.6372	1397.9001	1436.5068
1450.4630	1525.8962	2454.5590
2946.9839	2951.7533	2974.3544
3147.5604	3176.9373	3204.6656

i8 — i9

C	1.327681	0.002812	-0.000162
C	0.365490	1.205445	0.000094
C	-1.591174	-0.312970	-0.000102
C	-0.893389	0.845429	0.000072
C	0.534974	-1.283576	0.000139
H	1.980656	0.059200	-0.879249
H	1.981172	0.059274	0.878545
H	0.745768	2.220360	0.000210
H	-2.040437	-0.685983	0.917584
H	-2.040411	-0.685695	-0.917920
H	0.455932	-1.855254	-0.916543
H	0.455827	-1.854749	0.917130

Frequencies

-514.7720	103.6104	358.3837
463.8458	515.1293	614.6318
685.7939	736.7358	822.7148
878.0065	880.2140	906.8993
1025.2925	1025.8323	1069.3241
1098.7513	1237.2275	1242.4470
1322.4793	1458.9919	1478.9832
1491.5682	1832.7101	3006.3259
3034.6979	3097.4013	3137.4579
3166.1002	3177.3571	3232.4910

i18 — i19

C	-2.386059	-0.352146	0.000009
C	-0.143318	0.788576	0.000006
C	1.955713	-0.671874	0.000016
C	1.337219	0.504256	-0.000011
C	-1.080285	-0.416688	-0.000026
H	-3.165948	0.396116	0.000061
H	-0.368867	1.417684	0.870380
H	-0.368874	1.417729	-0.870334
H	3.038218	-0.727356	0.000010
H	1.430343	-1.619766	0.000049
H	1.950579	1.404077	-0.000044
H	-0.615076	-1.401227	-0.000090

Frequencies

-136.4848	79.9187	235.2087
374.7033	516.9762	559.8328
653.8563	798.0441	827.5901
935.2857	936.8432	955.4228
979.5655	1033.1981	1111.0535
1234.0061	1256.5255	1334.1037
1357.5772	1451.0142	1464.0132
1659.4093	1712.9924	3005.4831
3021.9813	3110.0114	3117.2366
3143.3448	3217.1049	3227.4647

i17 — i25

C	-1.472567	-0.367791	-0.567650
C	-0.360290	-0.418351	0.440739
C	1.906784	0.442250	-0.173277
C	1.079455	-0.566239	0.081845
C	-1.154486	0.827421	0.234525
H	-1.124745	0.777374	-1.056144
H	-2.397361	-0.914235	-0.703436
H	-0.651721	-0.972547	1.333944
H	2.942530	0.272868	-0.444576
H	1.566006	1.471457	-0.123800
H	1.445228	-1.590502	0.031650
H	-1.773316	1.451841	0.865276

Frequencies

-1879.2739	118.6839	250.0120
328.2117	556.1510	637.7222
679.1863	759.9474	786.7582
822.5878	946.4922	952.6924
1002.2741	1029.2352	1036.8813
1055.8365	1078.1747	1192.8227
1262.2459	1322.0199	1432.4161
1459.5293	1703.5151	2285.8098
3086.3261	3120.8753	3133.9633
3166.1384	3185.4574	3215.5876

i24 — i26

C	-1.323426	-0.100253	0.650692
C	-0.369446	-0.641778	-0.420112
C	1.565148	0.569427	0.166557
C	1.081751	-0.647356	-0.046634
C	-0.808735	0.788029	-0.424600
H	-2.368332	-0.395902	0.599277
H	-0.932978	-0.001409	1.658725
H	-0.747269	-1.365605	-1.133383
H	2.517341	0.940702	0.522193
H	1.645215	-1.569259	0.072653
H	-1.403712	1.298793	-1.170632
H	0.417992	1.284273	-0.104247

Frequencies

-1906.1497	289.7572	396.3753
585.2114	679.8358	715.7856
784.7059	808.5602	823.9655
895.6065	923.6551	930.1755
1021.8483	1046.0425	1057.6057
1071.8036	1124.1712	1154.8072
1204.2693	1263.5463	1346.9725
1463.8590	1615.0883	1699.3361
3090.5020	3139.1833	3156.2131
3171.2287	3187.4857	3209.6923

i16 — i15

C	1.807490	-0.286881	0.351899
C	0.220552	-0.169976	-0.603579
C	-2.052633	0.283110	0.209761
C	-1.064981	-0.586471	-0.057160
C	1.051636	0.881524	-0.222800
H	1.728352	-0.463509	1.423234
H	2.774423	-0.525316	-0.095421
H	1.164925	-1.148165	-0.283706
H	-3.061247	-0.058086	0.410910
H	-1.893006	1.355243	0.173789
H	-1.274065	-1.652813	-0.043736
H	0.788232	1.764812	0.346210

Frequencies

-1049.4334	115.4945	200.9529
256.0279	390.6851	544.4206
656.1478	707.9801	792.6500
899.6923	929.8041	938.0407
990.6340	1029.1229	1078.7902
1114.5344	1121.6261	1314.6016
1384.9281	1405.6624	1440.8059
1505.6259	1620.2501	2155.1747
3042.5605	3133.7647	3142.9302
3145.9093	3168.3139	3221.3874

i28 — p13

C	1.860974	-0.028716	-0.171382
C	0.534358	-0.034296	0.069371
C	-1.510171	-0.121023	-0.106447
C	-0.540719	-1.047373	-0.000123
C	-0.556738	1.064045	-0.008785
H	2.414291	0.901136	-0.230695
H	2.423517	-0.952962	-0.238579
H	0.699714	-0.024574	1.993389
H	-2.584475	-0.178142	-0.226832
H	-0.529248	-2.130000	0.009015
H	-0.656718	1.680102	0.888599
H	-0.493309	1.708619	-0.890697

Frequencies

-728.6792	260.4456	310.3618
383.6644	492.7858	503.4550
647.8885	719.0742	769.7647
867.1314	872.9201	909.4608
948.8998	972.9253	1007.5823
1097.7468	1106.3170	1183.2402
1217.7021	1310.1879	1435.4299
1470.3894	1592.7227	1641.4705
3037.8383	3084.0393	3136.5486
3186.8771	3216.1325	3224.9878

i17 — p5

C	-1.735387	0.441459	0.266849
C	-0.306930	0.078424	-0.093808
C	2.118228	-0.275746	0.124284
C	1.066393	0.535665	-0.017849
C	-1.176097	-0.902552	-0.092580
H	-1.987827	0.645163	1.309440
H	-2.345179	0.991402	-0.449449
H	-0.412150	0.673123	-2.072616
H	3.125527	0.118214	0.188650
H	2.001672	-1.352266	0.183370
H	1.214129	1.610320	-0.063715
H	-1.393404	-1.949456	-0.217054

Frequencies

-572.2154	91.1875	211.2526
267.9854	327.0135	377.2837
481.7862	628.3916	713.7011
747.4303	935.3847	950.2593
1002.7755	1018.0684	1024.2299
1062.3012	1089.6257	1103.6092
1150.2160	1325.8970	1439.7247
1511.2908	1664.1575	1752.3374
3032.4881	3100.2440	3138.5116
3157.3200	3226.8928	3265.3792

i15 — i31

C	2.084822	-0.577606	-0.000020
C	1.232506	0.671868	0.000101
C	-0.088753	0.726950	-0.000177
H	2.735669	-0.594152	0.880588
H	2.735574	-0.594048	-0.880702
H	1.488888	-1.490773	-0.000050
H	1.790489	1.608971	0.000403
C	-2.444950	-0.124297	0.000026
C	-1.116780	-0.277505	-0.000039
H	-3.097388	-0.989039	0.000236
H	-2.921015	0.845023	0.000011
H	-0.733293	-1.302441	0.000169

Frequencies

-105.8437	132.5797	181.4460
304.6909	362.4389	607.5728
691.7164	759.1261	855.1609
927.3802	965.3042	986.5846
1044.1899	1053.1571	1138.8754
1315.1180	1318.6936	1399.6779
1443.2514	1480.6210	1488.7959
1655.6106	1710.5276	3018.0839
3048.9491	3063.8001	3090.1028
3118.3204	3159.1143	3248.2551

i16 — i5

C	1.269211	-0.286646	0.323149
C	0.019920	-0.994194	-0.072908
C	1.880759	0.836174	-0.363437
H	1.971985	-0.922208	0.870132
H	1.073391	0.590208	1.052532
H	0.146240	-2.042016	-0.327450
H	1.087312	1.272067	-1.004459
C	-1.665780	0.822903	0.162282
C	-1.263638	-0.454289	-0.161732
H	-2.703703	1.114569	0.067664
H	-0.982292	1.578989	0.529373
H	-2.035769	-1.135300	-0.511914

Frequencies

-338.4314	99.8549	210.7183
261.5552	415.2233	536.9832
582.0760	729.1526	765.6625
808.6578	885.5726	944.4927
993.3477	1034.9462	1118.0504
1149.5722	1218.3763	1244.5947
1271.1050	1402.7649	1433.1816
1462.8947	1532.8135	2569.9560
2930.9981	3053.9367	3132.3714
3147.0104	3161.7989	3235.6303

i1 — i7

C	1.458600	-0.511079	0.136790
C	2.022218	0.783431	-0.289487
H	1.723940	-0.678895	1.197633
H	1.970499	-1.318097	-0.405034
H	2.166319	1.740555	0.197247
C	-0.030471	-0.688305	-0.040292
C	-2.331376	0.165846	-0.052252
C	-0.970606	0.321471	0.109054
H	-0.374605	-1.683559	-0.309961
H	-3.016276	0.988713	0.107135
H	-2.757342	-0.787732	-0.345054
H	-0.602722	1.310833	0.375162

Frequencies

-116.6426	165.1023	185.3414
237.9386	376.2459	541.7437
567.9237	686.1114	734.5719
801.1140	874.2465	965.2550
998.2721	1021.5591	1109.3499
1198.7488	1209.6561	1262.9626
1295.1653	1350.3815	1418.1463
1488.1569	1519.7263	2909.8530
3002.4971	3123.9528	3136.2422
3142.4451	3195.5592	3232.0532

i3 — i15

C	2.161389	-0.535298	0.000044
C	0.082845	0.074663	-0.000004
C	-2.326397	-0.451017	-0.000060
C	-1.315189	0.424180	0.000094
C	1.271794	0.673784	-0.000120
H	2.690978	-0.789700	0.918553
H	2.691204	-0.789878	-0.918287
H	0.865005	-1.117318	0.000191
H	-3.357849	-0.120448	0.000036
H	-2.144544	-1.519953	-0.000289
H	-1.533369	1.494420	0.000337
H	1.541928	1.725008	-0.000261

Frequencies

-2189.6045	111.6210	190.2051
208.2015	421.0733	503.5601
583.6645	680.5453	825.5782
901.7805	942.9117	966.3131
996.4844	1041.6017	1045.5921
1128.9195	1138.7463	1221.1711
1302.9494	1424.2077	1434.2278
1643.5403	1715.0418	1811.1577
3054.8201	3077.8732	3141.3970
3144.2331	3163.0561	3229.1957

i16 — p6

C	1.259549	0.335682	0.576613
C	0.371047	-0.671426	-0.129560
C	-1.832196	0.520312	0.144985
C	-1.116664	-0.589134	-0.040684
C	1.174013	0.470452	-0.708128
H	1.518659	0.744685	1.538075
H	3.133876	-0.930090	0.954293
H	0.753613	-1.683813	-0.252053
H	-2.913914	0.490812	0.196280
H	-1.363679	1.493600	0.251743
H	-1.639299	-1.538394	-0.140666
H	1.376252	1.027886	-1.607023

Frequencies

-297.4934	49.2796	141.9043
212.6366	254.2247	335.3846
566.5820	651.6443	671.3664
822.1120	849.7551	885.5929
931.5720	938.5429	1010.1486
1029.6421	1053.7792	1059.2590
1177.8488	1323.9665	1383.9297
1444.6277	1687.1419	1693.4072
3080.7834	3127.0541	3136.6515
3216.1436	3243.3968	3288.5411

i22 — i24

C	-1.206963	-0.306995	0.749566
C	-0.322823	0.673214	-0.000071
C	1.843238	-0.603858	0.000038
C	1.159637	0.514292	-0.000033
C	-1.206961	-0.307142	-0.749503
H	-0.698433	-1.117458	1.257608
H	-2.072574	0.087610	1.268543
H	-0.655367	1.704645	-0.000182
H	2.875641	-0.915709	0.000056
H	1.724972	1.454193	-0.000034
H	-0.698447	-1.117707	-1.257403
H	-2.072566	0.087364	-1.268568

Frequencies

-90.6381	235.2355	320.3055
535.2629	631.1315	747.9832
790.0712	805.8198	818.0219
836.9628	921.0823	994.6329
1050.4547	1075.1150	1109.2383
1126.1901	1203.7492	1220.8580
1271.8952	1398.2354	1463.9298
1498.5384	1662.7136	3011.2639
3119.6566	3122.9975	3155.8884
3201.0192	3216.7642	3252.2407

i16 — i7

C	-1.670179	-0.431946	-0.168153
C	-1.164683	0.945335	-0.117351
C	-0.335073	-0.094748	0.517812
H	-1.651929	-0.962045	-1.118822
H	-2.491333	-0.724183	0.481774
H	-0.926417	1.642148	-0.908676
H	-0.372906	-0.151129	1.606024
C	2.085155	0.209948	-0.057451
C	0.973079	-0.518839	-0.078751
H	3.011116	-0.157540	-0.485351
H	2.109221	1.198981	0.389936
H	0.992452	-1.504730	-0.541523

Frequencies

-123.7405	239.1186	297.8230
460.3948	624.0778	656.1346
795.1875	861.8720	873.1664
938.3643	953.0072	1015.6514
1026.3527	1046.1181	1074.0534
1094.3779	1157.2019	1239.4741
1321.4521	1347.7121	1444.8002
1467.3638	1694.1154	3072.8317
3074.3178	3112.3406	3129.1445
3146.7571	3206.1506	3210.9848

i3 — i7

C	-1.842230	-0.413880	-0.460720
C	-1.437750	0.521462	0.483897
C	-0.134570	-0.163260	0.475397
C	2.266562	-0.166800	-0.083880
C	1.010884	0.329430	-0.214880
H	-2.197680	-0.152340	-1.459140
H	-1.874130	-1.472670	-0.223870
H	-1.525940	1.587743	0.308732
H	-0.016270	-1.062690	1.075691
H	3.106494	0.283201	-0.597440
H	2.474219	-1.023750	0.548216
H	0.855885	1.198789	-0.851040

Frequencies

-829.8019	165.2582	234.1598
298.5959	487.5873	620.4267
668.6543	751.7353	834.0049
853.6492	923.4419	940.2310
985.9078	1006.5890	1108.3258
1199.0089	1258.9104	1292.4746
1303.9288	1350.1356	1459.8204
1505.9830	1576.9853	3068.2773
3120.4203	3129.0263	3136.6965
3161.1102	3174.1528	3227.1522

i4 — i2

C	-1.700740	-0.716770	0.199318
C	-0.152690	0.502040	0.205267
C	2.239170	-0.102320	0.175927
C	1.015867	-0.075060	-0.393100
C	-1.498210	0.532617	-0.390290
H	-2.482980	-0.910030	0.936880
H	-1.128540	-1.585450	-0.103140
H	-0.025140	1.003590	1.162418
H	3.093932	-0.516960	-0.343470
H	2.413787	0.308124	1.165223
H	0.887613	-0.499970	-1.386750
H	-2.179090	1.357634	-0.213900

Frequencies

-847.2805	152.2061	254.0031
282.7104	476.3807	641.9309
707.1993	769.6706	799.7909
880.6792	902.8302	933.6021
993.9885	1020.9009	1096.5652
1179.4700	1256.9776	1290.9449
1307.3834	1355.8187	1453.6195
1508.1641	1604.9287	3060.0198
3116.4437	3129.8897	3135.4417
3163.3280	3185.9246	3225.0005

i4 — i2' (with H shift)

C	-1.444827	0.422568	0.297862
C	0.003259	0.605292	-0.098789
C	2.340978	-0.125207	-0.133598
C	1.024870	-0.276988	0.235039
C	-1.967548	-0.815505	-0.347887
H	-2.003802	1.358101	0.161616
H	-1.504605	0.165866	1.376088
H	0.222588	1.454871	-0.738684
H	3.097243	-0.837656	0.169644
H	2.662440	0.714630	-0.740243
H	0.752927	-1.147574	0.827436
H	-2.967178	-0.569198	-0.771620

Frequencies

-439.9433	58.1805	168.9991
262.4078	417.3729	555.6446
576.2687	729.8885	785.9341
822.6203	876.9383	983.9816
996.1037	1073.1007	1095.1945
1132.5508	1214.5180	1285.6795
1321.1167	1362.8751	1426.1487
1479.1982	1523.7843	2882.1533
2888.0529	2994.5025	3135.5621
3139.6786	3155.9784	3233.2959

i26 — p5

C	-1.735389	-0.441463	0.266839
C	-0.306931	-0.078423	-0.093807
C	2.118229	0.275744	0.124281
C	1.066392	-0.535665	-0.017845
C	-1.176098	0.902553	-0.092570
H	-2.345177	-0.991396	-0.449469
H	-1.987834	-0.645180	1.309426
H	-0.412131	-0.673091	-2.072617
H	3.125527	-0.118218	0.188650
H	2.001677	1.352266	0.183356
H	1.214126	-1.610320	-0.063702
H	-1.393404	1.949459	-0.217029

Frequencies

-572.2332	91.1871	211.2529
267.9898	327.0148	377.2876
481.7857	628.3905	713.7010
747.4298	935.3846	950.2592
1002.7752	1018.0687	1024.2301
1062.3012	1089.6251	1103.6092
1150.2163	1325.8972	1439.7247
1511.2903	1664.1574	1752.3351
3032.4882	3100.2443	3138.5115
3157.3201	3226.8927	3265.3792

i4 — i11

C	-1.444181	0.451517	-0.035585
C	0.036480	0.668802	-0.042311
C	2.340831	-0.161313	-0.018488
C	1.001051	-0.370404	-0.000275
C	-2.058512	-0.807633	0.044401
H	-1.992754	1.374217	-0.256174
H	-0.972408	0.597978	1.056220
H	0.358571	1.704442	-0.039691
H	3.038134	-0.989312	-0.010175
H	2.761151	0.838229	-0.062855
H	0.613180	-1.384466	0.027825
H	-3.059887	-0.826898	-0.401599

Frequencies

-1428.0070	154.8012	201.8364
298.1703	381.3421	468.1248
611.5096	632.9304	759.8270
865.4962	882.1535	910.8224
952.9033	1033.3397	1035.2675
1118.3595	1192.8458	1239.8027
1289.9754	1327.6202	1417.9171
1467.3438	1577.8020	2339.9920
3015.1519	3054.9796	3135.0409
3158.5202	3174.2980	3229.4786

i7 — p11

C	1.525447	-0.234331	0.539801
C	1.464083	0.639224	-0.415112
C	0.244983	-0.247431	-0.280824
C	-2.238041	-0.149817	-0.065453
C	-1.024463	0.287895	0.267494
H	2.000653	-0.597700	1.434686
H	2.593060	-2.006380	-0.335981
H	1.895556	1.469084	-0.949015
H	0.111667	-1.057454	-0.999492
H	-3.135593	0.277292	0.365948
H	-2.373962	-0.953714	-0.782730
H	-0.923434	1.095638	0.991150

Frequencies

-352.6622	118.0863	154.3460
232.3435	302.3431	350.1390
473.0418	635.6949	675.2287
806.0513	857.0152	891.4626
928.4470	941.8298	1010.2142
1028.6058	1071.0548	1144.4636
1175.6001	1314.0117	1352.8932
1455.0666	1668.7637	1705.6815
3064.8773	3118.5911	3129.9247
3213.0913	3241.8150	3286.3085

i2 — i7

C	-1.549474	-0.682921	-0.017100
C	-0.270777	0.094964	0.409928
C	2.204748	-0.018231	0.107179
C	0.970545	-0.028282	-0.392854
C	-1.458217	0.757619	-0.131378
H	-2.143114	-1.132523	0.778925
H	-1.489096	-1.302642	-0.912393
H	-0.101254	0.159917	1.486062
H	3.075422	-0.110168	-0.531315
H	2.386408	0.082907	1.172731
H	0.827015	-0.123865	-1.467653
H	-1.936333	1.687478	-0.381008

Frequencies

-477.5040	120.6872	272.1253
317.8644	445.9704	676.5119
766.8394	845.0234	890.9784
924.6400	935.3518	956.0284
1017.9986	1044.2524	1075.2833
1094.0162	1179.5526	1246.5067
1311.6440	1347.4701	1454.4513
1464.9141	1693.9924	3046.5641
3064.4541	3110.6062	3123.7292
3132.2506	3213.9619	3278.6769

i16 — i17

C	1.471021	-0.254823	0.599774
C	0.381770	-0.410902	-0.505301
C	-1.870733	0.426656	0.219114
C	-1.052427	-0.564165	-0.127575
C	1.128095	0.823446	-0.310280
H	1.122842	-0.211807	1.631586
H	2.404601	-0.803418	0.472790
H	0.683151	-1.052772	-1.336357
H	-2.897989	0.236571	0.508024
H	-1.537861	1.459575	0.228125
H	-1.426943	-1.586362	-0.137383
H	1.305838	1.836946	-0.621172

Frequencies

-471.8252	109.3265	248.1958
298.7371	562.7911	654.7547
751.3644	852.8615	893.3105
928.8871	942.7083	985.5377
1024.4031	1045.4949	1047.7328
1091.0389	1131.5658	1242.0705
1324.0061	1380.8817	1442.1258
1463.1322	1695.6960	3048.3089
3048.8577	3116.9578	3120.9158
3133.4943	3214.6654	3278.3085

i4 — i15

C	2.227900	-0.097820	0.317608
C	0.101486	-0.288605	-0.086564
C	-2.247699	0.356454	0.261344
C	-1.315135	-0.505110	-0.178861
C	1.089810	0.515779	-0.447079
H	2.653050	0.445823	1.161329
H	2.931868	-0.725881	-0.227122
H	1.093100	-0.940534	0.663219
H	-3.303621	0.121443	0.193407
H	-1.974964	1.309231	0.700543
H	-1.629935	-1.467737	-0.577511
H	1.092331	1.373463	-1.112556

Frequencies

-2182.5473	104.6538	158.7111
259.9142	408.8028	489.6725
616.6266	697.5693	832.2779
885.8940	921.3435	964.4225
1002.1186	1032.5834	1052.9905
1065.2505	1111.9009	1242.0074
1310.3048	1427.3399	1433.5850
1608.4976	1742.3294	1795.7802
3061.7458	3123.0233	3137.8639
3153.6698	3161.4176	3226.2732

i15 — p10

C	-2.302199	-0.448592	-0.000005
C	0.055228	0.389942	0.000004
C	2.584532	-0.089899	-0.000005
C	1.267711	-0.020093	0.000002
C	-1.239260	0.617207	0.000004
H	-2.946186	-0.346428	-0.880222
H	-2.946209	-0.346423	0.880195
H	-1.864984	-1.446964	0.000004
H	3.110933	-1.036005	-0.000012
H	3.178915	0.818736	-0.000004
H	0.853880	-1.985848	0.000031
H	-1.582410	1.651544	0.000005

Frequencies

-598.2063	109.9511	131.9319
152.9935	249.4035	376.8682
456.7231	533.0914	563.2556
581.6426	802.4835	827.6409
882.5739	1020.5522	1035.8621
1048.9744	1100.6941	1316.7364
1400.3075	1442.9929	1481.3220
1487.8871	1690.5574	2118.0397
3016.5309	3061.7553	3101.6459
3126.5360	3127.0829	3214.3222

i23 — p13

C	-1.437730	0.107200	-0.140858
C	-0.459136	1.039932	-0.102538
C	1.928361	0.038702	0.081537
C	0.604470	0.034751	-0.013087
C	-0.464602	-1.066283	-0.084742
H	-2.506780	0.159193	-0.300214
H	-2.082578	0.102932	1.936125
H	-0.455103	2.122394	-0.128390
H	2.488471	-0.888354	0.129529
H	2.486400	0.968084	0.111745
H	-0.423156	-1.681993	-0.987319
H	-0.535431	-1.708070	0.796652

Frequencies

-557.2896	173.6407	255.8502
324.7809	346.9801	482.0022
705.4957	726.7573	817.3110
884.0913	907.3116	918.5691
957.4971	982.2518	1007.7306
1103.5589	1113.2043	1198.5283
1226.5052	1323.3704	1442.9815
1467.7854	1564.3600	1760.7276
3067.5067	3122.3851	3157.7060
3218.5509	3246.3766	3248.1148

i1 — i23

C	1.547430	-0.331890	-0.030671
C	0.192997	-0.951270	0.015726
C	-2.110273	0.127575	0.028275
C	-0.747760	0.065190	-0.092158
C	1.165848	1.162050	-0.048882
H	2.122939	-0.627786	-0.918778
H	2.147217	-0.605930	0.848779
H	-0.032380	-2.004556	0.162412
H	-2.656566	1.051784	-0.106617
H	-2.679183	-0.768309	0.260432
H	-0.197360	1.057942	-0.480122
H	1.005879	1.466924	1.000153

Frequencies

-417.6610	179.3814	262.6951
378.4501	433.6834	631.3396
697.4956	775.1525	790.0980
902.4769	928.8297	935.0666
982.6154	1019.5151	1080.1788
1204.4577	1231.7464	1254.5664
1282.8649	1362.8847	1444.4980
1478.0276	1500.3788	2016.5309
2974.3241	2978.9226	3005.3104
3124.3499	3139.3400	3229.3531

i4 — i14

C	-1.353082	0.575578	0.000000
C	-1.517224	-0.909826	-0.000001
C	0.854488	-0.136956	0.000005
C	2.167810	-0.297710	-0.000001
C	-0.070786	0.978883	0.000000
H	-2.199146	1.255784	0.000001
H	-1.929135	-1.358909	-0.904994
H	-0.158321	-1.088235	0.000011
H	-1.929167	-1.358908	0.904978
H	2.627979	-1.280483	0.000005
H	2.847597	0.555594	-0.000012
H	0.252964	2.015348	-0.000002

Frequencies

-1891.3100	166.8379	276.9910
296.8378	494.4039	542.5027
593.2211	744.5685	759.2376
888.3719	922.8616	939.7276
963.3243	1048.2457	1053.6981
1110.6587	1161.3919	1257.4723
1344.4578	1429.7589	1442.8894
1609.4243	1695.6175	1708.6489
3062.1627	3073.5873	3128.9585
3149.3088	3172.0595	3173.0587

i3 — i2' (with H shift)

C	-1.388489	0.407106	-0.332797
C	-2.210582	-0.473711	0.502997
H	-1.814280	0.532482	-1.344186
H	-1.325776	1.418856	0.099428
H	-3.194692	-0.448820	0.951292
C	-0.005431	-0.200535	-0.417780
C	2.388263	-0.208946	0.131378
C	1.124726	0.347200	0.168016
H	0.073252	-1.153660	-0.933083
H	3.235140	0.284576	0.590345
H	2.570091	-1.156994	-0.362630
H	1.005343	1.296883	0.687950

Frequencies

-272.6682	47.3930	164.6923
254.1193	305.7013	487.3647
548.6690	749.2913	782.4045
801.0358	857.4539	952.6734
995.7065	1079.5308	1097.3934
1163.0023	1208.3867	1274.6057
1284.2717	1354.9458	1444.6697
1492.4852	1518.3848	2914.7786
2955.2770	3117.8999	3138.6612
3152.2197	3214.9236	3234.5822

i24 — p14

C	1.340459	0.533170	0.551289
C	0.302838	0.256536	-0.522648
C	-2.162283	-0.301796	0.229238
C	-1.088497	0.115443	-0.156542
C	1.295954	-0.814984	-0.107764
H	2.145358	1.211523	0.296554
H	0.981949	0.612653	1.569486
H	0.474355	0.730803	-1.481761
H	-3.155143	-0.512307	0.544756
H	-1.556220	1.946085	-0.532487
H	2.069749	-1.070143	-0.821540
H	0.909135	-1.648827	0.463552

Frequencies

-681.9291	87.6937	223.3754
242.9796	463.2694	523.0392
535.8324	629.4073	681.0516
758.8458	814.0105	826.0533
901.1722	957.5268	1057.5805
1079.2284	1114.9821	1137.7417
1199.3677	1215.6769	1379.9634
1468.0298	1502.9390	2123.3738
3130.9650	3134.8855	3157.2503
3213.6808	3228.2070	3465.2618

i22 — p14

C	1.340501	-0.533229	0.551147
C	0.302845	-0.256493	-0.522700
C	-2.162292	0.301867	0.229024
C	-1.088448	-0.115552	-0.156401
C	1.295831	0.815072	-0.107632
H	0.982007	-0.612869	1.569333
H	2.145526	-1.211378	0.296280
H	0.474278	-0.730645	-1.481888
H	-3.155063	0.512026	0.545062
H	-1.555843	-1.946367	-0.531957
H	0.908865	1.648714	0.463869
H	2.069609	1.070523	-0.821332

Frequencies

-682.0973	87.9046	223.3909
242.9853	463.2512	523.0299
535.8323	629.4461	681.0642
758.8605	814.0237	826.0554
901.2104	957.5117	1057.5527
1079.2221	1114.9734	1137.7438
1199.3686	1215.6654	1379.9441
1468.0186	1502.9285	2123.3672
3130.9624	3134.8843	3157.2340
3213.6998	3228.2245	3465.2465

i10 — p4

C	1.307671	-0.079878	-0.041967
C	0.003207	-0.684811	-0.361271
C	-2.219691	0.457010	-0.119872
C	-1.139380	-0.087173	0.427089
C	2.348836	0.539852	-0.070502
H	1.433722	-0.828337	1.759459
H	0.058700	-1.762217	-0.165315
H	-0.178984	-0.562697	-1.433681
H	-3.020611	0.858041	0.490538
H	-2.345371	0.522813	-1.196402
H	-1.035300	-0.131320	1.507875
H	3.283988	1.033722	0.036660

Frequencies

-634.9028	86.2662	136.4561
226.0645	409.6385	417.4177
470.7895	493.6403	640.5880
658.9533	677.0498	896.8594
930.3318	953.5808	976.0849
1033.1573	1126.7855	1243.9729
1311.1820	1328.3364	1451.4524
1464.0303	1710.0776	2135.2698
3017.3993	3060.6795	3127.8473
3148.4321	3213.1270	3465.6190

i14 — i15

C	-1.298090	0.588206	-0.081221
C	-2.152096	-0.644424	0.072974
C	1.266726	0.121737	0.135555
C	2.484020	-0.402602	-0.033884
C	0.041824	0.550114	-0.154578
H	-1.806546	1.542535	-0.175202
H	-2.833765	-0.768789	-0.775768
H	-1.542154	-1.545934	0.152875
H	-2.774463	-0.575714	0.974250
H	3.339312	-0.068685	0.538012
H	2.626451	-1.228915	-0.724502
H	0.936866	1.367319	0.377257

Frequencies

-1660.6697	104.2780	121.8793
194.7258	355.9354	414.1339
482.7524	591.2528	714.6819
738.2271	799.8097	907.2907
999.3099	1029.6367	1035.5723
1098.8156	1316.6449	1402.2571
1420.4030	1478.1168	1485.4090
1546.9605	1819.7146	2180.0841
2998.4298	3042.7119	3102.6126
3115.6379	3148.4940	3213.8464

i14 — p10

C	-1.246380	0.552667	-0.000040
C	-2.220469	-0.591896	-0.000016
C	1.255184	-0.063017	0.000084
C	2.533164	-0.359669	-0.000057
C	0.066530	0.409086	0.000080
H	-1.665223	1.555221	-0.000134
H	-2.871759	-0.540005	-0.879644
H	-1.709554	-1.554837	0.000037
H	-2.871797	-0.539938	0.879581
H	2.879893	-1.388250	0.000038
H	3.289236	0.421286	-0.000229
H	0.621039	2.363498	0.000047

Frequencies

-551.4341	135.3776	154.3785
155.2077	231.4906	316.3061
454.3881	480.9086	567.9394
571.3670	802.8376	847.9757
864.5451	1011.9420	1030.1803
1050.5048	1109.6462	1328.5550
1403.0836	1435.0531	1480.1734
1487.0571	1690.2088	2123.5754
3014.6686	3058.6762	3109.2698
3118.3081	3144.7352	3185.4745

i8 — i14

C	1.338265	0.474138	0.019059
C	1.686739	-0.966516	0.041471
C	-1.120528	0.240642	0.020405
C	-2.203785	-0.482391	0.004569
C	-0.022045	0.977092	0.002642
H	2.121902	1.167177	0.303140
H	2.685655	-1.267197	0.320273
H	0.905905	-1.704760	-0.068693
H	-2.642031	-0.841728	-0.925510
H	-2.725246	-0.756922	0.919748
H	-0.136342	2.057466	-0.052512
H	1.718275	-0.111833	-1.025323

Frequencies

-1855.5087	145.8671	183.5916
301.0037	364.0834	409.8260
578.4494	639.2939	659.1615
803.2071	880.3335	885.5708
895.1587	1004.9941	1011.8093
1093.7479	1211.3647	1255.1704
1368.5745	1401.5963	1442.3085
1474.2560	1981.6591	2188.5508
3076.7463	3125.5177	3137.7282
3161.4555	3170.2186	3281.7042

i14 — p9

C	-1.289380	0.519440	0.066031
C	-1.683984	-0.919031	-0.028150
C	1.135412	0.219855	-0.129184
C	2.158388	-0.418690	-0.216649
C	-0.037247	1.004239	0.020553
H	-2.096827	1.237427	0.184027
H	-2.362036	-1.078465	-0.874128
H	-0.818158	-1.570915	-0.149019
H	-2.229235	-1.228284	0.870697
H	2.644924	-0.900563	2.001194
H	3.045090	-0.970668	-0.409815
H	0.117106	2.076591	0.101433

Frequencies

-240.3781	54.8375	140.7177
158.5927	184.1930	297.6164
376.0363	507.5680	661.7648
671.5543	674.2978	749.9122
902.2483	975.6056	985.9131
1062.7031	1121.9523	1265.1873
1399.1419	1430.6261	1482.1229
1483.2551	1673.7522	2169.2023
3015.9062	3056.7810	3115.4867
3138.3260	3157.1715	3473.9898

i25 — i27

C	-1.215580	0.828565	0.128018
C	-0.388883	-0.425567	0.475387
C	1.889108	0.431092	-0.178584
C	1.052034	-0.563526	0.099791
C	-1.440816	-0.442706	-0.541021
H	-1.926342	1.181727	0.875394
H	-0.728700	1.637139	-0.415591
H	-0.631102	-0.893635	1.433789
H	2.919362	0.238785	-0.456335
H	1.580053	1.470276	-0.139424
H	1.415643	-1.589161	0.057698
H	-2.004091	-1.012279	-1.257076

Frequencies

-496.5579	93.2956	256.0430
304.1712	516.6732	662.9829
767.4354	848.9278	896.9672
927.0931	942.7249	978.8135
1025.1720	1052.9926	1076.3255
1086.2443	1122.8025	1241.7673
1322.1415	1371.8602	1445.3551
1464.2287	1700.1896	3033.1526
3053.4662	3116.4747	3117.4225
3134.3380	3212.4927	3286.2311

i27 — p6

C	-1.271875	0.581924	0.405066
C	-0.373588	-0.635015	0.357044
C	1.834689	0.501420	-0.111596
C	1.082206	-0.586776	0.020635
C	-1.457335	-0.215659	-0.606847
H	-1.643502	1.366091	1.040760
H	-0.490327	2.328923	-0.477026
H	-0.618067	-1.468976	1.021372
H	2.885211	0.432970	-0.370800
H	1.426173	1.498110	0.023366
H	1.542855	-1.564671	-0.113795
H	-1.986925	-0.467819	-1.509688

Frequencies

-557.8886	54.6061	245.5046
289.0157	337.0860	354.0184
594.0576	637.0922	687.5503
793.2009	859.1780	869.7908
940.2638	949.3027	1006.1332
1023.4789	1045.7542	1073.6953
1198.5806	1327.4902	1379.9667
1443.0477	1652.8386	1701.1801
3028.9468	3113.8737	3124.7386
3207.7837	3248.0070	3289.1180

i12 — p7

C	1.151044	-0.135361	0.000004
C	1.879669	0.833540	0.000097
C	-0.005793	-1.038201	0.000052
C	-1.601660	0.943506	-0.000050
C	-1.359663	-0.360906	0.000004
H	2.472515	-1.565020	-0.000550
H	2.633096	1.583535	-0.000160
H	0.061510	-1.703399	0.869827
H	0.061519	-1.703514	-0.869630
H	-2.617816	1.320435	-0.000074
H	-0.800049	1.673364	-0.000070
H	-2.192359	-1.060870	0.000018

Frequencies

-641.9023	95.4826	166.0544
195.5698	351.5908	406.4738
468.5982	570.2041	617.3488
667.4709	674.7484	865.0490
946.2147	960.4500	964.1813
1027.5171	1090.6280	1245.1257
1324.6265	1352.2614	1441.2156
1461.8595	1713.1330	2137.2279
3014.1824	3030.4734	3130.4028
3143.6608	3223.5929	3465.5415

i11 — p4

C	-1.305491	0.115863	-0.042426
C	-2.198111	-0.698658	-0.134570
C	-0.004754	0.782165	0.135438
C	2.217087	-0.297045	-0.315034
C	1.108049	-0.203676	0.408797
H	-2.315129	1.775993	-0.305265
H	-3.065506	-1.303892	-0.239913
H	-0.088457	1.489995	0.969312
H	0.226970	1.378242	-0.752151
H	2.995063	-1.010453	-0.068617
H	2.389105	0.335547	-1.180557
H	0.957280	-0.857321	1.263963

Frequencies

-619.6065	87.7276	120.0602
218.7975	358.2650	410.4896
459.1576	501.6073	638.7054
667.5210	674.4640	897.9668
927.1289	954.9284	970.2192
1029.5872	1129.8746	1249.0678
1312.9477	1328.4962	1450.5047
1465.3671	1709.2538	2136.7903
3016.1276	3062.5152	3128.8383
3147.0199	3214.0547	3466.9338

i21 — p7

C	-1.137246	0.138884	0.061810
C	0.031788	1.023073	-0.032492
C	-2.135961	-0.503559	-0.183310
C	1.592165	-0.976230	-0.030902
C	1.377316	0.333270	-0.049709
H	-0.892434	-0.301469	1.936658
H	0.010157	1.740678	0.795982
H	-0.072954	1.621197	-0.947280
H	-3.009485	-1.105888	-0.248960
H	2.599132	-1.376404	-0.049422
H	0.775328	-1.688173	0.005941
H	2.221876	1.017429	-0.085310

Frequencies

-674.3154	116.0700	153.4362
201.2634	389.1813	419.7650
475.5023	565.9675	614.9878
653.4663	683.6950	865.5704
947.9714	964.8534	965.6240
1029.4692	1094.0168	1237.2615
1325.9674	1353.5860	1444.0817
1462.5840	1712.7708	2133.1050
3008.4867	3035.3334	3133.0898
3145.3028	3224.5539	3464.1375

i29 — p12

C	-0.415784	-0.026459	-0.030627
C	-1.882265	0.146814	-0.118565
C	1.637473	-0.020351	-0.054936
C	0.778456	0.992113	0.050586
C	0.461845	-1.034166	-0.136074
H	-0.638408	-0.803237	2.341365
H	-2.265865	0.706824	0.739450
H	-2.388556	-0.819549	-0.160901
H	-2.140198	0.717741	-1.018518
H	2.715101	-0.109200	-0.062897
H	0.862759	2.063718	0.164513
H	0.376816	-2.103997	-0.265310

Frequencies

-364.2054	135.5663	192.2243
230.5622	269.3993	314.6209
545.4749	608.2024	643.5811
746.2740	783.7617	873.8117
898.3233	1000.1954	1040.4599
1070.9362	1157.9628	1175.3673
1263.7754	1408.3091	1469.0859
1482.0989	1546.1834	1686.8292
3031.2383	3093.9140	3138.2040
3226.3646	3246.4623	3263.6272

i20 — p7

C	2.136087	-0.503410	-0.183279
C	-0.031764	1.023066	-0.032340
C	-1.592179	-0.976185	-0.031046
C	-1.377314	0.333315	-0.049725
C	1.137236	0.138825	0.061824
H	3.009661	-1.105661	-0.248974
H	0.073031	1.621373	-0.947002
H	-0.010134	1.740514	0.796274
H	-2.599146	-1.376355	-0.049642
H	-0.775340	-1.688128	0.005780
H	-2.221855	1.017497	-0.085304
H	0.891391	-0.302903	1.936262

Frequencies

-674.2349	116.1094	153.4731
201.3591	389.1781	419.7467
475.4396	565.9696	614.9835
653.4443	683.6954	865.5763
947.9708	964.8609	965.6264
1029.4663	1094.0172	1237.2559
1325.9669	1353.5846	1444.0835
1462.5852	1712.7699	2133.1174
3008.4850	3035.3127	3133.0917
3145.3010	3224.5508	3464.1415

i28 — i29

C	0.465100	-0.244414	0.603933
C	1.603997	-0.102188	-0.400663
C	-1.384804	0.182355	-0.298822
C	-0.769282	-0.963640	0.075707
C	-0.271351	1.042332	0.129383
H	0.732416	-0.376497	1.653451
H	1.731745	-0.847164	-1.182357
H	2.520442	0.360312	-0.041974
H	0.740719	0.991215	-0.822822
H	-2.303205	0.392079	-0.835180
H	-0.997288	-2.014709	-0.056335
H	-0.286791	2.008092	0.627988

Frequencies

-2129.7951	290.4894	408.5259
442.8956	630.9120	740.0700
789.7098	852.0294	884.6835
903.5627	935.2699	937.6809
987.9731	1021.9450	1055.9993
1107.4068	1155.8217	1192.3086
1260.7112	1307.5993	1326.7684
1428.1453	1544.8413	1684.7069
3079.7052	3090.5761	3141.9324
3170.1814	3188.4103	3198.7761

i18 — i20

C	2.136471	-0.453587	-0.263188
C	0.060493	0.945556	-0.021272
C	-1.705493	-0.873586	-0.042366
C	-1.347039	0.405093	-0.101267
C	1.107614	-0.063137	0.423666
H	2.980608	-0.773942	-0.826727
H	0.344443	1.368647	-0.991141
H	0.069030	1.785587	0.687250
H	-2.746079	-1.168225	-0.116601
H	-0.976920	-1.668768	0.072915
H	-2.118368	1.162692	-0.229338
H	0.935012	-0.468027	1.430203

Frequencies

-705.9103	87.2607	146.3980
261.4656	414.8430	525.3050
578.4155	661.9138	766.9948
899.2863	933.5154	952.1933
1001.8910	1035.2963	1096.3905
1195.9560	1283.0636	1323.8401
1340.3788	1444.3005	1465.6127
1670.5411	1705.5143	2981.8394
2995.6387	3041.2677	3119.2978
3137.0458	3216.3141	3437.6819

i29 — i30

C	-0.689658	-0.467974	0.451853
C	-1.666223	0.384543	-0.331337
H	-1.186517	-0.991921	1.275271
H	-2.108847	1.165336	0.292508
H	-2.492323	-0.250747	-0.679745
H	-1.201362	0.853851	-1.197724
C	1.382722	0.011203	-0.375335
C	0.947161	1.005915	0.425582
C	0.489267	-1.058739	-0.057391
H	2.222051	0.013351	-1.067296
H	1.210342	2.051595	0.572779
H	0.777038	-2.091157	0.123979

Frequencies

-673.0371	264.0032	286.8376
303.5896	483.9721	632.4591
740.3570	741.3697	852.5249
879.2012	906.2631	966.7640
1049.7205	1072.4799	1079.1195
1179.0455	1240.7311	1397.6814
1421.1567	1431.5395	1482.8679
1496.5933	1514.3082	2991.0647
3047.6127	3064.1171	3114.2125
3125.7025	3136.9765	3148.5380

i5 — i30

C	1.150176	0.570553	-0.026656
C	1.298534	-0.898904	0.026205
C	-1.295398	0.360266	0.024687
C	-1.273656	-0.968180	-0.044491
C	-0.062009	1.153456	0.025368
H	2.037320	1.186776	-0.158314
H	1.438685	-1.308471	1.030702
H	2.013222	-1.331520	-0.676145
H	0.081629	-1.303061	-0.194877
H	-2.240589	0.904876	0.031475
H	-2.084671	-1.685691	-0.061465
H	-0.151473	2.233943	-0.002057

Frequencies

-1581.2797	172.5470	352.3467
427.5580	520.5550	562.1910
614.9997	704.1404	763.2665
919.4956	932.0295	957.4266
968.7686	1033.2694	1045.4491
1112.1690	1212.7823	1274.0459
1328.0545	1412.1068	1443.9725
1530.9774	1586.1968	1670.4772
3044.6852	3086.8612	3109.2559
3122.2868	3174.4393	3194.6932

i14 — i30

C	-1.230219	0.550419	0.057261
C	-1.645326	-0.885044	-0.020890
C	1.188863	0.225601	-0.250944
C	1.980597	-0.742359	0.222997
C	0.047350	1.016275	0.015825
H	-2.025739	1.287771	0.112620
H	-2.213949	-1.085471	-0.937969
H	-2.303379	-1.144421	0.815851
H	-0.791202	-1.563545	0.004299
H	2.304308	0.555534	0.249719
H	2.774430	-1.129131	-0.431807
H	0.207940	2.089917	0.041794

Frequencies

-1076.5908	104.5648	117.2050
211.5692	272.1788	469.9590
498.3647	685.8370	750.0312
889.4163	922.9522	955.6070
976.0324	1042.1758	1107.7037
1232.8746	1247.3528	1394.2216
1424.4610	1475.2426	1483.0596
1562.3956	1644.5565	2231.4646
2989.3349	3002.5681	3044.8758
3105.9746	3142.5914	3161.1640

i30 — p9

C	1.213708	0.562787	0.028461
C	1.672324	-0.857612	-0.046604
C	-1.205493	0.150839	0.000041
C	-1.957710	-0.805932	0.051407
C	-0.054131	1.002926	0.044975
H	1.994052	1.318435	0.074618
H	2.267506	-1.115391	0.836874
H	2.324003	-1.005317	-0.915004
H	0.837118	-1.554632	-0.115643
H	-2.457223	1.501894	-0.493889
H	-2.734434	-1.531744	0.049273
H	-0.243207	2.068710	0.094088

Frequencies

-728.1593	22.9335	122.4887
188.9943	296.8966	410.6077
507.2691	524.8836	624.7440
653.3201	695.1906	746.7775
899.9434	968.3253	993.5846
1062.9889	1121.2010	1272.5740
1397.7895	1428.3015	1480.7644
1485.1735	1675.4422	2098.3421
3016.1894	3056.5604	3119.0148
3143.2158	3178.4430	3463.0839

i31 — i32

C	-1.190817	-0.505847	0.110124
C	-2.456588	0.279117	-0.077261
C	1.358252	0.075454	0.136251
C	2.676047	0.030354	-0.072933
C	0.053014	-0.042477	-0.089500
H	-1.286654	-1.557741	0.380015
H	-3.045942	0.310307	0.846638
H	-3.097138	-0.174989	-0.843285
H	-2.247133	1.306688	-0.380986
H	3.102973	-0.774876	-0.664003
H	3.354717	0.744518	0.373724
H	0.579732	1.126482	0.247816

Frequencies

-1660.1593	105.4645	131.5903
164.3010	316.4461	417.6515
488.7997	581.9132	719.6426
735.9787	799.8022	910.7900
1016.9849	1042.4901	1048.2276
1099.3857	1268.9713	1407.7919
1424.1858	1477.7743	1486.9748
1565.9214	1823.1322	2167.0769
3000.4725	3038.4410	3088.2441
3102.6488	3116.1207	3213.8702

i32 — p2

C	1.046420	-0.417534	-0.090728
C	2.333673	-0.052012	-0.159955
C	-1.321490	0.170142	-0.002447
C	-2.566700	-0.193478	0.071763
C	-0.063095	0.528137	-0.078451
H	0.786740	-1.470015	-0.022934
H	3.125051	-0.789743	-0.204397
H	2.930787	0.170057	1.978454
H	2.620097	0.989671	-0.263651
H	-3.061259	-0.310234	1.031125
H	-3.147427	-0.389974	-0.824334
H	0.173164	1.588716	-0.135357

Frequencies

-463.5121	105.2468	161.3516
193.2766	260.9379	357.1026
405.9263	539.3792	574.3906
758.2608	900.5587	911.5007
930.2060	952.1745	1014.6844
1030.5477	1119.4540	1197.2846
1310.4037	1337.2283	1444.6411
1492.1657	1668.8170	2065.6875
3139.7437	3158.1031	3162.5365
3185.1116	3221.6443	3259.3253

i32 — p15

C	1.004303	-0.373453	-0.119627
C	2.451518	-0.041832	0.057669
C	-1.374456	0.167757	-0.102147
C	-2.551775	-0.086531	-0.202159
C	-0.004257	0.491002	0.068286
H	0.765781	-1.390316	-0.421220
H	3.007716	-0.210939	-0.871292
H	2.909644	-0.686801	0.815954
H	2.595613	0.997893	0.359282
H	-3.069373	-0.878988	1.933878
H	-3.576165	-0.285560	-0.399690
H	0.214784	1.513050	0.370962

Frequencies

-221.9447	59.2615	144.0224
171.6044	194.0739	218.0072
389.3872	460.5453	546.3682
665.3568	676.3148	816.6019
912.6635	985.5400	1048.5597
1065.0245	1129.3934	1314.8482
1327.7314	1413.6674	1477.0633
1487.8745	1687.4317	2174.5350
3013.2941	3055.5690	3098.2795
3126.1396	3148.6422	3474.7654

i32 — i33

C	1.055183	-0.406049	0.000000
C	2.451399	0.130873	-0.000001
C	-1.400301	-0.185865	0.000002
C	-2.676569	0.054227	-0.000001
C	-0.055770	0.340722	0.000002
H	0.944428	-1.488262	-0.000002
H	3.005824	-0.219979	-0.877853
H	3.005826	-0.219982	0.877849
H	2.466128	1.222924	0.000001
H	-3.442240	0.831501	-0.000006
H	-2.247690	-1.160727	0.000002
H	0.024071	1.431077	0.000003

Frequencies

-2129.8742	79.5506	180.8918
182.3173	207.6937	286.8762
410.8173	490.9850	558.8918
822.3544	835.8421	910.7513
982.5288	1029.5624	1066.9004
1123.1373	1286.5909	1321.1115
1412.3276	1478.7627	1487.0607
1689.5652	1828.7898	2346.7128
3011.8839	3053.5193	3053.5528
3064.1468	3096.7515	3137.5823

i31 — i33

C	-1.079955	0.500064	-0.000001
C	-2.296461	-0.379949	-0.000011
C	1.549488	0.555885	0.000008
C	2.170071	-0.627507	-0.000028
C	0.178804	0.087582	0.000080
H	-1.253332	1.579608	-0.000140
H	-2.920842	-0.189541	-0.880095
H	-2.921550	-0.188611	0.879364
H	-2.019237	-1.435544	0.000646
H	1.940376	1.568415	-0.000023
H	3.192695	-0.992455	-0.000108
H	0.850211	-1.158322	0.000064

Frequencies

-2216.2748	142.5874	189.2030
230.1810	240.4307	488.5950
621.2779	625.9503	778.9131
869.2512	915.6882	954.3352
1046.9696	1060.0003	1064.9700
1114.5066	1229.3462	1297.1442
1411.3788	1482.6563	1491.2874
1577.5096	1743.0392	1861.8037
3011.7430	3053.3781	3060.4401
3106.2792	3149.4705	3183.5723

i33 — i34

C	1.036039	0.403757	0.000005
C	2.401470	-0.211556	0.000014
C	-1.436956	0.366595	0.000028
C	-2.592631	-0.242661	-0.000128
C	-0.116710	-0.276045	-0.000025
H	0.995912	1.492380	0.000030
H	2.976754	0.103390	0.878271
H	2.976773	0.103414	-0.878223
H	2.351490	-1.302790	-0.000002
H	-1.408165	1.465244	0.000026
H	-3.534105	-0.738953	0.000599
H	-0.105934	-1.363224	-0.000064

Frequencies

-704.0889	133.1726	203.9425
210.2996	270.1453	464.4387
485.6918	608.6913	770.3882
876.3051	933.2587	1003.1807
1064.2449	1074.8816	1132.6619
1241.4049	1317.2410	1334.8756
1413.2580	1479.1656	1490.0802
1632.6873	1698.7212	2979.0514
3009.1156	3049.7067	3092.3264
3119.3872	3141.9293	3437.9282

i34 — p15

C	-1.001893	0.384808	0.000022
C	-2.422078	-0.083407	-0.000018
C	1.437357	-0.032094	0.000022
C	2.653330	-0.072242	0.000018
C	0.063203	-0.425563	0.000009
H	-0.834271	1.458838	0.000063
H	-2.957139	0.296005	-0.877767
H	-2.957169	0.295943	0.877740
H	-2.492698	-1.173385	-0.000058
H	1.241083	1.948084	-0.000086
H	3.709292	0.048816	-0.000173
H	-0.088609	-1.503321	-0.000034

Frequencies

-633.1342	84.5570	182.2679
203.0727	219.8117	430.2555
464.8172	512.0502	531.7403
630.3705	667.3406	822.5765
908.2705	986.0161	1042.9643
1068.0493	1128.1833	1305.1972
1326.7250	1414.2943	1478.5207
1488.9815	1700.6669	2108.9185
3013.9549	3056.7324	3096.7012
3125.5190	3144.2810	3465.1167

i33 — i35

C	0.931286	-0.092307	0.386980
C	2.344844	0.180621	-0.035248
C	-0.109638	-0.176407	-0.439747
H	0.762708	-0.226919	1.454227
H	3.009960	-0.637224	0.263575
H	2.729489	1.088176	0.443263
H	2.424326	0.306286	-1.117578
H	0.041916	-0.040861	-1.509949
C	-1.513719	-0.460429	-0.001393
C	-2.434035	0.461960	0.132022
H	-1.767478	-1.503410	0.200773
H	-2.513348	1.533324	0.010004

Frequencies

-165.3589	171.8251	198.0992
256.0370	389.6056	483.3310
689.6156	773.8953	844.5044
887.3539	931.5445	988.7738
1048.7617	1069.4408	1117.3857
1246.0471	1294.2310	1328.4034
1412.6402	1479.5658	1490.8861
1648.2683	1711.9041	3012.7306
3056.2786	3070.1159	3092.4864
3111.1909	3126.8404	3223.8558

i35 — i36

C	-0.836661	-0.340142	-0.000290
C	-2.321051	-0.144310	0.000108
C	0.066272	0.645562	0.000140
C	1.537451	0.481852	-0.000198
C	2.228184	-0.625810	0.000221
H	-0.481782	-1.369503	-0.000998
H	-2.780885	-0.613036	0.877977
H	-2.781233	-0.612021	-0.878119
H	-2.589169	0.914856	0.000780
H	-0.281207	1.676678	0.000727
H	2.085532	1.433780	-0.000847
H	2.783575	-1.533668	0.000599

Frequencies

-690.8347	6.2455	197.4153
201.7842	250.4761	384.6990
604.0445	640.4756	738.8185
867.5623	891.4734	1002.3161
1030.9003	1066.2377	1121.7783
1262.7332	1327.6690	1339.9731
1413.9284	1478.6719	1490.0515
1625.4010	1707.6190	2980.0242
3006.9644	3047.0965	3089.7507
3122.4175	3130.6725	3436.3051

i36 — p15

C	-0.944115	-0.387109	-0.063246
C	-2.402001	-0.059141	0.008763
C	1.430568	0.162487	0.007460
C	2.490843	-0.434876	0.042408
C	0.042129	0.509818	0.069583
H	-0.681453	-1.427672	-0.236475
H	-2.888753	-0.620137	0.814454
H	-2.911905	-0.341093	-0.919266
H	-2.569780	1.005842	0.182517
H	2.060709	1.897318	-0.486550
H	3.482206	-0.817783	0.024210
H	-0.195566	1.556450	0.231300

Frequencies

-719.0065	41.6863	180.4338
198.9055	201.9972	398.5663
471.5628	512.4073	567.1619
627.8711	675.7954	816.4455
911.3163	990.6399	1037.1508
1066.0649	1128.7328	1314.2575
1330.8111	1413.8803	1478.2393
1488.4813	1688.1625	2103.8228
3013.7968	3056.3151	3099.5586
3146.1875	3158.7715	3464.3577

i11 — i36

C	-0.944220	-0.340704	-0.492340
C	-2.097943	-0.195211	0.289899
C	1.436522	0.443417	0.008244
C	2.008485	-0.728220	0.194152
C	-0.015107	0.663344	-0.098671
H	-0.782467	-1.065747	-1.288272
H	-2.003138	-0.378551	1.357839
H	-3.100736	-0.425637	-0.081539
H	-1.230356	0.941557	0.767808
H	2.078520	1.328949	-0.068360
H	3.005655	-1.130297	0.290356
H	-0.293895	1.673971	-0.385535

Frequencies

-1833.2773	150.1116	204.7649
273.9456	482.1852	570.0808
647.9727	747.9565	821.2820
849.2045	859.1365	887.4593
921.9045	1002.5597	1042.1471
1180.4980	1205.5582	1262.4357
1311.3376	1439.5257	1490.8793
1499.2817	1572.2530	1627.7028
3017.9435	3047.9307	3124.6267
3130.8551	3133.2435	3243.0754

i36 — i37

C	-0.845777	0.192014	-0.401766
C	-2.224917	-0.156298	0.058353
C	1.648879	0.557432	-0.014952
C	1.795924	-0.720616	-0.071070
C	0.271834	0.192810	0.431359
H	-0.699860	0.387254	-1.461057
H	-2.595091	-1.070046	-0.426877
H	-2.945186	0.634075	-0.186181
H	-2.259283	-0.317453	1.138983
H	2.161342	1.490960	-0.223632
H	2.356268	-1.596994	-0.352632
H	0.106155	0.080152	1.499860

Frequencies

-635.7234	127.0526	163.2760
278.7553	298.9143	458.8198
566.4059	679.4218	710.3957
839.4519	901.7427	934.6501
1019.3399	1045.9101	1116.3906
1162.5950	1247.2914	1308.0609
1409.1640	1458.0115	1473.6698
1508.6553	1714.1573	2984.9991
3023.1233	3082.9076	3122.8303
3140.4547	3143.0374	3259.7157

i37 — p11

C	-0.848631	-0.162071	-0.404258
C	-2.098456	-0.176287	0.073870
C	1.593946	0.688174	-0.121064
C	1.686736	-0.588483	-0.001170
C	0.360337	0.002458	0.430286
H	-0.680516	-0.255355	-1.475925
H	-2.950781	-0.338918	-0.574648
H	-2.656239	1.914525	0.056210
H	-2.292052	-0.127686	1.141089
H	2.016715	1.636879	-0.402459
H	2.244179	-1.502604	-0.109220
H	0.155109	0.090414	1.498974

Frequencies

-494.0415	100.4898	183.0574
275.3183	294.9459	381.4310
476.5957	629.2707	716.0340
824.4269	880.9310	893.1231
943.1131	952.3394	1016.6477
1035.8058	1076.5661	1156.1497
1187.8016	1320.7052	1363.3921
1458.6137	1671.0567	1756.9998
3091.3811	3152.6000	3161.9858
3251.5641	3277.8789	3327.7009

i37 — p16

C	-0.886033	0.605659	-0.122069
C	-2.059337	-0.320132	-0.048259
C	1.804808	0.411441	-0.104524
C	1.394969	-0.831059	-0.032926
C	0.389731	0.201185	0.069594
H	-1.073305	1.673196	-0.174813
H	-2.774390	-0.111583	-0.849974
H	-2.596316	-0.210016	0.901738
H	-1.747799	-1.364081	-0.134050
H	2.620683	1.107385	-0.200332
H	1.637010	-1.879994	-0.028775
H	0.069287	0.382533	1.915311

Frequencies

-823.5848	145.8037	181.0664
241.1227	309.1971	492.2277
526.3033	620.3237	701.2050
768.2237	790.2643	916.4957
929.3141	961.4628	1046.2615
1070.8816	1113.9132	1132.9184
1364.5166	1416.0995	1481.7668
1500.8538	1611.4463	1771.9876
3027.1206	3087.0375	3123.1623
3188.4862	3275.7963	3318.4461

i37 — i38

C	-0.864540	-0.627967	-0.113101
C	-2.016836	0.319084	-0.100513
H	-1.026327	-1.654539	-0.430238
H	-2.401712	0.484962	0.919469
H	-2.852014	-0.040760	-0.706103
H	-1.726339	1.309294	-0.475720
C	1.308051	0.843814	-0.041633
C	1.738411	-0.353536	-0.261424
C	0.438187	-0.272130	0.507723
H	1.425339	1.908158	-0.154315
H	2.474737	-1.012502	-0.689614
H	0.486670	-0.450206	1.590203

Frequencies

-125.8044	86.0229	225.9669
260.3168	439.1347	511.6096
623.7318	803.0126	856.8302
863.9806	929.8980	981.9884
1002.9922	1035.4557	1081.4489
1112.4214	1212.9585	1339.1579
1367.3611	1405.6975	1472.9398
1483.8132	1718.4284	2944.5535
2969.8903	3005.7571	3084.1836
3141.6881	3239.7775	3286.6510

i38 — p6

C	-0.415784	-0.026459	-0.030627
C	-1.882265	0.146814	-0.118565
C	1.637473	-0.020351	-0.054936
C	0.778456	0.992113	0.050586
C	0.461845	-1.034166	-0.136074
H	-0.638408	-0.803237	2.341365
H	-2.265865	0.706824	0.739450
H	-2.388556	-0.819549	-0.160901
H	-2.140198	0.717741	-1.018518
H	2.715101	-0.109200	-0.062897
H	0.862759	2.063718	0.164513
H	0.376816	-2.103997	-0.265310

Frequencies

-364.2054	135.5663	192.2243
230.5622	269.3993	314.6209
545.4749	608.2024	643.5811
746.2740	783.7617	873.8117
898.3233	1000.1954	1040.4599
1070.9362	1157.9628	1175.3673
1263.7754	1408.3091	1469.0859
1482.0989	1546.1834	1686.8292
3031.2383	3093.9140	3138.2040
3226.3646	3246.4623	3263.6272

i17 — i38

C	-1.039207	0.692935	0.026023
C	-1.498950	-0.630360	0.134944
C	0.997259	-0.558364	-0.614986
C	1.317988	-0.144192	0.629556
C	0.428860	0.812751	-0.087035
H	-1.664850	1.498448	-0.340784
H	-2.527442	-0.852265	-0.136864
H	-1.119454	-1.249618	0.950979
H	-0.346122	-1.092840	-0.614085
H	1.607805	-0.881407	-1.455760
H	1.981100	-0.228444	1.474666
H	0.833268	1.769507	-0.409162

Frequencies

-2051.2412	292.6577	381.6048
434.1473	525.6690	616.7512
665.6626	719.2699	801.4640
828.3483	905.7266	956.4257
987.2382	1002.6437	1021.5185
1048.3165	1102.9427	1203.2937
1274.6235	1316.8986	1401.8789
1479.9264	1493.1617	1520.9324
3053.7748	3108.6793	3114.6285
3155.6289	3183.2628	3246.5197

i5 — i17

C	1.132060	-0.501975	-0.244116
C	1.777263	0.598928	0.193973
C	-0.245758	-0.813577	0.032369
C	-1.473119	0.578328	-0.539986
C	-1.190048	0.065520	0.730506
H	1.666215	-1.212392	-0.870253
H	1.282112	1.321996	0.832680
H	2.813227	0.782978	-0.062535
H	-0.596898	-1.807693	-0.229771
H	-2.473282	0.552300	-0.977412
H	-0.724316	1.113688	-1.110076
H	-1.969452	-0.314219	1.380891

Frequencies

-782.8096	180.8288	239.4225
317.9919	558.2430	648.2267
726.5735	790.1404	807.5558
896.0229	913.6787	945.0642
994.2604	1003.8698	1060.1149
1158.0669	1229.7891	1292.8725
1316.0492	1398.3070	1437.1026
1501.7506	1608.2862	3065.0825
3128.1625	3137.2063	3147.3489
3167.6779	3194.5218	3228.9215

i4 — i28

C	0.908078	-1.095464	-0.035773
C	0.371619	1.050420	0.071146
C	-1.873128	-0.103895	-0.270352
C	-0.705417	0.074842	0.454317
C	1.431712	0.288898	-0.183274
H	1.269570	-1.734502	0.770275
H	0.614004	-1.636470	-0.930963
H	0.262948	2.130394	0.036367
H	-1.979991	0.299828	-1.271260
H	-2.673151	-0.733851	0.100651
H	-0.738754	-0.197056	1.509049
H	2.448187	0.582857	-0.430501

Frequencies

-622.9872	203.8788	285.9566
418.0628	470.6188	611.5873
702.7408	750.0532	771.4165
821.4563	922.6724	944.7890
975.0490	1035.4067	1061.6331
1100.4919	1111.1114	1248.5215
1324.3307	1407.8287	1451.0832
1506.2571	1668.2159	3077.1576
3096.9160	3129.7106	3135.2980
3165.7033	3167.0782	3222.0437

i5 — i25

C	-1.238798	1.008407	0.073383
C	-0.332701	-0.808645	0.252823
C	1.829803	0.539060	-0.029424
C	1.095038	-0.572246	-0.037476
C	-1.474798	-0.342644	-0.413809
H	-1.704590	1.345010	0.993576
H	-0.589140	1.704841	-0.441023
H	-0.467098	-1.634329	0.964551
H	2.879687	0.505320	-0.297755
H	1.424476	1.498370	0.265257
H	1.610899	-1.510320	-0.255377
H	-2.425507	-0.852484	-0.302212

Frequencies

-874.4866	119.6067	270.1352
333.7706	468.6086	617.5514
646.7805	690.8535	721.6429
838.7651	936.8852	944.8131
989.1963	1009.7232	1068.3113
1139.9907	1200.4422	1317.8046
1339.0799	1403.1304	1444.0986
1457.3029	1689.1528	2999.0635
3080.1806	3118.1550	3144.6507
3154.4481	3217.8342	3231.8929

3 REAGENTS**C₄H₆ (1,3-butadiene)**

C	1.844869	0.109468	-0.000133
C	0.608537	-0.399274	0.000236
C	-1.844801	-0.109628	-0.000309
C	-0.608697	0.399501	0.000084
H	2.015740	1.181622	-0.000088
H	2.722223	-0.525882	-0.000414
H	0.476381	-1.479581	0.000550
H	-2.722447	0.525421	0.000647
H	-2.015178	-1.181680	-0.000206
H	-0.476162	1.479696	0.000246

Frequencies

174.7374	299.6712	518.6950
539.4181	780.9923	899.2468
935.2060	936.3580	1001.5375
1004.0628	1058.3506	1226.9825
1314.7874	1320.0161	1415.4761
1473.5057	1653.3148	1706.1581
3122.3201	3131.6374	3135.0434
3135.9409	3219.4778	3219.9698

CH

C	0.000000	0.000000	0.161146
H	0.000000	0.000000	-0.966877

Frequencies

2803.9026

4 PRODUCTS

p1

C	0.736623	0.987585	0.000000
C	1.178765	-0.283674	0.000003
C	-0.732076	0.990950	-0.000042
C	-0.002784	-1.215526	0.000012
C	-1.180063	-0.278271	-0.000012
H	1.351623	1.878553	0.000008
H	2.208871	-0.612750	0.000074
H	-1.342974	1.884740	0.000182
H	-0.004416	-1.877171	0.877009
H	-0.004230	-1.877090	-0.877061
H	-2.211661	-0.602668	0.000024

Frequencies

348.6040	524.0849	681.4372
712.6337	816.8658	818.7255
917.4930	924.4380	954.1554
955.7283	970.8450	1012.4461
1111.9798	1125.8854	1129.9476
1266.1830	1314.9867	1397.1448
1414.9789	1552.2415	1638.8444
3010.5306	3032.0452	3186.7348
3196.8341	3215.4703	3222.0692

p2

C	1.246417	0.164206	-0.000008
C	-0.015825	0.524420	-0.000136
C	-2.423019	-0.032495	0.000111
C	-1.140523	-0.407808	-0.000148
C	2.497176	-0.194409	0.000090
H	-0.251149	1.587846	-0.000004
H	-3.224640	-0.760768	0.000239
H	-2.709453	1.014426	0.000274
H	-0.886707	-1.464206	-0.000212
H	3.043212	-0.350449	0.926638
H	3.043380	-0.350329	-0.926386

Frequencies

128.3752	166.0034	349.0876
401.1640	509.0084	568.5131
732.7050	878.9392	906.3957
919.2327	929.7325	1010.6104
1033.5679	1112.2682	1187.0084
1308.0442	1336.4696	1441.4101
1483.0362	1680.0310	2034.0520
3105.6866	3114.8395	3133.6526
3150.5828	3174.9934	3222.3421

p3

C	1.082951	0.235631	0.000051
C	-0.027104	0.934224	0.000228
C	-1.744360	-0.895463	0.000058
C	-1.396727	0.393504	-0.000224
C	2.181963	-0.460730	-0.000136
H	0.064251	2.018542	0.000699
H	-2.785965	-1.192330	-0.000231
H	-1.003498	-1.688040	0.000724
H	-2.180065	1.146565	-0.000708
H	2.662283	-0.764304	0.926469
H	2.662656	-0.763431	-0.926823

Frequencies

62.4014	151.4645	321.2813
395.1158	503.4724	654.9433
715.6226	875.7176	909.9486
912.8068	936.2907	1010.0872
1028.0158	1049.4939	1154.7942
1337.7733	1374.4764	1444.7785
1474.6992	1679.2160	2030.5745
3103.7385	3122.2214	3135.9200
3149.6274	3172.7222	3223.9267

p4

C	-1.338270	0.111976	-0.043656
C	-0.039083	0.772602	0.091737
C	2.193061	-0.313669	-0.301312
C	1.081494	-0.191272	0.414143
C	-2.399348	-0.441833	-0.144895
H	-0.113034	1.524078	0.889181
H	0.194377	1.317986	-0.828708
H	2.973102	-1.011742	-0.020010
H	2.364542	0.278153	-1.195387
H	0.931740	-0.805140	1.298553
H	-3.337848	-0.930163	-0.239728

Frequencies

89.3954	187.7194	337.6049
408.6864	475.0917	644.9942
664.4057	680.2830	898.3696
925.9499	953.1208	982.0640
1030.8713	1127.9109	1245.4688
1314.0050	1330.0467	1450.5476
1464.4171	1709.5795	2223.6181
3001.9565	3049.7914	3127.8671
3146.0430	3213.3811	3477.6481

p5

C	1.761599	-0.489549	0.002979
C	0.312786	-0.062184	-0.001771
C	-2.127524	0.243736	0.002438
C	-1.046363	-0.544167	-0.002732
C	1.185064	0.901729	-0.002002
H	2.204068	-0.887197	0.918520
H	2.209447	-0.891454	-0.908061
H	-3.127376	-0.173797	0.001265
H	-2.042419	1.324903	0.007622
H	-1.170659	-1.623381	-0.007550
H	1.413566	1.953538	-0.005266

Frequencies

61.8754	220.4274	292.9325
467.6382	627.4367	716.2182
776.5796	936.5846	950.8538
1012.5347	1017.8187	1025.2337
1058.5794	1101.9637	1110.6724
1158.9382	1327.2907	1443.6907
1520.1417	1666.7390	1817.9521
3022.2578	3082.7542	3138.0520
3151.1196	3226.5515	3266.7490

p6

C	-1.326178	-0.299187	-0.644256
C	-0.415589	0.725445	0.000079
C	1.724220	-0.608608	-0.000040
C	1.067452	0.551441	0.000014
C	-1.326133	-0.299363	0.644203
H	-1.629200	-0.728654	-1.584052
H	-0.736908	1.767126	0.000233
H	2.807066	-0.642848	-0.000103
H	1.204251	-1.561396	-0.000040
H	1.641185	1.476414	0.000002
H	-1.629020	-0.729009	1.583959

Frequencies

46.3672	243.9208	327.7042
557.6669	655.0084	668.5262
819.6444	855.1614	880.1675
929.2777	941.7518	1006.3480
1029.5046	1051.5428	1061.1557
1179.6793	1323.5052	1388.2846
1443.2912	1691.8075	1729.7643
3069.7672	3124.7463	3135.8526
3215.5342	3241.6687	3290.3903

p7

C	-1.163693	0.167288	0.000096
C	-2.133665	-0.541117	-0.000019
C	0.012695	1.031130	0.000113
C	1.538108	-0.994979	-0.000148
C	1.348571	0.318440	-0.000019
H	-2.995522	-1.162115	-0.000082
H	-0.032561	1.697068	0.872207
H	-0.032649	1.697226	-0.871856
H	2.537300	-1.414736	-0.000236
H	0.705184	-1.689370	-0.000169
H	2.206159	0.987355	-0.000002

Frequencies

147.5206	162.0456	332.3985
378.7846	568.0392	614.7230
663.9413	681.5658	866.6468
947.0140	965.1155	966.7503
1030.0920	1093.1564	1237.7560
1325.0798	1353.6219	1441.0304
1463.1201	1712.5303	2226.1384
3000.4644	3016.9398	3131.0362
3143.4622	3223.0748	3476.4354

p8

C	2.568573	0.159298	-0.000024
C	-0.066040	-0.229606	-0.000039
C	-2.413055	0.466827	0.000023
C	-1.466149	-0.478287	0.000032
C	1.129171	-0.061316	-0.000149
H	2.871725	0.781474	-0.847692
H	3.113478	-0.786804	-0.066757
H	2.888973	0.666457	0.915322
H	-3.463267	0.201246	0.000032
H	-2.163062	1.521235	-0.000031
H	-1.762848	-1.525097	0.000077

Frequencies

22.8317	140.9556	185.0418
325.9990	376.6336	537.5901
700.3439	722.4331	941.1626
1010.1677	1047.9865	1049.6705
1056.4442	1195.1913	1321.6636
1415.7175	1448.0138	1478.1799
1478.4361	1669.8715	2334.3371
3019.5650	3073.9152	3079.4274
3126.0596	3143.9889	3232.5357

p9

C	-1.202292	0.542763	-0.000079
C	-1.645730	-0.885237	-0.000019
C	1.219844	0.145766	0.000002
C	2.221543	-0.524619	0.000053
C	0.066812	0.978728	0.000028
H	-1.987388	1.294487	-0.000082
H	-2.268509	-1.096578	-0.876600
H	-0.798957	-1.572565	-0.002829
H	-2.263492	-1.097953	0.879832
H	3.100856	-1.120378	-0.000332
H	0.256429	2.048577	0.000096

Frequencies

136.6859	157.8647	274.8248
374.7152	502.7787	630.2292
661.7995	679.5908	749.8505
901.1060	973.5395	987.8983
1063.3332	1120.7954	1265.7218
1398.6581	1430.3399	1482.6620
1483.8772	1683.1863	2199.3013
3015.0403	3055.6654	3113.9473
3136.8641	3156.1774	3476.3682

p10

C	-2.302339	0.469137	-0.000051
C	0.080887	-0.297358	-0.000034
C	2.607944	0.223575	0.000038
C	1.319785	-0.040913	-0.000011
C	-1.209023	-0.562833	-0.000023
H	-2.944826	0.350513	0.879666
H	-2.945021	0.350618	-0.879640
H	-1.896270	1.481012	0.000009
H	2.976616	1.244664	0.000736
H	3.348536	-0.570269	-0.000558
H	-1.522560	-1.606192	0.000275

Frequencies

139.7794	145.3217	228.1596
313.1212	488.0139	529.0218
571.9209	800.8118	844.6482
867.7941	1029.1745	1040.0907
1049.8782	1107.7729	1322.1202
1402.9365	1446.8614	1480.7149
1489.4716	1699.2533	2198.7043
3013.0217	3056.2503	3104.3061
3116.3469	3122.7037	3190.7161

p11

C	1.574687	0.644345	-0.060072
C	1.574096	-0.644245	-0.064296
C	0.291989	-0.001075	0.431893
C	-2.178785	-0.000382	0.079797
C	-0.935580	0.001444	-0.399601
H	2.067387	1.580527	-0.261573
H	2.067638	-1.579619	-0.267437
H	0.096882	-0.004076	1.506456
H	-3.042160	0.001550	-0.575030
H	-2.374469	-0.003901	1.148037
H	-0.773718	0.004996	-1.476782

Frequencies

122.3555	291.1705	338.4087
471.3951	623.3542	678.6315
798.5870	866.8975	886.5404
924.9696	945.0840	1008.3736
1030.8747	1073.8610	1148.6470
1173.4682	1312.9871	1356.4724
1454.9231	1684.5220	1737.1928
3052.6081	3117.9046	3128.8667
3211.5106	3239.0276	3287.3868

p12

C	0.431814	0.050461	-0.000115
C	1.901743	-0.109433	0.000029
C	-1.623272	0.031715	0.000071
C	-0.763027	-0.980823	-0.000014
C	-0.440091	1.056482	-0.000014
H	2.231468	-0.670503	0.881682
H	2.401321	0.861656	-0.002244
H	2.231218	-0.674536	-0.879117
H	-2.701494	0.117183	0.000026
H	-0.846101	-2.059001	-0.000086
H	-0.359413	2.134790	-0.000011

Frequencies

177.7788	240.0033	310.8300
552.8133	585.7288	643.1515
736.4258	769.1127	894.7487
942.1349	1004.5957	1049.0006
1068.8275	1170.1764	1215.8309
1263.9311	1412.2267	1467.8142
1484.9917	1661.5933	1751.7038
3028.6347	3083.2052	3134.1394
3221.8258	3242.4530	3260.7162

p13

C	-1.881630	-0.030485	-0.000029
C	-0.552121	-0.036100	-0.000040
C	1.498229	-0.121199	-0.000099
C	0.518047	-1.046095	0.000000
C	0.533773	1.062481	0.000032
H	-2.441364	0.898098	-0.000032
H	-2.450582	-0.953956	-0.000043
H	2.579317	-0.178503	-0.000150
H	0.509500	-2.129439	0.000359
H	0.552689	1.696506	-0.891780
H	0.552656	1.695684	0.892469

Frequencies

219.5350	347.6044	492.1782
706.9335	717.1392	779.2688
872.3004	889.0620	909.6364
952.2949	974.0754	1014.0919
1102.2439	1103.0951	1184.9896
1213.4411	1315.0415	1440.8947
1472.0925	1587.8724	1737.1593
3030.8469	3073.1519	3132.2329
3181.9049	3212.6440	3213.9197

p14

C	-1.301031	0.749843	-0.238143
C	-0.257511	-0.000048	0.575770
C	2.270805	0.000133	-0.183217
C	1.118193	-0.000119	0.161450
C	-1.301058	-0.749783	-0.238228
H	-2.075622	1.269166	0.312826
H	-0.953998	1.259527	-1.127713
H	-0.405678	-0.000099	1.650713
H	3.288600	-0.000211	-0.486463
H	-2.075672	-1.269142	0.312684
H	-0.954020	-1.259389	-1.127842

Frequencies

202.5242	208.2961	504.5454
517.9661	627.3706	686.3617
756.1626	813.4217	821.8630
894.5771	964.0323	1057.8261
1078.0634	1113.4563	1138.4289
1200.7868	1215.1196	1382.5695
1468.5512	1503.2178	2218.3207
3129.5624	3133.1580	3141.3089
3212.4586	3227.1617	3477.9736

p15

C	0.925056	-0.394350	0.000012
C	2.371246	-0.011169	-0.000008
C	-1.466238	0.109466	0.000001
C	-2.639574	-0.165085	0.000016
C	-0.093017	0.477133	-0.000018
H	0.697974	-1.457539	0.000054
H	2.884328	-0.419494	-0.878030
H	2.884334	-0.419427	0.878041
H	2.502368	1.073139	-0.000050
H	-3.671109	-0.417575	0.000030
H	0.117264	1.544925	-0.000060

Frequencies

167.0357	170.9676	199.8552
390.5346	450.1885	544.8979
626.0470	681.2255	816.2460
912.4616	986.8754	1046.6087
1065.7194	1128.4006	1314.4868
1328.7208	1414.4391	1477.7085
1489.6826	1695.6858	2203.1267
3012.8784	3054.9688	3097.4517
3125.2985	3147.4522	3477.9955

p16

C	0.876785	-0.619324	-0.000314
C	2.058863	0.308951	0.000148
C	-1.807997	-0.424697	0.000154
C	-1.394991	0.822027	-0.000097
C	-0.382361	-0.209702	-0.000122
H	1.068712	-1.687917	0.000007
H	2.695896	0.152946	-0.877541
H	2.689232	0.160470	0.883993
H	1.737464	1.353973	-0.005576
H	-2.638856	-1.110578	0.000589
H	-1.654241	1.867572	-0.000078

Frequencies

95.9312	202.7348	259.7389
444.5624	515.8458	680.3526
780.7003	786.0342	901.7894
923.7492	953.5827	1050.6706
1074.2207	1112.2941	1122.5335
1364.9250	1412.9358	1481.7765
1498.4472	1634.5866	1877.6686
3027.5617	3081.7621	3110.6937
3176.7892	3266.5736	3308.8008