

Supporting Information for

**Astrochemistry Prefers the Biomolecule:
Isomer-Selective Production of Ethanolamine
(HOCH₂CH₂NH₂) in Interstellar Model Ices**

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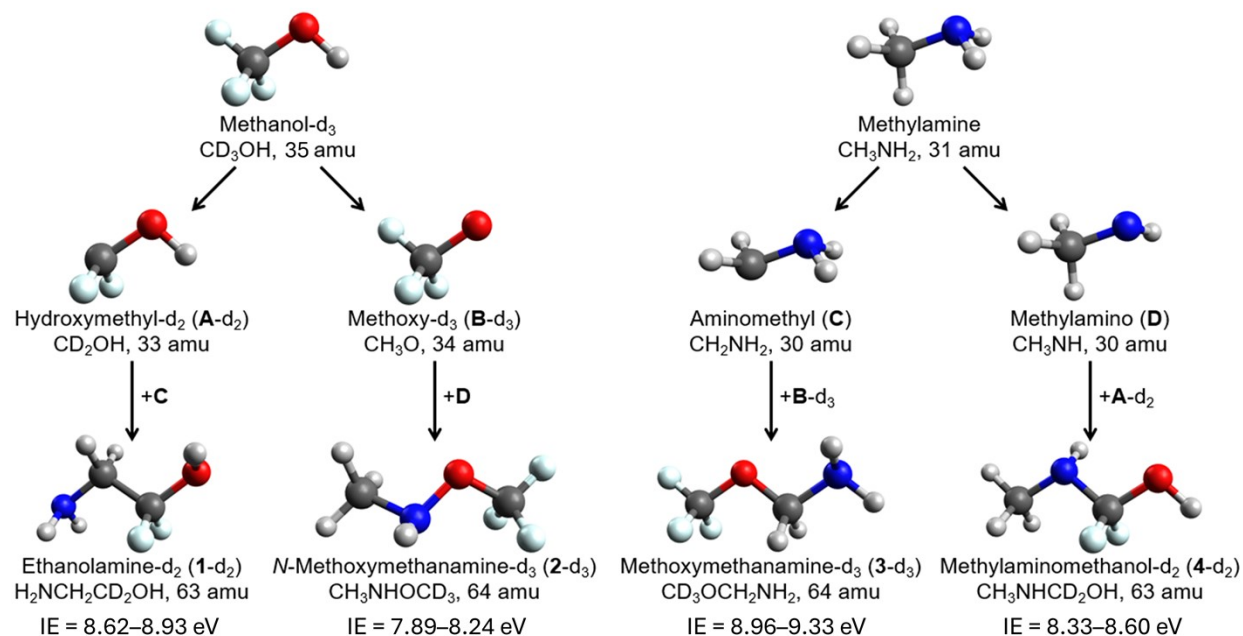


Figure S1. Isomers of C₂H₅D₂NO and C₂H₄D₃NO achievable through a single $\dot{\text{H}}$ elimination initiated by an incident electron simulating secondary electrons produced in the track of a galactic cosmic ray (GCR) followed by radical-radical recombination in methanol-d₃–methylamine ices.

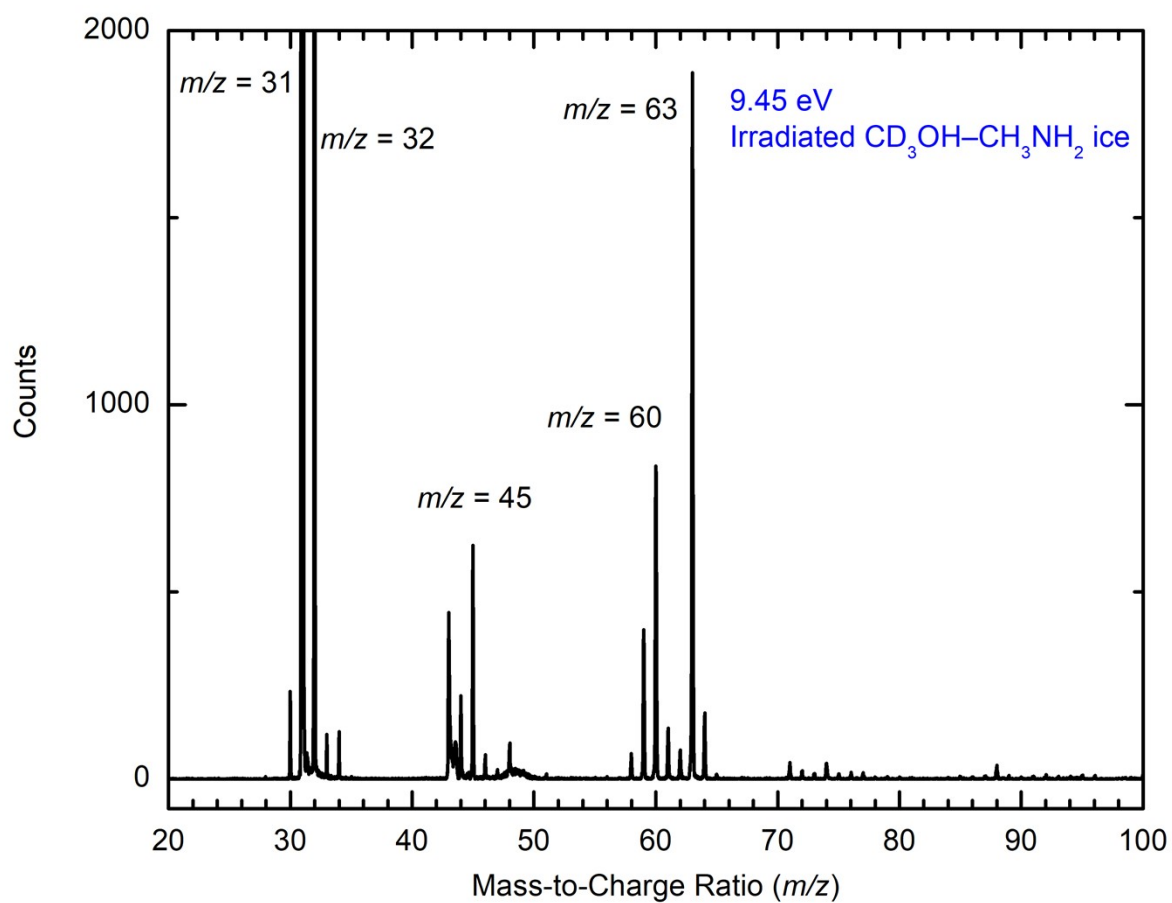


Figure S2. Mass spectra (integrated ion signals) of masses recorded at 9.45 eV for irradiated $\text{CD}_3\text{OH}-\text{CH}_3\text{NH}_2$ ice.

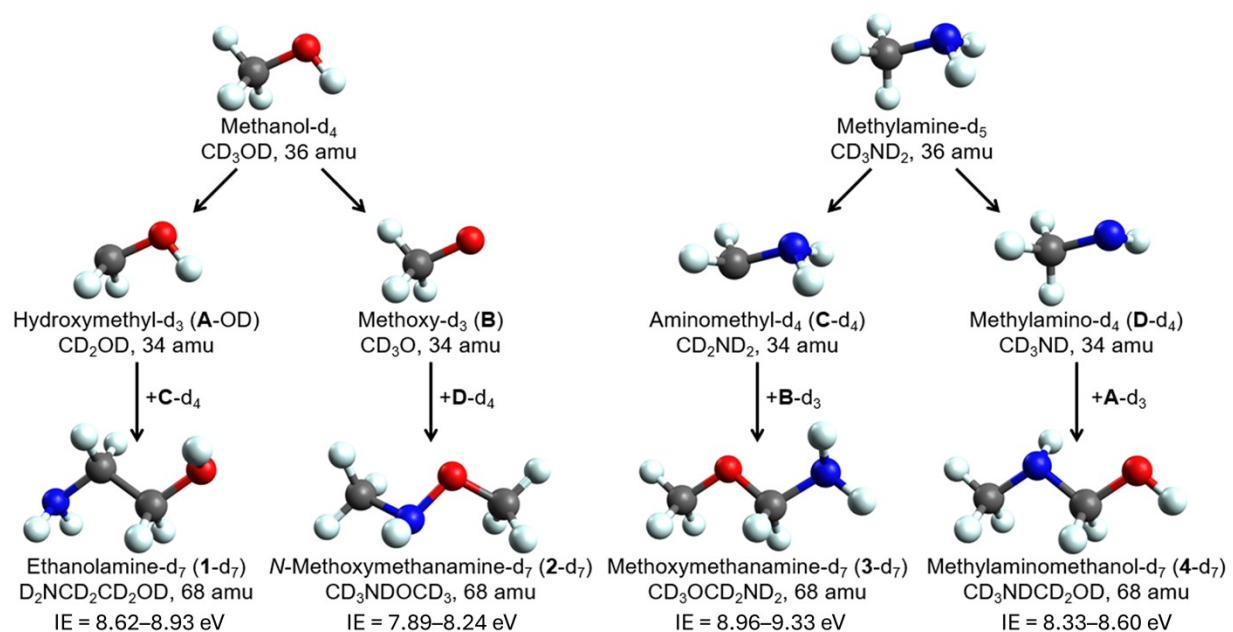


Figure S3. Isomers of C_2D_7NO achievable through a single $\dot{H}$ elimination initiated by an incident electron simulating secondary electrons produced in the track of a galactic cosmic ray (GRC) followed by radical-radical recombination in methanol- d_4 –methylamine- d_5 ices.

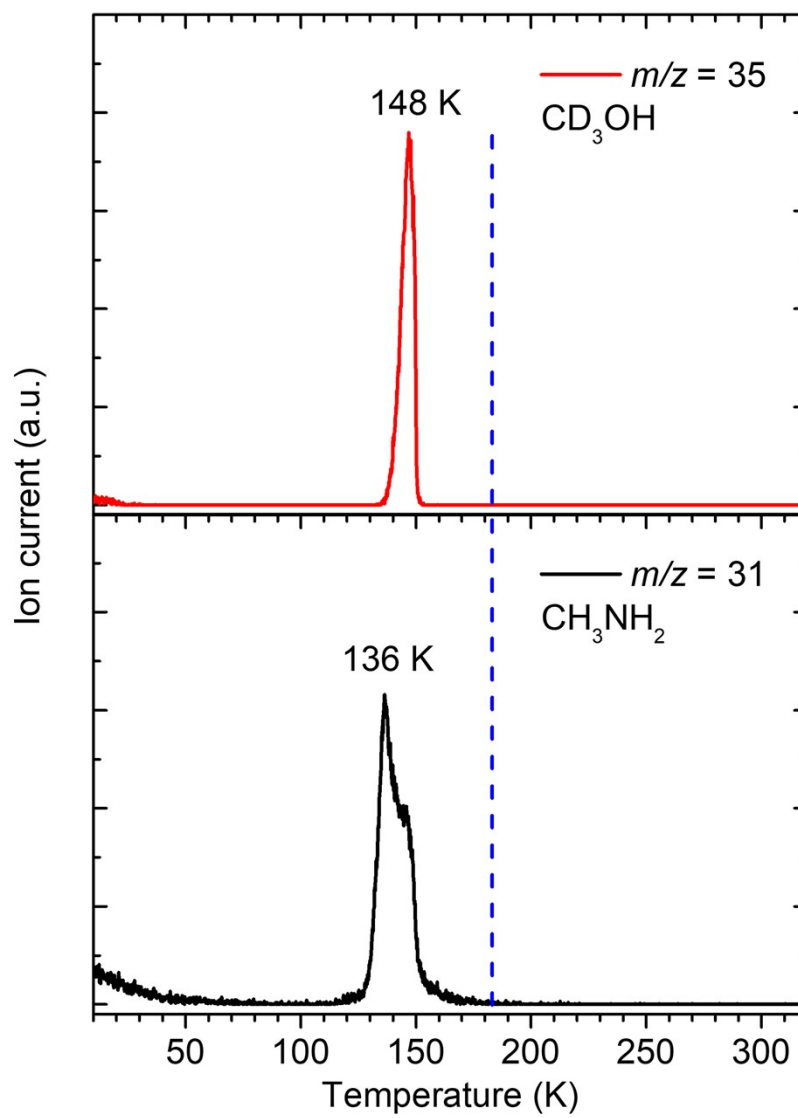


Figure S4. TPD profiles of methanol- d_3 (CD_3OH , top) at $m/z = 35$ and methylamine (CH_3NH_2 , bottom) at $m/z = 31$ in unirradiated CD_3OH – CH_3NH_2 ice recorded by electron impact quadrupole mass spectrometer (QMS) operating at 70 eV and an current of 2 mA. The dashed blue line indicate the peak sublimation temperature of ethanolamine.

Table S1. Conformers of ethanolamine (**1**) with calculated energetics, vibrational frequencies (cm^{-1}) & intensities (km mol^{-1}), and Cartesian coordinates ($\text{\AA}$).

1a

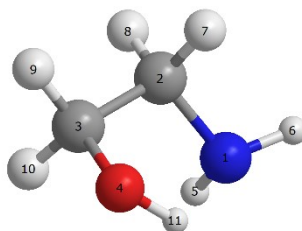
Relative Energy = 0.0 kJ mol^{-1}

Total Energy = -210.039697 hartree

Ionization Product $\rightarrow \mathbf{1c}^+$

Adiabatic Ionization Energy = 8.91 eV

Dipole Moment = 3.2 D



Frequency	Intensity	Frequency	Intensity	Frequency	Intensity
188.4598	6.6724	1061.1942	32.122	1515.534	0.4158
271.216	12.7946	1103.1717	52.397	1659.8757	30.57
327.8656	0.3972	1191.9136	8.3661	2934.7308	78.1325
539.6919	11.6252	1255.8764	24.8424	2970.2673	86.5447
588.7156	125.7529	1325.7349	2.6241	3061.2615	32.6402
820.0067	89.9578	1377.1282	3.8034	3071.0793	49.6665
877.7014	13.3264	1407.7585	7.2916	3500.9953	0.2034
926.4879	61.6641	1453.3987	82.5602	3583.7432	1.812
1005.407	8.1209	1495.6971	6.6625	3710.7111	69.511

AtomX Y Z

N	0.029618	0.01357	0.009848
C	-0.000534	-0.028587	1.481014
C	1.440099	0.000499	1.99061
O	2.136193	1.106233	1.448378
H	0.231208	-0.904452	-0.374282
H	-0.861824	0.309452	-0.370011
H	-0.509748	0.875125	1.827121
H	-0.534855	-0.896301	1.89605
H	1.458758	0.092976	3.07984
H	1.938683	-0.948929	1.730439
H	1.829437	1.151465	0.530066

1b

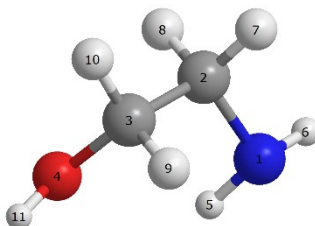
Relative Energy = 5.4 kJ mol^{-1}

Total Energy = -210.037640 hartree

Ionization Product $\rightarrow \mathbf{1a}^+$

Adiabatic Ionization Energy = 8.79 eV

Dipole Moment = 0.9 D



Frequency	Intensity	Frequency	Intensity	Frequency	Intensity
178.4071	2.9614	504.9703	13.4033	1038.4958	59.4512
247.0926	127.5568	860.8023	58.8813	1097.0035	37.2048
282.9790	46.4472	884.2241	92.6322	1103.9053	9.8276
361.4260	9.4595	904.2532	20.8601	1177.8913	1.1859
				1257.4719	2.6190

Frequency Intensity		1500.953	4.9311		3025.5100	71.6533
1288.2222	46.1962	1508.9704	4.9496		3044.7195	47.0597
1345.6756	5.9600	1655.9508	38.1336		3491.9759	1.9026
1418.7811	5.4132	2943.9989	65.9869		3567.9306	1.0360
1460.1308	3.0412	2979.3708	62.9349		3850.5728	29.6044

AtomX Y Z

N	-0.120676	-0.267024	0.154656
C	-0.029082	0.102700	1.514884
C	1.438167	0.031000	1.996895
O	2.040491	-0.979886	1.222327
H	0.594993	-0.903293	-0.209300
H	-0.884078	0.033535	-0.447763
H	-0.529755	1.056924	1.697496
H	-0.603397	-0.664456	2.084498
H	1.902822	1.007910	1.809040
H	1.467429	-0.175403	3.069265
H	2.830016	-1.332177	1.649228

1c

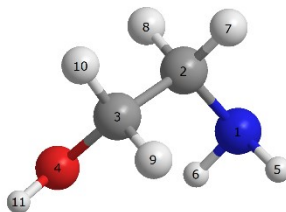
Relative Energy = 6.5 kJ mol⁻¹

Total Energy = -210.037219 hartree

Ionization Product → **1b**⁺

Adiabatic Ionization Energy = 8.81 eV

Dipole Moment = 2.7 D



Frequency	Intensity	Frequency	Intensity	Frequency	Intensity
167.8305	14.1345	1080.8124	75.3134	1513.6611	4.3825
246.7399	102.7577	1129.6942	10.0549	1670.9416	24.4634
285.2259	24.7466	1162.1836	7.4942	2955.4005	67.4683
355.5006	34.6944	1255.198	14.4518	2987.3863	59.3065
509.4791	19.9877	1297.9123	38.7647	3029.7588	59.0831
832.2218	33.6651	1390.4447	9.7780	3066.037	41.2095
865.5737	50.6671	1397.5363	0.7256	3478.1001	1.8917
919.3058	141.0833	1442.2989	0.5614	3554.5341	1.2013
1013.0918	18.7122	1478.6531	3.1870	3848.203	29.4353

AtomX Y Z

N	-0.251651	-0.193794	0.133400
C	-0.062865	-0.041942	1.481859
C	1.627939	-0.086751	1.918578
O	2.294121	0.958483	1.381509
H	-0.337335	-1.111229	-0.290454
H	-0.165305	0.591154	-0.503124
H	-0.374485	0.936089	1.845536
H	-0.464342	-0.874072	2.059746

H 1.560140 -0.102275 3.008929
H 1.976660 -1.022810 1.488206
H 2.318073 1.719821 1.978363

1d

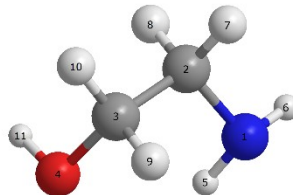
Relative Energy = 7.8 kJ mol⁻¹

Total Energy = -210.036731 hartree

Ionization Product → **1b**⁺

Adiabatic Ionization Energy = 8.79 eV

Dipole Moment = 2.5 D



Frequency	Intensity	Frequency	Intensity	Frequency	Intensity
182.2357	3.8094	1062.942	58.7567	1508.9222	2.1634
287.2191	17.7296	1113.546	8.162	1655.8773	37.0245
328.2489	52.3841	1187.9952	6.3155	2893.8699	107.305
372.1016	109.6566	1212.9852	26.5929	2996.1435	60.0201
519.4927	32.7959	1335.3703	4.8547	3032.1218	53.8201
849.8969	73.5941	1384.0817	3.1696	3093.9503	29.8593
866.908	72.1999	1408.5314	24.8443	3493.5333	2.0675
901.9591	24.9416	1434.261	16.1323	3572.0784	1.3434
1040.628	30.0854	1497.3467	4.0622	3818.2108	18.0314

Atom	X	Y	Z
N	-0.331958	-0.260820	0.09464
C	-0.163371	-0.111745	1.443622
C	1.522597	0.097651	1.922691
O	1.978596	1.313269	1.562854
H	-0.294823	-1.171011	-0.349895
H	-0.464122	0.537893	-0.515191
H	-0.602034	0.803807	1.834903
H	-0.417068	-1.010452	0.005195
H	1.383797	0.047275	3.00291
H	2.044586	-0.760339	1.498327
H	2.500833	1.28552	0.749019

1e

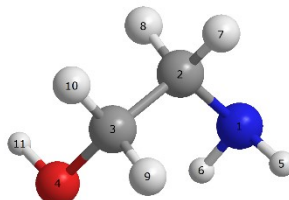
Relative Energy = 8.1 kJ mol⁻¹

Total Energy = -210.036602 hartree

Ionization Product → **1b**⁺

Adiabatic Ionization Energy = 8.79 eV

Dipole Moment = 1.3 D



Frequency	Intensity	Frequency	Intensity	Frequency	Intensity
180.9734	3.6764	323.6781	109.0613	825.7519	33.3371
269.3976	44.7244	367.8184	35.3022	871.2694	25.3948
		525.9907	6.053	918.1515	161.8828

996.3091	48.5623	1387.0579	12.4721	2974.4727	65.6145
Frequency Intensity		1397.9055	1.044	2997.7273	52.1108
1078.5986	24.0867	1413.739	32.9768	3046.3546	36.3331
1105.3483	50.6525	1484.4713	1.6497	3069.0113	56.8163
1158.3703	11.7837	Frequency Intensity		3475.3709	1.0993
1258.8015	3.8129	1500.6173	2.2079	3548.3111	1.0087
1370.1362	4.8485	1673.3232	25.2034	3816.8659	19.4321

AtomX Y Z

N	-0.245823	-0.138128	0.135231
C	-0.097865	-0.126544	1.491227
C	1.633279	-0.087738	1.97071
O	1.686317	-0.225498	3.306574
H	-0.230581	-1.003662	-0.392359
H	-0.285375	0.718291	-0.405333
H	-0.475333	0.780439	1.958377
H	-0.408951	-1.048669	1.975987
H	2.025407	-0.974677	1.479735
H	1.992437	0.857755	1.563774
H	1.675543	0.625314	3.768859

1f

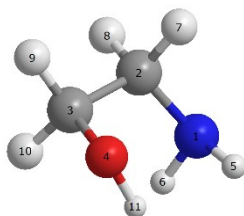
Relative Energy = 9.4 kJ mol⁻¹

Total Energy = -210.036108 hartree

Ionization Product → **1c⁺**

Adiabatic Ionization Energy = 8.81 eV

Dipole Moment = 1.4 D



Frequency Intensity		Frequency Intensity		Frequency Intensity	
158.1195	4.011	1065.0047	74.7741	1500.5715	1.8531
238.8227	150.1081	1108.9465	13.9139	1657.8651	21.4463
312.1484	8.483	1173.0979	8.6568	2958.6182	66.7911
383.9451	60.2231	1236.6333	22.7753	3021.2911	36.7996
507.2327	4.5724	1374.263	0.9955	3065.397	37.2699
786.269	138.1624	1384.1815	5.8198	3073.9194	50.0827
856.7294	28.7809	1391.543	5.9607	3486.7108	1.3617
863.8825	67.2598	1413.4468	34.3921	3574.4073	0.0276
1003.639	7.4321	1476.6407	3.9608	3819.9673	12.9457

AtomX Y Z

N	-0.110006	-0.053495	-0.007783
C	0.011105	-0.007407	1.450914
C	1.439792	0.011299	2.000694
O	2.186306	1.136334	1.545257
H	0.254065	0.79233	-0.433092
H	0.391872	-0.845183	-0.39848

H -0.512395 0.88843 1.798219
H -0.519338 -0.870767 1.868961
H 1.421089 0.08494 3.091367
H 1.951047 -0.928809 1.739309
H 2.293905 1.041407 0.593708

1g

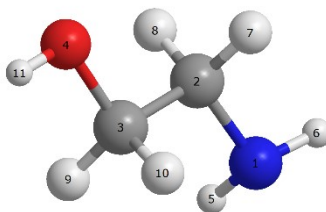
Relative Energy = 11.1 kJ mol⁻¹

Total Energy = -210.035473 hartree

Ionization Product → **1d⁺**

Adiabatic Ionization Energy = 8.79 eV

Dipole Moment = 1.1 D



Frequency	Intensity	Frequency	Intensity	Frequency	Intensity
133.4142	10.1144	1078.1927	4.1932	1529.2964	3.2228
225.9989	38.527	1102.4941	8.6015	1664.3399	27.8191
251.9553	123.0553	1201.3065	3.0289	2956.6244	90.457
294.2791	22.1794	1238.5007	43.804	2962.973	38.4625
477.6285	1.8042	1306.8229	9.7369	3014.1141	67.2669
819.9408	40.8033	1328.7758	2.5578	3067.2264	45.5047
860.3914	102.1718	1399.9795	1.8719	3492.3985	0.8202
962.7425	15.1879	1468.3099	1.0748	3569.9478	0.0876
1058.8847	110.9996	1514.8044	0.2634	3848.0176	27.0402

AtomX Y Z

N -0.000236 0.000812 -5.7e-05
C -6.4e-05 0.000321 1.466919
C 1.430396 -0.000798 1.98526
O 1.371518 -0.004839 3.409355
H 0.243292 -0.920321 -0.351921
H -0.929874 0.204305 -0.350201
H -0.487628 0.914768 1.815645
H -0.535274 -0.845004 1.925574
H 1.957319 -0.891378 1.608141
H 1.94915 0.885301 1.597823
H 2.270457 0.033715 3.746246

1h

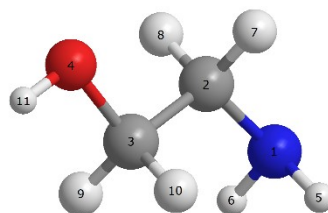
Relative Energy = 11.4 kJ mol⁻¹

Total Energy = -210.035356 hartree

Ionization Product → **1d⁺**

Adiabatic Ionization Energy = 8.79 eV

Dipole Moment = 2.7 D



Frequency	Intensity	Frequency	Intensity	Frequency	Intensity
137.998	5.2861	253.6544	82.6897	302.952	78.9894
		282.1576	0.8613	466.9381	17.4628

801.4756	0.2315	1244.7969	63.4628	1666.3718	23.5252
837.5435	199.9732	1312.1684	1.3266	2948.5268	70.2539
1004.6398	0.2707	1366.7152	2.2377	2976.1884	65.3448
1012.8427	22.2995	1378.6529	0.2607	3039.7673	38.3439
Frequency Intensity		1454.7152	0.3307	3079.6872	41.7295
1060.5728	91.3138	1498.6257	2.0813	3483.8111	1.44
1098.1879	4.4542	Frequency Intensity		3561.3606	0.1207
1206.4805	1.0607	1522.3558	2.1675	3842.6789	24.2318

AtomX Y Z

N -0.051086 -0.04129 -0.00936
C 0.040824 0.012894 1.449234
C 1.460351 -0.018912 0.13556
O 1.368373 0.040763 3.43363
H 0.442855 0.74029 -0.429497
H 0.380727 -0.888858 -0.365063
H -0.453326 0.923795 1.799188
H -0.520094 -0.827358 1.868447
H 1.962698 -0.941498 1.682827
H 2.030389 0.83385 1.612609
H 2.257753 0.021234 3.797212

li

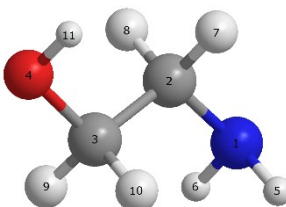
Relative Energy = 11.7 kJ mol⁻¹

Total Energy = -210.035234 hartree

Ionization Product → **1d⁺**

Adiabatic Ionization Energy = 8.79 eV

Dipole Moment = 1.4 D



Frequency	Intensity	Frequency	Intensity	Frequency	Intensity
146.8106	2.3439	1063.5836	61.1373	1512.206	0.3185
265.4075	38.4235	1094.9997	1.2053	1665.9288	23.9898
290.321	68.2445	1141.5027	11.822	2958.5342	73.4514
329.6196	78.2962	1303.0633	5.6587	3007.8669	37.94
464.5874	9.7605	1335.6962	5.5613	3054.9485	22.3549
786.256	1.2005	1373.8807	7.8856	3074.0442	62.3281
842.2317	181.4065	1402.0258	19.5529	3483.1777	1.0543
990.3184	21.3279	1421.879	19.4541	3560.2927	0.0342
1032.418	67.9802	1491.5799	1.5795	3824.0505	19.146

AtomX Y Z

N -0.043331 -0.042906 -0.034461
C 0.011274 0.00911 1.426691
C 1.418701 -0.005546 2.036005
O 1.404678 -0.014268 3.459684
H 0.472229 0.732725 -0.439997

H 0.392485 -0.89451 -0.375554
H -0.512329 0.91596 1.754783
H -0.553056 -0.836424 1.830782
H 1.939994 -0.919813 1.73812
H 1.999726 0.844729 1.644983
H 0.991184 0.802759 3.755587

1j

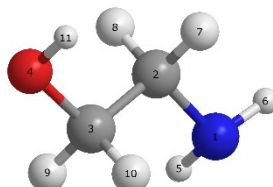
Relative Energy = 11.9 kJ mol⁻¹

Total Energy = -210.035152 hartree

Ionization Product → **1d⁺**

Adiabatic Ionization Energy = 8.79 eV

Dipole Moment = 1.7 D



Frequency	Intensity	Frequency	Intensity	Frequency	Intensity
138.8771	8.4673	1060.7555	109.3409	1506.7536	0.0932
231.524	45.0359	1075.7085	15.3851	1520.8545	1.3172
282.9968	16.5539	1111.4002	8.7382	1663.7955	29.6459
324.8323	116.091	1134.7848	9.5324	2957.8448	61.9342
Frequency	Intensity	1284.6343	9.6785	3004.3804	72.5204
475.0341	5.757	1319.6032	0.576	3024.0995	20.7247
808.0035	39.7462	1362.079	1.4242	3068.582	63.308
853.3411	113.3601	1411.2497	38.554	3491.0721	0.6803
961.8576	7.6976	1438.3165	0.9568	3568.012	0.1109
				3827.0391	19.0095

AtomX Y Z

N -0.007539 0.012146 -0.019011
C -0.039145 0.00038 1.447033
C 1.384547 0.011091 2.002857
O 1.411647 -0.034316 3.425864
H 0.302206 -0.889841 -0.368658
H -0.938525 0.160665 -0.392992
H -0.551944 0.910481 1.780473
H -0.577349 -0.850856 1.891929
H 1.920071 -0.882544 1.669198
H 1.920585 0.88306 1.606978
H 1.046591 0.79352 3.752951

1k

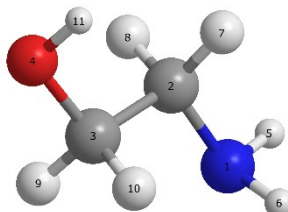
Relative Energy = 12.1 kJ mol⁻¹

Total Energy = -210.035076 hartree

Ionization Product → **1d⁺**

Adiabatic Ionization Energy = 8.78 eV

Dipole Moment = 2.8 D



Frequency	Intensity	Frequency	Intensity
143.7594	2.5457	224.6451	18.5389

274.1201	14.3523	1165.761	7.7264	2905.8396	112.6182
329.3167	143.7955	1268.3888	2.6415	2963.0231	67.987
474.9466	4.2174	1326.2697	8.1226	3063.7581	30.4291
807.2306	32.0397	1375.6748	0.1831	3100.1973	34.7911
844.2955	136.696	1396.0956	54.0089	3493.5994	0.678
970.6451	2.1101	1437.0632	0.6834	3571.4668	0.1217
1055.041	70.0735	1505.3765	0.0308	3824.5802	16.6861
Frequency Intensity		Frequency Intensity			
1068.488	54.2638	1519.9469	1.1727		
1093.7817	1.897	1662.4743	29.4142		

AtomX Y Z

N	0.063369	0.042137	-0.030439
C	0.000725	0.079479	1.432851
C	1.405987	-0.008743	2.026031
O	1.391021	-0.045939	3.44883
H	-0.863853	-0.07474	-0.423888
H	0.424481	0.919174	-0.393314
H	-0.500613	0.976334	1.840804
H	-0.569532	-0.785806	1.781494
H	1.878281	-0.934894	1.696011
H	2.021666	0.825783	1.655732
H	1.030834	0.789313	3.762511

II

Relative Energy = 17.2 kJ mol⁻¹

Total Energy = -210.033176 hartree

Ionization Product → **1b**⁺

Adiabatic Ionization Energy = 8.70 eV

Dipole Moment = 2.1 D

Frequency Intensity		Frequency Intensity		Frequency Intensity	
105.0914	40.2488	1081.0646	12.6899	1511.8093	5.5499
170.4818	35.7309	1113.0031	33.1994	1663.4902	26.5114
188.6883	95.3571	1171.6182	9.6601	2929.1782	48.6926
327.6887	3.3429	1270.5468	32.5849	2958.2308	114.4085
492.3293	14.5348	1307.8679	13.5297	2983.2228	76.2748
797.411	111.4045	1346.9088	15.6066	3063.7069	32.0744
875.9992	20.218	1417.5096	10.138	3493.416	1.1003
932.6891	108.9051	1458.9377	2.1489	3573.347	0.0213
994.1868	1.6703	1489.8927	4.4103	3846.8723	24.1881

Atom X Y Z

N	-0.01944	-0.082311	-0.019382
C	0.018362	0.019541	1.441852
C	1.444192	0.014835	1.975633

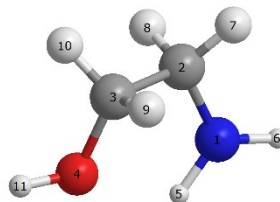
O	2.055146	1.262164	1.671425
H	0.117997	-1.045413	-0.30991
H	-0.926636	0.20261	-0.37107
H	-0.434922	0.971369	1.733616
H	-0.541965	-0.776602	1.960816
H	1.412538	-0.152374	3.063498
H	1.996746	-0.82307	1.524102
H	2.998932	1.181925	1.831965

1a⁺

Relative Energy = 0.0 kJ mol⁻¹

Total Energy = -209.714585 hartree

Dipole Moment = 2.3 D



Frequency	Intensity	Frequency	Intensity	Frequency	Intensity
123.5069	1.3114	1038.2032	57.7314	1507.5645	4.4912
247.0276	131.9223	1067.5868	75.0857	1571.0333	56.4214
329.7734	30.4039	1120.5278	13.6609	2825.7139	56.6661
337.3129	47.4812	1159.0055	37.9572	3002.5593	20.4011
561.1636	24.4978	1232.1618	67.7104	3088.5389	3.2074
684.468	124.8307	1272.4751	23.1760	3090.7149	6.8459
767.7324	4.9520	1357.4701	19.2019	3410.8096	175.9294
863.9617	20.9541	1395.9174	27.5740	3575.3511	186.3453
1022.1075	30.9065	1409.0167	20.2944	3825.6029	273.1766

AtomX Y Z

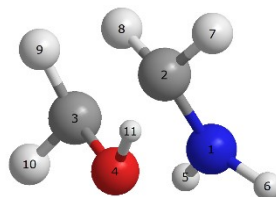
N	-0.120676	-0.267024	0.154656
C	-0.029082	0.102700	1.514884
C	1.438167	0.0310000	1.996895
O	2.040491	-0.979886	1.222327
H	0.594993	-0.903293	-0.209300
H	-0.884078	0.033535	-0.447763
H	-0.529755	1.056924	1.697496
H	-0.603397	-0.664456	2.084498
H	1.902822	1.00791	1.809040
H	1.467429	-0.175403	3.069265
H	2.830016	-1.332177	1.649228

1b⁺

Relative Energy = 2.6 kJ mol⁻¹

Total Energy = -209.71361 hartree

Dipole Moment = 2.0 D

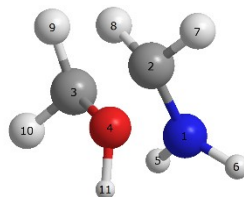


Frequency	Intensity	Frequency	Intensity	Frequency	Intensity
369.6451	0.7547	473.8419	147.8427		
148.1347	5.6726	425.9405	70.961	632.2427	213.2661
235.6132	8.2717	463.6156	8.7689	848.4856	15.1889

924.8076	20.1356	1349.7157	7.0804	3162.5307	1.347
1055.5398	87.7016	1392.1566	29.2639	3171.2451	0.4309
1095.2504	97.4836	1489.158	18.613	3520.4224	216.4713
1181.9294	22.721	1509.2189	0.6875	3633.4757	115.3701
1229.9888	81.292	1663.8174	45.0059	3771.1607	231.0369
1258.5581	8.3591	3055.8246	6.458		
1311.5574	3.9786	3076.7451	1.752		

AtomX Y Z

N -0.251651 -0.193794 0.1334
 C -0.062865 -0.041942 1.481859
 C 1.627939 -0.086751 9.18578
 O 2.294121 0.958483 1.381509
 H -0.337335 -1.111229 -0.290454
 H -0.165305 0.591154 -0.503124
 H -0.374485 0.936089 1.845536
 H -0.464342 -0.874072 2.059746
 H 1.56014 -0.102275 3.008929
 H 1.97666 -1.022811 4.88206
 H 2.318073 1.719821 1.978363



1c⁺

Relative Energy = 5.8 kJ mol⁻¹

Total Energy = -209.712363 hartree

Dipole Moment = 3.2 D

Frequency	Intensity	Frequency	Intensity	Frequency	Intensity
138.7317	3.9992	1055.2328	97.9807	1507.5279	0.3646
234.5934	2.3426	1112.1262	32.1394	1663.7606	48.3242
380.8443	24.2071	1163.1891	79.5105	3060.7109	9.5594
410.2959	9.2855	1236.7198	83.9289	3079.8641	3.6904
433.7888	32.1991	1256.8952	8.2277	3159.0377	3.7331
504.4097	197.7089	1306.8862	4.1282	3176.785	2.6059
609.9644	102.1267	1353.9237	11.1095	3526.6051	206.2417
851.2142	22.3214	1390.0306	20.8737	3640.3807	113.052
912.518	5.7021	1485.8281	19.1489	3775.2684	180.6848

AtomX Y Z

N -0.331958 -0.260820 0.09464
 C -0.163371 -0.111745 1.443622
 C 1.522597 0.097651 1.922691
 O 1.978596 1.313269 1.562854
 H -0.294823 -1.171011 -0.349895
 H -0.464122 0.537893 -0.515191
 H -0.602034 0.803807 1.834903
 H -0.417068 -1.010452 0.05195

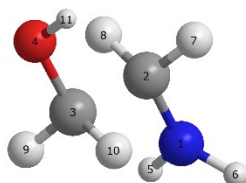
H 1.383797 0.047275 3.00291
H 2.044586 -0.760339 1.498327
H 2.500833 1.28552 0.749019

1d⁺

Relative Energy = 6.0 kJ mol⁻¹

Total Energy = -209.712299 hartree

Dipole Moment = 3.2 D



Frequency	Intensity	Frequency	Intensity	Frequency	Intensity
917.4124	10.6824	1494.1815	14.6264		
113.0349	4.054	1076.4058	47.5789	1519.7446	1.773
265.9399	13.5835			1668.8574	53.4936
290.026	4.2461	1127.9857	135.8261	3073.8419	6.9801
417.139	6.7159	1174.9045	21.612	3092.4197	3.315
493.1238	45.7523	1222.9293	88.2265	3178.6432	2.4031
		1272.1054	36.8572	3194.8524	0.9568
512.7664	198.5627	1285.7047	1.5317	3527.4857	242.9211
618.7909	157.8202	1344.5423	1.3002	3639.0204	112.9352
831.9252	10.2	1392.6336	32.2106	3764.4123	243.4435

Atom X Y Z

N	-0.245823	-0.138128	0.135231
C	-0.097865	-0.126544	1.491227
C	1.633279	-0.087738	1.97071
O	1.686317	-0.225498	3.306574
H	-0.230581	-1.003662	-0.392359
H	-0.285375	0.718291	-0.405333
H	-0.475333	0.780439	1.958377
H	-0.408951	-1.048669	1.975987
H	2.025407	-0.974677	1.479735
H	1.992437	0.857755	1.563774
H	1.675543	0.625314	3.768859

Table S2. Conformers of *N*-methoxymethanamine (**2**) with calculated energetics, vibrational frequencies (cm⁻¹) & intensities (km mol⁻¹), and Cartesian coordinates (Å).

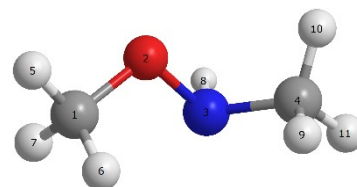
2a

Relative Energy = 0.0 kJ mol⁻¹

Total Energy = -209.974809 hartree

Adiabatic Ionization Energy = 8.22 eV

Dipole Moment = 0.6 D



Frequency	Intensity	Frequency	Intensity
113.0349	4.054	1076.4058	47.5789
265.9399	13.5835	1127.9857	135.8261
290.026	4.2461	1174.9045	21.612
417.139	6.7159	1222.9293	88.2265
493.1238	45.7523	1272.1054	36.8572
512.7664	198.5627	1285.7047	1.5317
618.7909	157.8202	1344.5423	1.3002
831.9252	10.2	1392.6336	32.2106
917.4124	10.6824	1494.1815	14.6264

Frequency	Intensity
1519.7446	1.773
1668.8574	53.4936
3073.8419	6.9801
3092.4197	3.315
3178.6432	2.4031
3194.8524	0.9568
3527.4857	242.9211
3639.0204	112.9352
3764.4123	243.4435

AtomX Y Z

C	-0.000135	0.000277	-0.000228
O	0.000107	-0.000786	1.419519
N	1.364095	-0.000767	1.888900
C	1.508649	-1.138405	2.794337
H	-1.05144	-0.028223	-0.294631
H	0.517491	-0.87708	-0.404027
H	0.467989	0.905967	-0.402783
H	1.415156	0.853971	2.440492
H	1.471073	-2.064973	2.218654
H	0.735275	-1.175684	3.572696
H	2.493068	-1.065968	3.266056

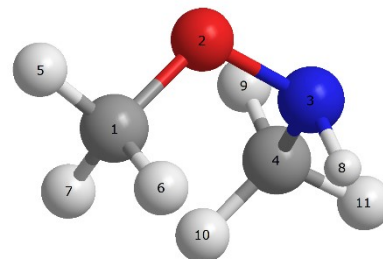
2b

Relative Energy = 16.5 kJ mol⁻¹

Total Energy = -209.968531 hartree

Adiabatic Ionization Energy = 7.97 eV

Dipole Moment = 2.9 D



Frequency	Intensity	Frequency	Intensity
930.6329	25.8155	930.6329	25.8155
98.6743	0.3955	1007.1567	17.5652
221.3308	1.6526	1069.1747	40.7819
264.1206	1.5844	1152.4972	2.3555
395.2266	3.8428	1165.1117	2.8212
489.4997	3.6863	1186.1268	5.6406
785.5174	55.0539		

Frequency	Intensity
1237.8687	11.8731
1434.3221	0.154
1455.3981	4.6715
1469.8672	8.0072
1479.6836	6.1945
1492.202	4.5121

1504.2761	1.3855	2979.3184	65.9283	3110.8547	13.0721
1526.7004	12.025	3036.5278	70.2016	3111.7732	28.5509
2970.2627	36.0537	3069.4728	31.8829	3423.8137	5.058

AtomX Y Z

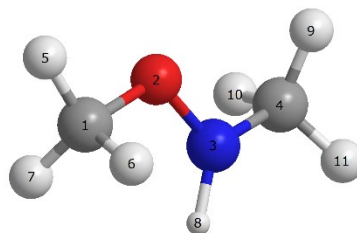
C	-0.311198	-0.235136	0.037164
O	0.209261	0.416480	1.189409
N	1.411015	-0.171483	1.687988
C	2.556593	0.157162	0.842764
H	-1.248819	0.272844	-0.193114
H	-0.523077	-1.294843	0.241063
H	0.353162	-0.161338	-0.831809
H	1.256945	-1.180542	1.693474
H	2.703917	1.238101	0.862605
H	2.481886	-0.170621	-0.203978
H	3.435136	-0.316500	1.289219

2a⁺

Relative Energy = 0.0 kJ mol⁻¹

Total Energy = -209.675704 hartree

Dipole Moment = 2.4 D



Frequency Intensity

77.258	0.0661
106.6838	8.4736
157.6932	11.1064
297.5787	3.1766
384.5558	68.7866
496.866	1.9476
874.6151	42.1953
972.1938	16.7747
1097.0441	8.1737

Frequency Intensity

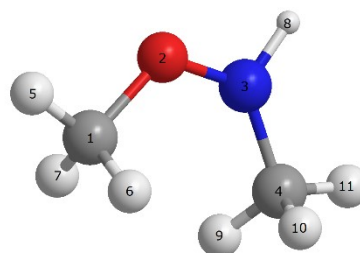
1143.5075	0.5072
1155.0233	4.9208
1200.0424	18.9562
1321.1961	80.6162
1437.0453	8.8177
1449.0984	15.9263
1459.0905	3.8331
1463.0043	19.7598
1470.964	13.0274

Frequency Intensity

1478.9446	26.1789
1542.8464	13.0148
3023.8752	14.9777
3056.962	1.2774
3118.68	2.6291
3157.0427	0.0746
3163.6806	3.8960
3200.1999	3.3458
3469.8238	66.2847

AtomX Y Z

C	-0.676023	-0.353584	0.109386
O	0.570580	0.373873	0.400835
N	1.571428	-0.354395	0.818619
C	2.837383	0.313420	1.050285
H	-1.351408	0.423575	-0.234900
H	-1.035894	-0.809553	1.031969
H	-0.481545	-1.08386	-0.677060
H	1.460982	-1.370472	0.797545
H	2.637142	1.297994	1.472260
H	3.377683	0.415167	0.102071
H	3.414494	-0.298042	1.743776



2b⁺

Relative Energy = 8.1 kJ mol⁻¹

Total Energy = -209.672627 hartree

Dipole Moment = 2.1 D

Frequency Intensity		Frequency Intensity		Frequency Intensity	
80.7069	0.1567	1137.9998	1.7799	1486.4605	3.619
192.9394	0.4242	1143.8144	3.2269	1540.3831	3.4239
214.9984	1.5792	1210.5942	6.8257	3026.306	9.2563
300.8308	1.0394	1332.5835	61.2948	3061.2003	2.5386
456.2209	105.9664	1432.0077	5.6916	3105.1511	1.2916
562.5762	11.1645	1453.3483	13.7037	3158.4973	2.83
827.4582	25.633	1461.5292	22.2304	3160.2903	0.122
959.6686	8.7868	1463.329	15.5319	3199.051	2.5946
1085.4848	1.3814	1483.5904	41.7439	3529.7875	160.0648

AtomX Y Z

C	-0.016396	-0.219898	0.196004
O	0.238669	0.686292	1.321069
N	1.029793	0.282107	2.284874
C	1.596124	-1.046186	2.434641
H	-0.716315	0.343526	-0.413533
H	-0.466668	-1.141811	0.562945
H	0.916686	-0.395968	-0.339598
H	1.111205	1.006980	2.995860
H	2.169060	-1.319727	1.545846
H	0.802776	-1.780500	2.611162
H	2.256395	-1.006487	3.299715

Table S3. Conformers of Methoxymethanamine (**3**) with calculated energetics, vibrational frequencies (cm^{-1}) & intensities (km mol^{-1}), and Cartesian coordinates ($\text{\AA}$).

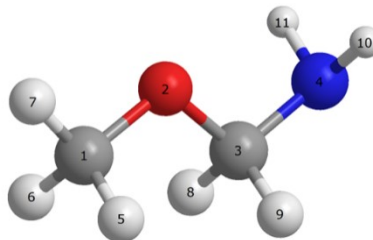
3a

Relative Energy = 0.0 kJ mol^{-1}

Total Energy = -210.030838 hartree

Adiabatic Ionization Energy = 9.31 eV

Dipole Moment = 0.8 D



Frequency	Intensity	Frequency	Intensity	Frequency	Intensity
113.6214	2.1893	1158.7412	52.0853	1522.6241	0.0251
212.0925	0.0427	1172.6813	2.245	1681.3694	29.96
298.7336	12.5718	1225.792	19.6856	2956.0002	40.8304
385.493	60.5596	1255.6938	5.7008	2973.5646	92.2656
487.8636	18.7272	1387.4287	0	2996.712	115.003
838.6657	159.4894	1421.5478	36.5527	3002.5016	39.072
948.0799	2.1273	1479.8053	1.6193	3109.1141	31.9372
960.6000	210.1098	1484.7602	6.5581	3499.3793	0.086
1103.312	125.8179	1506.7301	6.1061	3574.5837	1.1699

AtomX Y Z

C -0.004242 0.004873 -0.019442

O -0.017638 0.12385 1.388222

C 1.288296 0.031698 1.965032

N 1.24794 0.154878 3.387916

H 0.400649 -0.965502 -0.344199

H 0.590521 0.801267 -0.49172

H -1.035516 0.086931 -0.364036

H 1.925048 0.827507 1.552216

H 1.735437 -0.937215 1.699604

H 0.666195 -0.574667 3.787314

H 0.839819 1.045903 3.651915

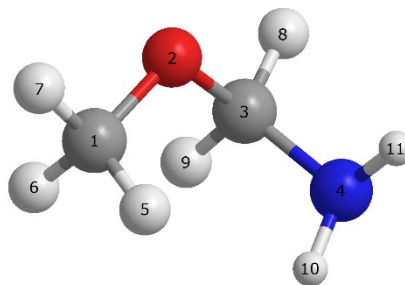
3b

Relative Energy = 2.3 kJ mol^{-1}

Total Energy = -210.02997 hartree

Adiabatic Ionization Energy = 9.29 eV

Dipole Moment = 1.5 D



Frequency	Intensity	Frequency	Intensity	Frequency	Intensity
134.56	1.64	913.68	129.09	1295.88	7.70
201.24	1.13	929.47	36.61	1388.51	2.20
338.60	12.28	1085.21	139.55	1415.10	12.68
421.49	45.01	1122.65	61.50	1473.95	3.21
521.03	54.02	1170.99	3.22	1488.14	3.04
795.59	150.02	1197.18	31.17	1492.90	1.32

1508.72	8.33	2996.37	83.82	3109.53	29.26
1672.08	24.37	3005.90	61.32	3509.38	0.35
2961.38	60.56	3099.97	34.08	3592.88	1.15

AtomX Y Z

C	-0.095948	0.021364	-0.010959
O	-0.020134	0.008841	1.40011
C	1.313715	-0.031173	1.910688
N	2.039083	-1.2636	1.746656
H	0.277973	-0.909735	-0.459191
H	0.466803	0.865502	-0.437864
H	-1.147753	0.13111	-0.276554
H	1.198969	0.171562	2.976142
H	1.904553	0.776136	1.456465
H	2.265696	-1.455441	0.777944
H	1.513635	-2.049241	2.115263

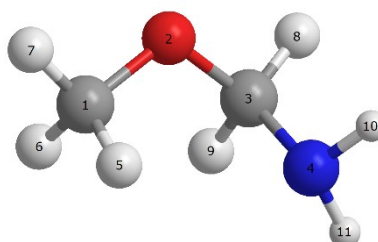
3c

Relative Energy = 7.9 kJ mol⁻¹

Total Energy = -210.027838 hartree

Adiabatic Ionization Energy = 9.12 eV

Dipole Moment = 1.8 D



Frequency Intensity

150.443	2.9924
207.7736	15.8526
220.1813	38.4369
363.0758	4.6965
559.1954	4.5171
763.3622	143.6052
919.2991	27.3439
976.8099	9.1103
1060.4382	50.1941

Frequency Intensity

1139.9129	177.2723
1172.5897	5.5268
1195.2984	28.7398
1281.9154	7.5017
1354.9594	3.489
1428.7701	20.7497
1471.5659	7.5129
1480.9605	7.2177
1507.0485	0.5204

Frequency Intensity

1515.5853	6.8877
1653.0713	34.0264
2961.9994	60.2327
2971.3651	103.0068
3020.2348	70.0695
3057.547	41.5266
3116.716	30.1076
3517.3911	0.0705
3605.1556	2.0448

AtomX Y Z

C	-0.023039	0.027955	-0.023293
O	0.007848	0.023672	1.395944
C	1.312676	-0.025658	1.929553
N	1.976174	-1.281266	1.623944
H	0.482043	-0.850472	-0.435043
H	0.453665	0.934529	-0.425847
H	-1.073043	0.020946	-0.316615
H	1.169612	0.157797	3.000971
H	1.930118	0.786541	1.515803
H	1.700226	-2.016581	2.264288
H	2.984379	-1.191308	1.645211

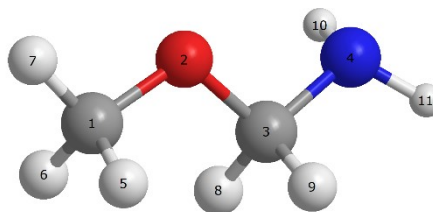
3d

Relative Energy = 16.0 kJ mol⁻¹

Total Energy = -210.024734 hartree

Adiabatic Ionization Energy = 9.04 eV

Dipole Moment = 2.3 D



Frequency Intensity

111.525 3.5464

153.3069 45.7664

224.0978 2.9614

321.5479 6.3028

514.9277 11.8798

751.1244 156.2345

933.2887 46.4488

1046.0272 39.5356

1101.9182 2.1182

Frequency Intensity

1142.6846 189.6573

1173.2219 2.2296

1216.3865 44.6588

1256.3681 9.8667

1346.9875 2.8867

1447.5454 49.2481

1479.9923 10.7816

1486.8168 8.9998

1508.2862 5.1363

Frequency Intensity

1534.7243 0.3236

1657.6545 33.021

2871.6507 111.1547

2954.1934 72.4468

2967.6101 89.196

2992.5513 80.6249

3112.4861 30.6364

3522.9931 0.4728

3611.9863 2.1575

AtomX Y Z

C 2.6e-05 0.000206 -3.6e-05

O -0.000314 0.00053 1.410832

C 1.307503 -6.1e-05 1.953453

N 1.192018 0.110129 3.384423

H 0.475748 -0.90364 -0.410203

H 0.519245 0.879510 -0.411457

H -1.041228 0.023843 -0.321966

H 1.880868 0.818763 1.475599

H 1.819925 -0.946221 1.719416

H 1.021800 1.066175 3.673279

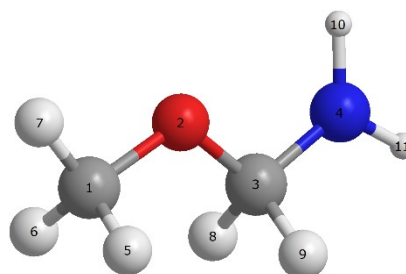
H 2.024542 -0.228793 3.848976

3a⁺

Relative Energy = 0.0 kJ mol⁻¹

Total Energy = -209.692615 hartree

Dipole Moment = 3.8 D



Frequency Intensity

39.8007 1.3355

131.1587 4.5702

285.5631 25.9455

287.555 6.6796

490.4497 6.549

496.4117 177.8226

809.5399 16.5786

871.8786 3.7173

1036.1104 73.7488

Frequency Intensity

1120.2597 87.7747

1139.5668 0.5924

1161.8825 1.1198

1191.9321 7.3694

1248.5849 291.3253

1302.3869 58.6651

1337.06 8.0854

1481.2696 23.3552

1483.8245 1.399

Frequency Intensity

1490.0283 21.4212

1603.7481 49.0732

2719.1589 7.8727

2761.6815 24.2985

3040.1759 7.2999

3120.7032 7.7091

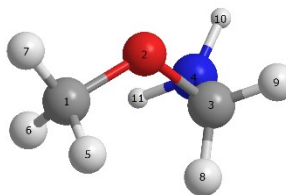
3186.2163 0.8773

3476.9525 455.9464

3615.5038 179.6837

AtomX Y Z

C -0.015297 0.02695 -0.037738
 O 0.118745 0.211469 1.396027
 C 1.348705 0.032637 1.92501
 N 1.352052 0.238563 3.313314
 H 0.247807 -0.997631 -0.309861
 H 0.611701 0.746919 -0.56836
 H -1.063261 0.214011 -0.250554
 H 2.128903 0.703151 1.475663
 H 1.774989 -0.986849 1.727193
 H 0.490639 0.490968 3.795578
 H 2.20515 0.140254 3.856043



3b⁺

Relative Energy = 10.4 kJ mol⁻¹

Total Energy = -209.688666 hartree

Dipole Moment = 2.3 D

Frequency Intensity

43.1282 0.0754

148.7541 6.3677

296.8291 13.5725

400.256 4.9744

468.509 39.0241

649.571 199.7829

801.2203 34.2999

895.022 12.6275

926.1588 19.8379

Frequency Intensity

1112.4622 15.3799

1114.5441 8.6544

1156.1533 35.7987

1241.2654 11.5187

1321.8098 9.2857

1375.7476 53.3781

1441.6627 26.8552

1462.4098 12.1978

1468.5719 20.6173

Frequency Intensity

1500.0073 8.1347

1638.3915 46.7907

3017.555 17.2995

3089.2881 1.2675

3093.5409 0.3594

3173.1429 2.7377

3176.124 1.1164

3491.3673 256.294

3611.5776 111.802

AtomX Y Z

C -0.035979 0.16182 0.080886

O 0.210991 -0.598454 1.281686

C 1.453776 -0.397299 1.957004

N 1.002702 0.380452 3.073003

H 0.755508 -0.051125 -0.643815

H -0.063710 1.235243 0.294680

H -1.009924 -0.164532 -0.274689

H 2.179875 0.145549 1.350827

H 1.834053 -1.363662 2.279086

H 0.611175 -0.087293 8.87178

H 0.698043 1.33882 2.926974

Table S4. Conformers of Methylaminoethanol (**4**) with calculated energetics, vibrational frequencies (cm^{-1}) & intensities (km mol^{-1}), and Cartesian coordinates ($\text{\AA}$).

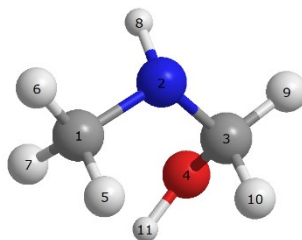
4a

Relative Energy = 0.0 kJ mol^{-1}

Total Energy = $-210.034243 \text{ hartree}$

Adiabatic Ionization Energy = 8.58 eV

Dipole Moment = 1.5 D



Frequency	Intensity	Frequency	Intensity	Frequency	Intensity
152.0662	8.2551	1131.9248	26.3312	1504.1067	6.651
208.9271	3.9744	1144.7216	1.0466	1530.3634	14.8234
302.4207	52.1235	1186.1513	64.5167	2948.8198	89.3989
381.9701	80.6571	1303.5755	13.6772	3004.0874	57.5156
543.7166	17.8003	1380.5306	5.5706	3045.1584	41.3781
743.4384	128.5331	1419.8352	24.8523	3092.4881	31.2806
929.9826	10.3003	1455.3024	3.4402	3100.8633	34.9128
978.9496	182.6783	1490.7249	10.6946	3523.666	0.3997
1005.5303	20.1773	1493.5981	0.8097	3833.8802	18.1703

Atom X Y Z

C	1.521131	0.440305	0.086894
N	0.618717	-0.665436	-0.220254
C	-0.714867	-0.534630	0.301045
O	-1.496493	0.550452	-0.217460
H	1.605830	0.543217	1.173563
H	2.518342	0.216217	-0.297608
H	1.212434	1.414030	-0.325759
H	0.580235	-0.820525	-1.222334
H	-1.276098	-1.432878	0.041101
H	-0.647692	-0.465342	1.394417
H	-1.189711	1.365660	0.190442

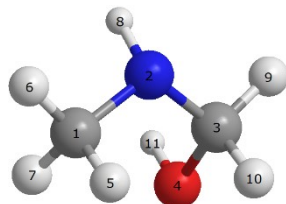
4b

Relative Energy = 0.7 kJ mol^{-1}

Total Energy = $-210.033972 \text{ hartree}$

Adiabatic Ionization Energy = 8.58 eV

Dipole Moment = 1.7 D

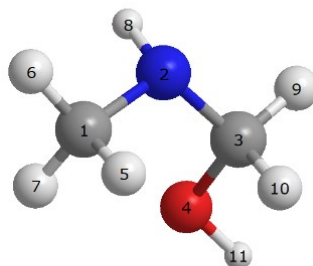


Frequency	Intensity	Frequency	Intensity	Frequency	Intensity
169.1089	2.4202	941.0412	11.0797	1306.3548	14.4552
198.3734	3.0857	967.4373	170.5527	1377.41	0.9067
300.1512	92.0114	1003.2192	28.2978	1422.2347	24.1161
382.5331	39.8638	1129.5847	25.7863	1458.3188	8.1437
564.1791	23.5236	1154.3555	8.483	1484.3182	7.673
716.5643	120.7424	1168.6796	72.8461	1493.9313	0.516

1504.8055	2.201		3013.7733	64.1578		3095.1067	35.7146
1527.286	15.4411		3055.8035	38.0372		3521.9638	0.4606
2990.5108	71.2942		3086.0364	30.3958		3814.5762	14.1553

AtomX Y Z

C	-1.520049	-0.449039	0.096740
N	-0.618993	0.652413	-0.240364
C	0.709261	0.544345	0.293168
O	1.442358	-0.641060	-0.051149
H	-1.651582	-0.481900	1.182439
H	-2.499449	-0.263872	-0.349528
H	-1.160834	-1.434523	-0.227138
H	-0.598596	0.810020	-1.242197
H	1.268358	1.439220	-0.004799
H	0.648480	0.516228	1.383256
H	1.652440	-0.595425	-0.989743



4c

Relative Energy = 1.3 kJ mol⁻¹

Total Energy = -210.033744 hartree

Adiabatic Ionization Energy = 8.57 eV

Dipole Moment = 1.0 D

Frequency Intensity

159.4761	3.1247
184.6451	41.424
215.5538	77.2165
347.756	24.0897
537.9209	22.3407
748.6314	117.0942
947.2754	2.3007
971.1002	114.3352
1028.9017	25.4638

Frequency Intensity

1124.6476	44.8587
1157.7247	50.3797
1208.2095	11.5195
1277.6682	56.1547
1319.1577	1.113
1433.1982	10.1457
1462.2905	6.9803
1485.962	7.8872
1509.4219	3.4012

Frequency Intensity

1515.7289	0.7733
1531.5257	20.7312
2978.4646	89.3403
2998.2873	40.6919
3015.7509	73.9551
3056.7937	41.8632
3092.9614	36.1457
3526.8974	0.4269
3815.7453	9.741

AtomX Y Z

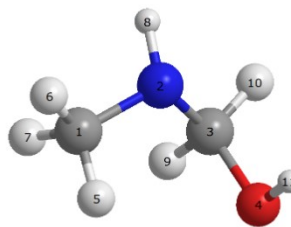
C	-1.516844	-0.449525	0.116031
N	-0.619030	0.649236	-0.244502
C	0.700479	0.547562	0.285307
O	1.375245	-0.620432	-0.218169
H	-1.649403	-0.459285	1.202338
H	-2.496916	-0.272716	-0.332385
H	-1.156649	-1.438485	-0.193063
H	-0.575062	0.753389	-1.252639
H	1.256906	1.451410	0.005519
H	0.631471	0.500437	1.381016
H	2.219090	-0.704170	0.238048

4dRelative Energy = 1.5 kJ mol⁻¹

Total Energy = -210.033656 hartree

Adiabatic Ionization Energy = 8.53 eV

Dipole Moment = 2.0 D

**Frequency Intensity**

154.408 4.6318

201.0783 0.5354

351.638 29.6429

392.1026 98.3557

563.9842 46.652

726.3202 99.3042

922.3268 14.1013

1024.6767 12.6692

1043.3172 105.1109

Frequency Intensity

1139.4051 28.4354

1157.3303 64.5166

1187.4224 6.4501

1276.8948 13.2522

1374.2563 4.6132

1432.7452 44.9526

1457.5351 22.6849

1482.3674 14.5181

1497.5067 7.7359

Frequency Intensity

1516.3458 6.2398

1529.4312 4.8153

2944.7291 85.7976

2962.9098 106.2216

2996.4964 77.3187

3068.4826 34.7676

3110.5008 19.2433

3542.2609 0.3094

3792.7129 18.6622

AtomX Y Z

C 1.537741 -0.438300 0.117120

N 0.558047 0.513433 -0.403350

C -0.702704 0.524619 0.306272

O -1.493324 -0.593674 -0.054587

H 1.092106 -1.434315 0.111076

H 2.416054 -0.457898 -0.531768

H 1.866196 -0.220202 1.146749

H 0.945911 1.447824 -0.456339

H -0.598928 0.449713 1.399157

H -1.207785 1.471721 0.069965

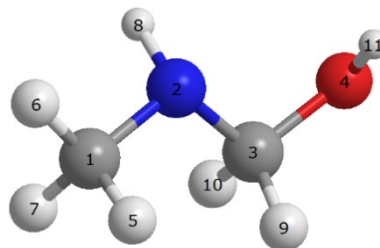
H -1.483511 -0.619398 -1.019045

4eRelative Energy = 3.5 kJ mol⁻¹

Total Energy = -210.032914 hartree

Adiabatic Ionization Energy = 8.55 eV

Dipole Moment = 1.7 D

**Frequency Intensity**

154.408 4.6318

201.0783 0.5354

351.638 29.6429

392.1026 98.3557

563.9842 46.652

726.3202 99.3042

922.3268 14.1013

1024.6767 12.6692

1043.3172 105.1109

Frequency Intensity

1139.4051 28.4354

1157.3303 64.5166

1187.4224 6.4501

1276.8948 13.2522

1374.2563 4.6132

1432.7452 44.9526

1457.5351 22.6849

1482.3674 14.5181

1497.5067 7.7359

Frequency Intensity

1516.3458 6.2398

1529.4312 4.8153

2944.7291 85.7976

2962.9098 106.2216

2996.4964 77.3187

3068.4826 34.7676

3110.5008 19.2433 3542.2609 0.3094

3792.7129 18.6622

AtomX Y Z

C	1.537741	-0.438300	0.117120
N	0.558047	0.513433	-0.403350
C	-0.702704	0.524619	0.306272
O	-1.493324	-0.593674	-0.054587
H	1.092106	-1.434315	0.111076
H	2.416054	-0.457898	-0.531768
H	1.866196	-0.220202	1.146749
H	0.945911	1.447824	-0.456339
H	-0.598928	0.449713	1.399157
H	-1.207785	1.471721	0.069965
H	-1.483511	-0.619398	-1.019045

4f

Relative Energy = 13.3 kJ mol⁻¹

Total Energy = -210.029179 hartree

Adiabatic Ionization Energy = 8.41 eV

Dipole Moment = 2.4 D

Frequency Intensity

66.3141	16.0531
196.6822	10.1571
257.3645	82.923
378.4254	25.0692
517.3838	25.2866
695.6822	108.0391
913.3113	25.4712
1013.531	73.9934
1052.8677	51.9038

AtomX Y Z

C	1.541690	-0.451857	0.090436
N	0.584925	0.545883	-0.370546
C	-0.699074	0.510675	0.299726
O	-1.559219	-0.494362	-0.208353
H	1.190079	-1.452686	-0.177186
H	2.497858	-0.307642	-0.416290
H	1.719634	-0.435520	1.180874
H	0.979884	1.476721	-0.311493
H	-0.593203	0.382011	1.394847
H	-1.202660	1.459924	0.110191
H	-1.268013	-1.341999	0.138732

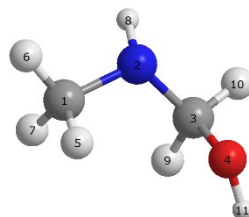
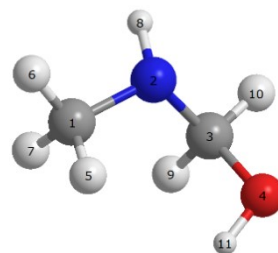
4g

Frequency Intensity

1134.5616	10.8941
1153.2733	36.9719
1159.0161	78.8454
1297.0698	20.6962
1389.2525	7.435
1432.2404	40.2433
1458.8843	5.7571
1481.3756	10.2364
1491.7465	3.8371

Frequency Intensity

1508.3478	2.5486
1520.0633	9.5811
2878.5594	121.373
2918.8388	117.5666
3048.0771	39.968
3088.157	36.3702
3097.3275	27.3348
3544.9044	0.3814
3842.0204	19.5566



Relative Energy = 13.5 kJ mol⁻¹

Total Energy = -210.029098 hartree

Adiabatic Ionization Energy = 8.41 eV

Dipole Moment = 2.4 D

Frequency Intensity		Frequency Intensity		Frequency Intensity	
138.5524	4.1817	1140.6006	8.3327	1517.8211	5.8017
194.8209	53.6724	1165.3341	94.0997	1528.9844	5.3723
203.7331	53.4644	1202.0904	14.8381	2856.5022	137.979
355.111	7.3243	1276.8758	46.2081	2922.0216	119.5653
523.1297	30.1815	1315.878	21.0537	2994.9508	81.1026
690.991	112.9004	1438.506	8.5962	3070.4535	35.2828
932.1979	9.5289	1464.9666	22.3589	3112.9323	19.5884
1029.5462	99.1227	1492.0107	13.942	3559.6878	1.1335
1042.6336	8.0048	1497.0497	2.0006	3842.0996	19.3136

Atom	X	Y	Z
C	1.517780	-0.476587	0.108253
N	0.592923	0.548288	-0.359468
C	-0.691547	0.533698	0.281085
O	-1.441950	-0.552980	-0.254164
H	1.072672	-1.456065	-0.072330
H	2.447958	-0.421079	-0.460970
H	1.760197	-0.403425	1.183447
H	1.001030	1.473209	-0.314594
H	-0.625717	0.417164	1.382330
H	-1.183766	1.491564	0.065935
H	-2.044632	-0.858207	0.429739

4h

Relative Energy = 16.3 kJ mol⁻¹

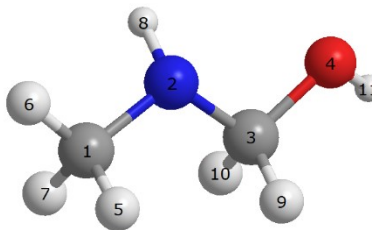
Total Energy = -210.028051 hartree

Adiabatic Ionization Energy = 8.41 eV

Dipole Moment = 2.3 D

Frequency Intensity		Frequency Intensity		Frequency Intensity	
104.9136	1.5785	1140.1463	46.8228	1522.3095	29.1934
215.4941	109.513	1151.9913	91.4989	1543.4936	1.9628
229.4704	1.189	1220.881	18.3788	2840.4665	152.8053
290.7449	5.8203	1257.5265	35.2368	2917.4639	123.9379
501.0777	11.3012	1314.8106	35.7856	2964.5943	76.4334
796.6203	110.8433	1437.2788	3.5508	3045.6129	41.8031
964.3225	23.442	1464.8078	0.7186	3096.8644	30.8507
1043.4512	24.4841	1487.8983	23.5245	3520.8439	0.2954
1077.0137	45.5775	1505.6638	13.1517	3846.6295	22.9844

Atom	X	Y	Z
------	---	---	---



C	-1.821839	0.093659	-0.016005
N	-0.491163	-0.494984	-0.072971
C	0.574758	0.466472	0.045465
O	1.794749	-0.242092	-0.102466
H	-1.965225	0.758945	-0.873029
H	-2.570738	-0.697582	-0.086293
H	-2.026920	0.679115	0.898308
H	-0.375510	-1.203511	0.644184
H	0.441823	1.213287	-0.752253
H	0.570747	1.009319	1.014618
H	2.488458	0.281268	0.308229

4i

Relative Energy = 16.9 kJ mol⁻¹

Total Energy = -210.027785 hartree

Adiabatic Ionization Energy = 8.41 eV

Dipole Moment = 2.5 D

Frequency	Intensity	Frequency	Intensity
53.6132	5.5618	1118.6057	132.3968
219.8344	15.059	1139.678	19.6212
264.6298	77.7537	1174.3336	15.7875
308.1229	10.3492	1289.2086	26.9233
499.2847	3.723	1385.8417	6.2515
796.3833	136.9251	1431.3761	40.7407
967.3545	20.0835	1463.7621	9.8231
1014.9579	23.35	1488.4803	13.5805
1080.5914	79.1421	1498.9838	3.9015

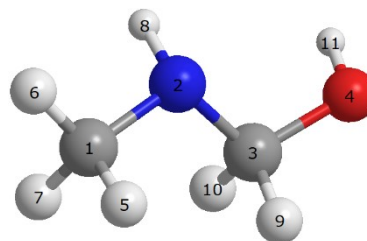
AtomX Y Z

C	-1.821190	0.098421	-0.040032
N	-0.493186	-0.507043	-0.097004
C	0.579942	0.446362	0.138086
O	1.849828	-0.078927	-0.185004
H	-1.927245	0.817946	-0.857230
H	-2.578283	-0.675242	-0.182930
H	-2.047022	0.627359	0.902708
H	-0.437265	-1.257751	0.585597
H	0.421637	1.292686	-0.534650
H	0.582607	0.836962	1.175179
H	2.086736	-0.729932	0.482064

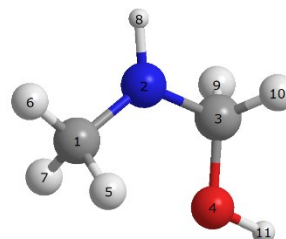
4a⁺

Relative Energy = 0.0 kJ mol⁻¹

Total Energy = -209.720001 hartree



Frequency	Intensity
1518.5662	11.8283
1527.0564	3.2313
2873.2784	133.3192
2924.0954	121.5688
3049.1105	35.6491
3070.0101	32.8562
3096.6197	32.0133
3492.5151	0.9537
3831.3499	22.2581



Dipole Moment = 2.5 D

Frequency	Intensity	1038.7203	55.5569	1439.9851	12.6943
15.5474	5.5042	1058.5019	4.8533	1484.6981	3.8384
145.7464	68.5088	Frequency	Intensity	1493.7744	16.2524
229.424	44.4423	1112.1175	77.6561	2879.0172	61.2506
283.3921	5.0112	1204.6886	4.0955	2886.0931	7.9991
545.4101	136.4603	1208.4279	90.0752	2980.1632	40.5025
Frequency	Intensity	1229.1574	18.9525	3025.8403	10.6155
627.3692	10.2682	1373.5134	39.9553	3178.4193	3.9128
866.4814	10.7655	1396.8262	50.4135	3524.4978	140.45
910.7915	1.5151	1418.1702	28.7352	3816.9537	226.7553

AtomX Y Z

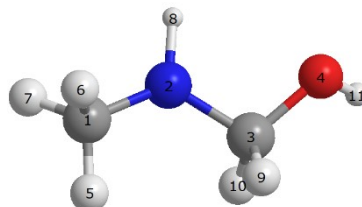
C	1.462454	-0.496282	-0.004115
N	0.609961	0.658437	-0.002118
C	-0.822871	0.590470	-0.000726
O	-1.198939	-0.730103	0.008789
H	1.173350	-1.156888	-0.832114
H	2.503032	-0.191673	-0.071763
H	1.279999	-1.080464	0.910961
H	1.023868	1.589232	0.014386
H	-1.166802	1.166122	0.884135
H	-1.170179	1.157212	-0.889513
H	-2.158982	-0.816908	-0.042526

4b⁺

Relative Energy = 3.0 kJ mol⁻¹

Total Energy = -209.718851 hartree

Dipole Moment = 2.4 D



Frequency Intensity

97.9252 8.3976
 127.2832 2.6151
 150.0391 149.3797
 295.9631 0.6185
 501.0626 7.0091
 554.7374 82.4671
 880.2126 16.7279
 927.7853 8.3932
 1041.242 27.0749

Frequency Intensity

1067.8716 10.4202
 1135.6035 107.2748
 1184.0347 48.9911
 1197.2175 65.6569
 1309.6382 38.2675
 1364.5357 6.7627
 1393.8959 34.9591
 1405.2424 19.7788
 1435.4605 20.6764

Frequency Intensity

1472.6502 11.0642
 1506.9462 40.2045
 2918.1321 90.2293
 2941.4926 1.2231
 2974.6075 37.5877
 3055.5509 7.4683
 3154.208 5.1823
 3465.8403 104.941
 3824.9881 216.920

AtomX Y Z

C 1.866337 -0.053166 -0.051278
 N 0.502182 0.363770 0.112885
 C -0.651178 -0.506590 0.042274
 O -1.767704 0.269883 -0.153139
 H 1.946541 -1.137862 -0.003130
 H 2.233081 0.303222 -1.027010
 H 2.483541 0.425951 0.716355
 H 0.284170 1.360702 0.196129
 H -0.466415 -1.202264 -0.797566
 H -0.659832 -1.117054 0.963869
 H -2.485687 0.020391 0.440291

Table S5. Ices studied in this experiment containing methanol and methylamine or their isotopomers, all of which were deposited to a thickness of 730 ± 30 nm. The ratio of the concentration of the components, irradiation parameters, and photon energy used are listed.

Ice	Methanol:Methylamine	Irradiation Time (s)	Irradiation Current (nA)	Methanol Dose (eV molecule ⁻¹)	Methylamine Dose (eV molecule ⁻¹)	Photon Energy (eV)
CD ₃ OH–CH ₃ NH ₂	1:1.6 ± 0.8	-	-	0.63 ± 0.05	0.56 ± 0.05	9.45
CD ₃ OH–CH ₃ NH ₂	1:2.5 ± 0.5	900 ± 10	20 ± 1	0.63 ± 0.05	0.56 ± 0.05	9.45
CD ₃ OH–CH ₃ NH ₂	1:1.7 ± 0.5	900 ± 10	20 ± 1	0.63 ± 0.05	0.56 ± 0.05	8.89
CD ₃ OH–CH ₃ NH ₂	1:1.3 ± 0.5	900 ± 10	20 ± 1	0.63 ± 0.05	0.56 ± 0.05	8.45
CH ₃ OH–CH ₃ NH ₂	1:1.5 ± 0.4	900 ± 10	20 ± 1	0.56 ± 0.05	0.58 ± 0.05	8.95
CH ₃ OH–CH ₃ NH ₂	1:1.4 ± 0.3	900 ± 10	20 ± 1	0.56 ± 0.05	0.58 ± 0.05	8.89
CH ₃ OH–CH ₃ NH ₂	1:1.6 ± 0.4	900 ± 10	20 ± 1	0.56 ± 0.05	0.58 ± 0.05	8.61
CD ₃ OD–CD ₃ ND ₂	1:1.4 ± 0.2	1800 ± 10	40 ± 2	2.5 ± 0.1	2.6 ± 0.1	8.89

Table S6. Parameters Used in Irradiation Dose Calculation and Resulting Doses

Irradiated area	$1.6 \pm 0.1 \text{ cm}^2$		
Initial kinetic energy of e^-	5.000 keV		
Irradiation current	20 nA	20 nA	40 nA
Irradiation time	900 s	900 s	1800 s
Total number of e^-	$(1.12 \pm 0.05) \times 10^{14}$		
Total molecules irradiated	7.88×10^{17}		
	Methanol– Methylamine	Methanol- d_3 – Methylamine	Methanol- d_5 – Methylamine- d_4
Approximate density of mixed ice*	0.756 g cm^{-1}	0.779 g cm^{-1}	0.825 g cm^{-1}
Average Penetration depth	$340 \pm 10 \text{ nm}$	$330 \pm 10 \text{ nm}$	$310 \pm 10 \text{ nm}$
Fraction of backscattered e^-	0.319	0.318	0.319
Average energy of backscattered e^-	1.109 keV	1.015 keV	1.017 keV
Fraction of Transmitted e^-	0.001	0.001	0.000
Average energy of transmitted e^-	0.001 keV	0.000 keV	0.000 keV
Dose per molecule of methanol	0.56 ± 0.05	0.63 ± 0.05	2.5 ± 0.1
Dose per molecule of methylamine	0.58 ± 0.05	0.56 ± 0.05	2.6 ± 0.1

*average density with 0.779 g cm^{-3} for methanol and 0.732 g cm^{-3} for methylamine, with corrections made for isotopic labelling¹

Table S7. These structures and associated energies form the basis of the computational results that form the basis of the Discussion. These calculations represent an exploration of the potential energy surfaces of reactions [7]–[9]. ZPVE-corrected energy was calculated at the ω B97X-D/6-311G(d,p) level of theory and polarizable continuum model (PCM) calculations were used to calculate empirically-derived single-point energy corrections. The index of refraction and dielectric constants of liquid methanol,² solid methanol,³ and liquid methylamine⁴ were input as parameters for these calculations. Reaction molecules that serve a role as solvent are indicated with *italic* text. Transition states that were identified without ZPVE correction may not represent physical states but are provided for completeness, these are marked with an asterisk (*).

	Relative Energy			
	ω B97X-D/ 6-311G(d,p)	SCRF-PCM liquid methanol	SCRF-PCM solid methanol	SCRF-PCM liquid methylamine
$\dot{\text{C}}\text{H}_2\text{OH} \rightarrow \text{CH}_3\dot{\text{O}}$				
R1	0	0	0	0
TS1	158	160	159	160
P1	25	29	27	29
$\dot{\text{C}}\text{H}_2\text{OH} + \text{CH}_3\text{OH} \rightarrow \text{CH}_3\dot{\text{O}} + \text{CH}_3\text{OH}$				
R2	0	0	0	0
TS2	135	135	135	135
P2	36	42	40	41
$\dot{\text{C}}\text{H}_2\text{OH} + \text{CH}_3\text{NH}_2 \rightarrow \text{CH}_3\dot{\text{O}} + \text{CH}_3\text{NH}_2$ (1)				
R3	0	0	0	0
TS3	139	93	111	94
P3	50	57	55	57
$\dot{\text{C}}\text{H}_2\text{OH} + \text{CH}_3\text{NH}_2 \rightarrow \text{CH}_3\dot{\text{O}} + \text{CH}_3\text{NH}_2$ (2)				
R4	0	0	0	0
TS4	112	85	96	85
P4	50	57	55	57
$\dot{\text{C}}\text{H}_2\text{OH} + 2\text{CH}_3\text{OH} \rightarrow \text{CH}_3\dot{\text{O}} + 2\text{CH}_3\text{OH}$				
R5	0	0	0	0
TS5	88	80	83	80
P5	40	40	40	40
$\dot{\text{C}}\text{H}_2\text{OH} + \text{CH}_3\text{OH} + \text{CH}_3\text{NH}_2 \rightarrow \text{CH}_3\dot{\text{O}} + \text{CH}_3\text{OH} + \text{CH}_3\text{NH}_2$ (1)				
R6	0	0	0	0
TS6	81	66	72	66
P6	41	41	41	41
$\dot{\text{C}}\text{H}_2\text{OH} + \text{CH}_3\text{OH} + \text{CH}_3\text{NH}_2 \rightarrow \text{CH}_3\dot{\text{O}} + \text{CH}_3\text{OH} + \text{CH}_3\text{NH}_2$ (2)				
R7	0	0	0	0
TS7	70	40	52	42
P7	53	55	54	55
$\dot{\text{C}}\text{H}_2\text{OH} + \text{CH}_3\text{OH} + \text{CH}_3\text{NH}_2 \rightarrow \text{CH}_3\dot{\text{O}} + \text{CH}_3\text{OH} + \text{CH}_3\text{NH}_2$ (3)				
R8	0	0	0	0
TS8*	63	38	49	39

I8	68	40	52	41
TS9*	63	44	52	45
P9	52	55	54	54
$\dot{\text{C}}\text{H}_2\text{OH} + 2\text{CH}_3\text{NH}_2 \rightarrow \text{CH}_3\dot{\text{O}} + 2\text{CH}_3\text{NH}_2$				
R10	0	0	0	0
TS10	82	48	62	50
P10	53	55	54	56
$\dot{\text{C}}\text{H}_2\text{OH} + 3\text{CH}_3\text{OH} \rightarrow \text{CH}_3\dot{\text{O}} + 3\text{CH}_3\text{OH}$				
R11	0	0	0	0
TS11	78	70	73	72
P11	47	46	46	46
$\dot{\text{C}}\text{H}_2\text{OH} + 2\text{CH}_3\text{OH} + \text{CH}_3\text{NH}_2 \rightarrow \text{CH}_3\dot{\text{O}} + 2\text{CH}_3\text{OH} + \text{CH}_3\text{NH}_2$ (1)				
R12	0	0	0	0
TS12	78	70	73	70
P12	45	45	45	43
$\dot{\text{C}}\text{H}_2\text{OH} + 2\text{CH}_3\text{OH} + \text{CH}_3\text{NH}_2 \rightarrow \text{CH}_3\dot{\text{O}} + 2\text{CH}_3\text{OH} + \text{CH}_3\text{NH}_2$ (2)				
R13	0	0	0	0
TS13	65	51	57	52
P13	50	50	50	49
$\dot{\text{C}}\text{H}_2\text{OH} + 2\text{CH}_3\text{OH} + \text{CH}_3\text{NH}_2 \rightarrow \text{CH}_3\dot{\text{O}} + 2\text{CH}_3\text{OH} + \text{CH}_3\text{NH}_2$ (3)				
R14	0	0	0	0
TS14	61	39	49	39
I14	58	32	44	33
TS15*	52	36	44	36
P15	25	29	27	52
$\dot{\text{C}}\text{H}_2\text{OH} + \text{CH}_3\text{OH} + 2\text{CH}_3\text{NH}_2 \rightarrow \text{CH}_3\dot{\text{O}} + \text{CH}_3\text{OH} + 2\text{CH}_3\text{NH}_2$ (1)				
R16	0	0	0	0
TS16	66	46	55	47
I16	63	42	51	43
TS17	59	41	49	42
P17	51	51	51	51
$\dot{\text{C}}\text{H}_2\text{OH} + \text{CH}_3\text{OH} + 2\text{CH}_3\text{NH}_2 \rightarrow \text{CH}_3\dot{\text{O}} + \text{CH}_3\text{OH} + 2\text{CH}_3\text{NH}_2$ (2)				
R18	0	0	0	0
TS18*	54	31	41	32
I18	60	36	46	37
TS19	64	55	59	55
P19	44	47	46	47
$\dot{\text{C}}\text{H}_2\text{OH} + \text{CH}_3\text{OH} + 2\text{CH}_3\text{NH}_2 \rightarrow \text{CH}_3\dot{\text{O}} + \text{CH}_3\text{OH} + 2\text{CH}_3\text{NH}_2$ (3)				
R20	0	0	0	0
TS20	62	31	44	32
I20	57	28	41	29
TS21	52	35	43	37
P21	54	51	52	51
$\dot{\text{C}}\text{H}_2\text{OH} + 3\text{CH}_3\text{NH}_2 \rightarrow \text{CH}_3\dot{\text{O}} + 3\text{CH}_3\text{NH}_2$				
R22	0	0	0	0

TS22	68	42	53	42
I22	59	33	44	34
TS23	74	46	58	47
I23	65	29	52	43
TS24*	63	43	52	43
P24	53	54	54	53
$\dot{\text{C}}\text{H}_2\text{NH}_2 \rightarrow \text{CH}_3\dot{\text{N}}\text{H}$				
R25	0	0	0	0
TS25	183	181	182	182
P25	27	26	26	26
$\dot{\text{C}}\text{H}_2\text{NH}_2 + \text{CH}_3\text{OH} \rightarrow \text{CH}_3\dot{\text{N}}\text{H} + \text{CH}_3\text{OH}$				
R26	0	0	0	0
TS26	178	182	181	182
P26	21	25	23	25
$\dot{\text{C}}\text{H}_2\text{NH}_2 + \text{CH}_3\text{NH}_2 \rightarrow \text{CH}_3\dot{\text{N}}\text{H} + \text{CH}_3\text{NH}_2$				
R27	0	0	0	0
TS27	153	136	143	137
P27	36	38	37	39
$\dot{\text{C}}\text{H}_2\text{NH}_2 + 2\text{CH}_3\text{OH} \rightarrow \text{CH}_3\dot{\text{N}}\text{H} + 2\text{CH}_3\text{OH}$				
R28	0	0	0	0
TS28	107	103	104	104
P28	28	25	27	26
$\dot{\text{C}}\text{H}_2\text{NH}_2 + \text{CH}_3\text{OH} + \text{CH}_3\text{NH}_2 \rightarrow \text{CH}_3\dot{\text{N}}\text{H} + \text{CH}_3\text{OH} + \text{CH}_3\text{NH}_2$ (1)				
R29	0	0	0	0
TS29	113	100	105	99
P29	40	40	40	22
$\dot{\text{C}}\text{H}_2\text{NH}_2 + \text{CH}_3\text{OH} + \text{CH}_3\text{NH}_2 \rightarrow \text{CH}_3\dot{\text{N}}\text{H} + \text{CH}_3\text{OH} + \text{CH}_3\text{NH}_2$ (2)				
R30	0	0	0	0
TS30	107	89	97	90
P30	40	40	40	40
$\dot{\text{C}}\text{H}_2\text{NH}_2 + \text{CH}_3\text{OH} + \text{CH}_3\text{NH}_2 \rightarrow \text{CH}_3\dot{\text{N}}\text{H} + \text{CH}_3\text{OH} + \text{CH}_3\text{NH}_2$				
R31	0	0	0	0
TS31	152	118	133	120
P31	49	40	44	40
$\dot{\text{C}}\text{H}_2\text{NH}_2 + 2\text{CH}_3\text{NH}_2 \rightarrow \text{CH}_3\dot{\text{N}}\text{H} + 2\text{CH}_3\text{NH}_2$				
R32	0	0	0	0
TS32	124	105	113	105
P32	37	37	37	36
$\dot{\text{C}}\text{H}_2\text{NH}_2 + 3\text{CH}_3\text{OH} \rightarrow \text{CH}_3\dot{\text{N}}\text{H} + 3\text{CH}_3\text{OH}$				
R33	0	0	0	0
TS33	100	96	98	97
P33	30	25	27	25
$\dot{\text{C}}\text{H}_2\text{NH}_2 + 3\text{CH}_3\text{OH} \rightarrow \text{CH}_3\dot{\text{N}}\text{H} + 3\text{CH}_3\text{OH}$ (2)				
R34	0	0	0	0

TS34	105	109	107	109
P34	5	8	6	8
$\dot{\text{C}}\text{H}_2\text{NH}_2 + 2\text{CH}_3\text{OH} + \text{CH}_3\text{NH}_2 \rightarrow \text{CH}_3\dot{\text{N}}\text{H} + 2\text{CH}_3\text{OH} + \text{CH}_3\text{NH}_2$ (1)				
R35	0	0	0	0
TS35	102	82	91	83
P35	27	26	26	20
$\dot{\text{C}}\text{H}_2\text{NH}_2 + 2\text{CH}_3\text{OH} + \text{CH}_3\text{NH}_2 \rightarrow \text{CH}_3\dot{\text{N}}\text{H} + 2\text{CH}_3\text{OH} + \text{CH}_3\text{NH}_2$ (2)				
R36	0	0	0	0
TS36	99	84	90	86
P36	32	29	30	26
$\dot{\text{C}}\text{H}_2\text{NH}_2 + 2\text{CH}_3\text{OH} + \text{CH}_3\text{NH}_2 \rightarrow \text{CH}_3\dot{\text{N}}\text{H} + 2\text{CH}_3\text{OH} + \text{CH}_3\text{NH}_2$ (3)				
R37	0	0	0	0
TS37	87	72	78	72
P37	41	40	41	40
$\dot{\text{C}}\text{H}_2\text{NH}_2 + 2\text{CH}_3\text{OH} + \text{CH}_3\text{NH}_2 \rightarrow \text{CH}_3\dot{\text{N}}\text{H} + 2\text{CH}_3\text{OH} + \text{CH}_3\text{NH}_2$ (4)				
R38	0	0	0	0
TS38	91	72	79	72
P38	36	38	37	37
$\dot{\text{C}}\text{H}_2\text{NH}_2 + 2\text{CH}_3\text{OH} + \text{CH}_3\text{NH}_2 \rightarrow \text{CH}_3\dot{\text{N}}\text{H} + 2\text{CH}_3\text{OH} + \text{CH}_3\text{NH}_2$ (5)				
R39	0	0	0	0
TS39	90	81	85	81
P39	11	5	8	5
$\dot{\text{C}}\text{H}_2\text{NH}_2 + \text{CH}_3\text{OH} + 2\text{CH}_3\text{NH}_2 \rightarrow \text{CH}_3\dot{\text{N}}\text{H} + \text{CH}_3\text{OH} + 2\text{CH}_3\text{NH}_2$ (1)				
R40	0	0	0	0
TS40	119	96	106	96
I40	122	98	108	99
TS41	114	95	103	95
P41	27	26	26	21
$\dot{\text{C}}\text{H}_2\text{NH}_2 + \text{CH}_3\text{OH} + 2\text{CH}_3\text{NH}_2 \rightarrow \text{CH}_3\dot{\text{N}}\text{H} + \text{CH}_3\text{OH} + 2\text{CH}_3\text{NH}_2$ (2)				
R42	0	0	0	0
TS42	109	97	102	98
P42	35	34	35	34
$\dot{\text{C}}\text{H}_2\text{NH}_2 + \text{CH}_3\text{OH} + 2\text{CH}_3\text{NH}_2 \rightarrow \text{CH}_3\dot{\text{N}}\text{H} + \text{CH}_3\text{OH} + 2\text{CH}_3\text{NH}_2$ (3)				
R43	0	0	0	0
TS43	94	76	84	77
P43	45	43	44	44
$\dot{\text{C}}\text{H}_2\text{NH}_2 + \text{CH}_3\text{OH} + 2\text{CH}_3\text{NH}_2 \rightarrow \text{CH}_3\dot{\text{N}}\text{H} + \text{CH}_3\text{OH} + 2\text{CH}_3\text{NH}_2$				
R44	0	0	0	0
TS44	95	78	85	78
P44	24	27	26	25
$\dot{\text{C}}\text{H}_2\text{NH}_2 + 3\text{CH}_3\text{NH}_2 \rightarrow \text{CH}_3\dot{\text{N}}\text{H} + 3\text{CH}_3\text{NH}_2$				
R45	0	0	0	0
TS45	122	99	109	100
P45	37	37	37	37
$\dot{\text{C}}\text{H}_2\text{NH}_2 + 4\text{CH}_3\text{OH} \rightarrow \text{CH}_3\dot{\text{N}}\text{H} + 4\text{CH}_3\text{OH}$				

R46	0	0	0	0
TS46	103	102	102	103
P46	27	30	28	30
$\dot{\text{C}}\text{H}_2\text{NH}_2 + 3\text{CH}_3\text{OH} + \text{CH}_3\text{NH}_2 \rightarrow \text{CH}_3\dot{\text{N}}\text{H} + 3\text{CH}_3\text{OH} + \text{CH}_3\text{NH}_2$ (1)				
R47	0	0	0	0
TS47	91	77	83	78
P47	37	32	34	32
$\dot{\text{C}}\text{H}_2\text{NH}_2 + 3\text{CH}_3\text{OH} + \text{CH}_3\text{NH}_2 \rightarrow \text{CH}_3\dot{\text{N}}\text{H} + 3\text{CH}_3\text{OH} + \text{CH}_3\text{NH}_2$ (2)				
R48	0	0	0	0
TS48	89	73	80	73
P48	15	8	11	8
$\dot{\text{C}}\text{H}_2\text{NH}_2 + 3\text{CH}_3\text{OH} + \text{CH}_3\text{NH}_2 \rightarrow \text{CH}_3\dot{\text{N}}\text{H} + 3\text{CH}_3\text{OH} + \text{CH}_3\text{NH}_2$ (3)				
R49	0	0	0	0
TS49	85	64	73	65
P49	44	46	46	46
$\dot{\text{C}}\text{H}_2\text{NH}_2 + 2\text{CH}_3\text{OH} + 2\text{CH}_3\text{NH}_2 \rightarrow \text{CH}_3\dot{\text{N}}\text{H} + 2\text{CH}_3\text{OH} + 2\text{CH}_3\text{NH}_2$ (1)				
R50	0	0	0	0
TS50	97	69	81	71
P50	50	47	48	47
$\dot{\text{C}}\text{H}_2\text{NH}_2 + 2\text{CH}_3\text{OH} + 2\text{CH}_3\text{NH}_2 \rightarrow \text{CH}_3\dot{\text{N}}\text{H} + 2\text{CH}_3\text{OH} + 2\text{CH}_3\text{NH}_2$ (2)				
R51	0	0	0	0
TS51	92	82	86	82
P51	35	34	34	34
$\dot{\text{C}}\text{H}_2\text{NH}_2 + 2\text{CH}_3\text{OH} + 2\text{CH}_3\text{NH}_2 \rightarrow \text{CH}_3\dot{\text{N}}\text{H} + 2\text{CH}_3\text{OH} + 2\text{CH}_3\text{NH}_2$ (3)				
R52	0	0	0	0
TS52	63	55	58	55
I52	55	46	49	46
TS53	60	54	56	55
P53	11	7	9	8
$\dot{\text{C}}\text{H}_2\text{NH}_2 + \text{CH}_3\text{OH} + 3\text{CH}_3\text{NH}_2 \rightarrow \text{CH}_3\dot{\text{N}}\text{H} + \text{CH}_3\text{OH} + 3\text{CH}_3\text{NH}_2$				
R54	0	0	0	0
TS54	93	76	83	77
I54	98	78	86	79
TS55	98	79	87	80
P55	27	30	29	29
$\text{CH}_3\dot{\text{N}}\text{H} + \text{CH}_3\text{OH} \rightarrow \text{CH}_3\dot{\text{O}} + \text{CH}_3\text{NH}_2$				
R56	0	0	0	0
TS56	48	49	50	50
P56	32	35	34	35
$\text{CH}_3\dot{\text{N}}\text{H} + \text{CH}_3\text{OH} + \text{CH}_3\text{OH} \rightarrow \text{CH}_3\dot{\text{O}} + \text{CH}_3\text{NH}_2 + \text{CH}_3\text{OH}$				
R57	0	0	0	0
TS57	90	84	87	85
P57	39	42	41	42
$\text{CH}_3\dot{\text{N}}\text{H} + \text{CH}_3\text{OH} + \text{CH}_3\text{NH}_2 \rightarrow \text{CH}_3\dot{\text{O}} + \text{CH}_3\text{NH}_2 + \text{CH}_3\text{NH}_2$				

R58	0	0	0	0
TS58	111	105	108	106
P58	43	50	47	50
$\text{CH}_3\dot{\text{N}}\text{H} + \text{CH}_3\text{OH} + 2\text{CH}_3\text{OH} \rightarrow \text{CH}_3\dot{\text{O}} + \text{CH}_3\text{NH}_2 + 2\text{CH}_3\text{OH}$				
R59	0	0	0	0
TS59	81	68	74	68
P59	37	33	35	33
$\text{CH}_3\dot{\text{N}}\text{H} + \text{CH}_3\text{OH} + \text{CH}_3\text{OH} + \text{CH}_3\text{NH}_2 \rightarrow \text{CH}_3\dot{\text{O}} + \text{CH}_3\text{NH}_2 + \text{CH}_3\text{OH} + \text{CH}_3\text{NH}_2$ (1)				
R60	0	0	0	0
TS60	98	90	93	92
P60	43	43	43	45
$\text{CH}_3\dot{\text{N}}\text{H} + \text{CH}_3\text{OH} + \text{CH}_3\text{OH} + \text{CH}_3\text{NH}_2 \rightarrow \text{CH}_3\dot{\text{O}} + \text{CH}_3\text{NH}_2 + \text{CH}_3\text{OH} + \text{CH}_3\text{NH}_2$ (2)				
R61	0	0	0	0
TS61	93	78	85	79
P61	42	44	44	43
$\text{CH}_3\dot{\text{N}}\text{H} + \text{CH}_3\text{OH} + 2\text{CH}_3\text{NH}_2 \rightarrow \text{CH}_3\dot{\text{O}} + \text{CH}_3\text{NH}_2 + 2\text{CH}_3\text{NH}_2$				
R62	0	0	0	0
TS62	89	73	80	75
I62	94	76	83	79
TS63	106	92	98	92
P63	49	49	49	50
$\text{CH}_3\dot{\text{N}}\text{H} + \text{CH}_3\text{OH} + \text{CH}_3\text{NH}_2 + 2\text{CH}_3\text{OH} \rightarrow \text{CH}_3\dot{\text{O}} + \text{CH}_3\text{NH}_2 + \text{CH}_3\text{NH}_2 + 2\text{CH}_3\text{OH}$				
R64	0	0	0	0
TS64	96	83	89	85
P64	43	44	44	45

Table S8. Cartesian coordinates (Å) and vibrational frequencies (cm⁻¹) of all structures listed in Table S7.

R1

Cartesian coordinates

C	0.680560	0.027688	-0.067946
O	-0.667746	-0.124655	0.024302
H	1.118455	0.989503	0.181386
H	1.227553	-0.888964	0.103269
H	-1.087401	0.730572	-0.071392

Vibrational frequencies

442.1865	604.2929	1080.2675
1242.3323	1379.3581	1503.5482
3133.7153	3278.7155	3927.8599

TS1

Cartesian coordinates

C	-0.631687	-0.000013	0.013857
O	0.740307	-0.000096	-0.088837
H	-1.157227	-0.938026	-0.172266
H	-1.157749	0.937387	-0.173998
H	0.182637	0.001485	0.973817

Vibrational frequencies

-2065.0152	744.4136	986.8042
1158.7083	1195.4448	1498.2655
2499.9685	3057.9681	3169.9566

P1

Cartesian coordinates

C	0.571193	-0.000001	-0.013495
O	-0.788333	0.000001	-0.007834
H	1.006571	0.908545	-0.455213
H	1.006551	-0.908605	-0.455112
H	0.866387	0.000060	1.053965

Vibrational frequencies

824.5846	977.1160	1141.6066
1380.8309	1383.4200	1532.4628
2925.9776	2997.9437	3039.1324

R2

Cartesian coordinates

C	1.881562	0.472731	0.336666
O	1.421732	-0.513591	-0.466180
H	1.160619	1.071764	0.888611
H	2.824804	0.902864	0.026639
H	-1.322100	-0.488309	1.320097

C	-1.762881	0.502681	-0.308120
O	-1.194887	-0.605024	0.378433
H	-2.842855	0.565138	-0.141607
H	-1.580571	0.339549	-1.369460
H	-1.290951	1.447934	-0.018187
H	0.524217	-0.742487	-0.175393

Vibrational frequencies

55.1231	68.9894	75.8942
137.6280	228.4415	258.9257
405.1742	565.0619	817.2510
1076.7662	1095.3891	1121.8374
1187.0688	1263.4005	1377.1538
1458.1435	1495.4630	1498.7145
1505.4970	1513.4440	3025.5228
3093.5463	3106.2663	3154.5274
3252.5129	3683.7787	3929.1317

TS2

Cartesian coordinates

C	1.484427	-0.580316	-0.029513
O	1.336113	0.674839	0.296729
H	1.266579	-1.354778	0.729349
H	2.279624	-0.851794	-0.736181
H	0.103834	-0.554039	-0.661735
C	-1.795606	-0.170274	0.311805
O	-0.785015	0.234787	-0.613614
H	-2.430903	-0.907597	-0.177162
H	-2.390419	0.704071	0.576033
H	-1.348018	-0.597155	1.213633
H	-0.022416	0.787821	-0.102617

Vibrational frequencies

-1422.2347	85.1405	128.9091
144.0585	331.3063	472.3898
539.9789	1035.1137	1068.7716
1076.4589	1139.2984	1195.0485
1205.0120	1290.1777	1328.1948
1440.6504	1483.1716	1501.0412
1512.9094	1524.0039	1625.1270
2323.8088	2922.4800	3044.8942
3057.5906	3143.8353	3170.0481

P2

Cartesian coordinates

C	1.768081	0.513842	0.207401
O	1.462907	-0.647520	-0.439070
H	1.501957	1.316784	-0.508900

H	2.839120	0.617653	0.422346
H	1.135086	0.679451	1.089515
C	-1.908998	0.319947	-0.349302
O	-1.192433	-0.402544	0.623579
H	-2.762740	0.784808	0.146658
H	-2.291786	-0.323027	-1.153066
H	-1.309270	1.120316	-0.807731
H	-0.430661	-0.798206	0.186509

Vibrational frequencies

45.6333	76.4663	101.4886
111.2856	158.4893	198.7230
643.8409	877.6154	990.6086
1106.2644	1127.3481	1134.3025
1184.6464	1376.6696	1383.7744
1438.5421	1496.7191	1499.2957
1513.2914	1517.4900	2921.6341
2983.1724	3012.3125	3035.7190
3071.0143	3120.6644	3815.6545

R3

Cartesian coordinates

C	-1.885083	-0.474086	0.309443
O	-1.389742	0.485365	-0.500302
H	-2.927120	-0.716281	0.140554
H	-1.461967	-0.580321	1.307228
H	-0.476446	0.691344	-0.200519
N	1.248616	0.630734	0.325004
C	1.680006	-0.650568	-0.243034
H	1.809962	1.392085	-0.037405
H	1.363398	0.633534	1.331471
H	1.030110	-1.441432	0.136019
H	2.722253	-0.909710	-0.022765
H	1.547898	-0.619358	-1.325655

Vibrational frequencies

64.7151	85.8368	103.3203
180.8396	251.9823	269.8432
422.6109	611.5160	874.4362
984.7830	998.9286	1078.2979
1143.1628	1195.5195	1270.6455
1350.2142	1472.5526	1495.4224
1507.6233	1518.6667	1535.8977
1670.9563	3024.2540	3093.4711
3109.9983	3141.0450	3236.9349
3425.8838	3551.1800	3629.1766

TS3

Cartesian coordinates

C	-1.735228	0.146967	0.435345
O	-1.198687	-0.451708	-0.608134
H	-1.849228	-0.413270	1.381112
H	-2.513574	0.912755	0.275832
H	-0.090605	0.585511	0.019206
N	0.998261	0.735727	-0.129743
C	1.627070	-0.558879	0.212305
H	1.102599	0.947996	-1.118121
H	1.358106	1.508196	0.421896
H	1.463842	-0.738666	1.273550
H	2.692959	-0.552001	-0.014156
H	1.086519	-1.315476	-0.351943

Vibrational frequencies

-656.2659	58.8112	154.5854
166.5056	256.5371	298.8334
408.1562	849.8246	920.5755
968.4600	1041.4234	1182.2465
1221.6584	1260.4577	1331.8456
1388.0413	1442.0635	1501.8199
1518.1403	1529.4922	1572.6860
1648.0779	2177.7062	2911.1860
2967.1961	3085.4000	3180.7699
3199.3028	3528.6600	3609.6044

P3**Cartesian coordinates**

C	-1.694177	0.458784	0.330903
O	-1.664285	-0.659606	-0.426944
H	-1.823628	0.257971	1.406922
H	-2.404967	1.220649	-0.024944
H	-0.663713	0.890050	0.229402
N	1.434710	0.718945	-0.233702
C	1.628338	-0.647437	0.249935
H	1.362384	0.727775	-1.244145
H	2.221094	1.306264	0.013961
H	1.752858	-0.628406	1.335093
H	2.492814	-1.167431	-0.184069
H	0.729502	-1.230719	0.034225

Vibrational frequencies

46.4486	75.8275	107.2238
169.9919	193.2741	244.8811
369.1165	870.4695	959.7876
993.9404	1032.2139	1084.9099
1164.6886	1185.9957	1351.6319
1372.0265	1386.3773	1472.6031

1508.8047	1523.1633	1529.4453
1669.2902	2745.2003	2963.1284
3005.1296	3017.7209	3088.2635
3125.3863	3546.6869	3629.7703

R4

Cartesian coordinates

C	-1.885256	-0.474071	0.309431
O	-1.389779	0.485298	-0.500330
H	-2.927318	-0.716145	0.140527
H	-1.462162	-0.580349	1.307219
H	1.363371	0.633543	1.331485
C	1.680218	-0.650512	-0.243011
N	1.248593	0.630714	0.325017
H	2.722528	-0.909436	-0.022783
H	1.548055	-0.619356	-1.325626
H	1.030509	-1.441504	0.136093
H	-0.476474	0.691200	-0.200524
H	1.809804	1.392163	-0.037395

Vibrational frequencies

64.6661	85.7734	103.2940
180.8267	252.1121	269.8398
422.6147	611.4666	874.4420
984.7880	998.9327	1078.3015
1143.1637	1195.5199	1270.6468
1350.2151	1472.5574	1495.4229
1507.6242	1518.6760	1535.8974
1670.9571	3024.2534	3093.4766
3110.0113	3141.0623	3236.9387
3425.9117	3551.1779	3629.1737

TS4

Cartesian coordinates

C	1.592296	-0.193438	0.480673
O	1.331712	0.536197	-0.556327
H	1.747978	0.294285	1.460469
H	2.178503	-1.125435	0.358198
H	0.046548	-0.775647	0.432173
C	-1.750734	0.429090	0.257564
N	-0.884098	-0.635121	-0.264800
H	-2.249636	0.090395	1.165306
H	-2.492649	0.727567	-0.483702
H	-1.101624	1.274529	0.483211
H	-0.270969	-0.259618	-1.015460
H	-1.372533	-1.483717	-0.525406

Vibrational frequencies

-487.8271	67.7433	136.5311
206.2690	335.4159	403.3517
497.5324	826.0918	971.0424
988.0047	1068.7857	1072.7036
1209.3341	1279.2558	1325.2482
1354.9444	1453.9934	1501.6496
1511.8973	1520.8122	1534.8978
1601.2182	1814.5794	2888.4601
2945.0697	3075.4280	3162.1387
3177.4298	3212.8492	3596.9275

P4

Cartesian coordinates

C	-1.693768	0.458572	0.331400
O	-1.664474	-0.659087	-0.427550
H	-1.821645	0.256655	1.407407
H	-2.405354	1.220491	-0.022726
H	-0.663575	0.890270	0.228970
C	1.628039	-0.647442	0.250166
N	1.434722	0.718799	-0.234004
H	1.752467	-0.628021	1.335330
H	2.492455	-1.167766	-0.183560
H	0.729094	-1.230611	0.034600
H	1.362461	0.727246	-1.244456
H	2.221209	1.306062	0.013467

Vibrational frequencies

46.6227	75.8675	107.3826
170.0968	193.3964	244.9995
369.1223	870.4922	959.6876
993.9404	1032.3258	1084.9015
1164.6989	1186.0095	1351.6340
1372.0192	1386.4036	1472.6118
1508.8186	1523.1496	1529.4608
1669.2977	2745.1948	2963.1152
3005.1414	3017.7191	3088.2698
3125.3854	3546.6799	3629.7604

R5

Cartesian coordinates

O	-0.652255	1.939933	-0.264836
C	0.611914	2.070012	0.177726
H	0.852211	1.675690	1.165162
H	1.109828	2.969732	-0.164959
C	-2.303057	-1.204083	-0.156114
O	-1.272022	-0.552450	0.563952
H	-3.256127	-0.835381	0.224752

H	-2.268183	-2.288743	-0.006785
H	-2.249154	-0.992532	-1.230379
H	-1.038286	1.127407	0.126324
H	-0.414829	-0.852940	0.211957
C	2.333653	-1.179647	0.197304
O	1.210045	-0.786449	-0.571092
H	3.270906	-0.958389	-0.324196
H	2.266811	-2.257812	0.344140
H	2.349544	-0.692618	1.179547
H	1.236064	0.179625	-0.663251

Vibrational frequencies

32.1877	55.2849	84.6558
94.4739	106.4038	116.1686
130.3328	138.3354	188.5327
244.8533	274.7482	328.2303
647.5621	795.6241	797.5125
942.9200	1090.4097	1099.7931
1129.3233	1138.2841	1162.8608
1187.6102	1189.0557	1278.5705
1431.2144	1460.3095	1489.5706
1491.3181	1497.2525	1500.7519
1503.3203	1517.5128	1521.5501
1534.6006	3016.7764	3018.1290
3080.8041	3082.0682	3086.8515
3134.3150	3140.0635	3230.2610
3469.9384	3617.6562	3667.5809

TS5

Cartesian coordinates

O	-0.611385	1.762798	0.033518
C	0.687910	1.888674	-0.020947
H	1.256651	1.827166	0.927487
H	1.088792	2.627804	-0.728191
C	-2.217272	-0.957621	-0.222281
O	-1.083020	-0.571647	0.544728
H	-3.130804	-0.699665	0.317367
H	-2.187793	-2.038400	-0.369835
H	-2.222100	-0.455485	-1.194457
H	-0.999436	0.482860	0.506251
H	0.032114	-0.767028	-0.067259
C	2.080864	-1.215333	0.216249
O	1.036364	-0.648590	-0.573297
H	3.032555	-1.049217	-0.288775
H	1.904757	-2.287201	0.307600
H	2.109402	-0.764476	1.212561
H	1.071180	0.488839	-0.500475

Vibrational frequencies

-1093.0690	71.3562	88.8665
120.7971	123.4599	155.4167
166.2109	186.1781	219.9459
408.0759	440.9442	492.6839
631.2741	1032.1853	1073.4727
1094.2925	1105.8199	1165.2542
1172.2723	1173.4671	1211.4015
1216.9611	1265.6048	1354.9373
1395.7326	1475.4659	1478.1134
1501.0651	1502.7225	1508.3926
1517.7863	1521.1173	1570.7896
1606.7885	1631.9907	1864.4694
2239.6178	2903.3052	3028.2982
3047.0603	3053.6308	3123.4319
3137.3722	3142.4890	3161.0042

P5**Cartesian coordinates**

O	-0.740724	1.994317	-0.047175
C	0.604330	2.142223	0.032189
H	0.970786	1.996486	1.061963
H	0.975026	3.076552	-0.405585
C	-2.330107	-1.177957	-0.167501
O	-1.166133	-0.704051	0.484573
H	-3.235036	-0.925171	0.396174
H	-2.253985	-2.264248	-0.225737
H	-2.423124	-0.778971	-1.184173
H	-1.196609	0.264791	0.498871
H	0.424352	-0.913179	-0.353191
C	2.213665	-1.229969	0.312288
O	1.327439	-0.801624	-0.696561
H	3.230228	-1.148656	-0.077118
H	2.038943	-2.275153	0.595683
H	2.142379	-0.614958	1.220942
H	1.035050	1.267590	-0.516389

Vibrational frequencies

37.8517	50.2207	66.6893
92.5371	103.3078	113.4119
119.6428	123.0300	187.3136
222.9206	248.2718	253.3970
637.7155	820.8669	899.8883
1074.1936	1097.9673	1106.7654
1139.7922	1143.8680	1186.9882
1187.5582	1195.6656	1354.5794
1403.2744	1457.2909	1472.3663

1492.9480	1495.5034	1500.7311
1502.1523	1516.5648	1519.4400
1524.8298	2778.8748	2970.8241
2991.4034	3017.3121	3050.3929
3065.4580	3079.6416	3119.3828
3135.8280	3631.3270	3706.1852

R6

Cartesian coordinates

O	-0.688812	1.883279	-0.268910
C	0.580395	2.019188	0.147245
H	0.843971	1.627058	1.130984
H	1.076016	2.917213	-0.204752
C	-2.421001	-1.146214	-0.279531
N	-1.405180	-0.581613	0.611618
H	-3.389672	-0.687100	-0.071261
H	-2.526685	-2.234444	-0.196727
H	-2.155186	-0.906394	-1.310530
H	-1.066165	1.059397	0.143407
H	-1.621240	-0.788670	1.578936
H	-0.492269	-0.983894	0.398096
C	2.539716	-1.043697	0.171093
O	1.333725	-0.842044	-0.534713
H	3.409212	-0.689472	-0.395547
H	2.651697	-2.117061	0.331018
H	2.537154	-0.546071	1.149990
H	1.215466	0.115187	-0.638794

Vibrational frequencies

29.6721	53.0083	74.1291
91.1772	100.4201	113.2549
143.1284	158.6574	176.2921
206.4635	297.2229	323.6157
505.4483	673.9580	783.2916
964.7076	1015.1015	1068.7128
1087.8824	1102.2021	1126.6812
1161.7677	1186.1366	1210.5264
1286.3321	1373.3286	1435.5581
1467.9781	1492.4142	1497.7172
1499.2970	1507.3803	1519.1668
1524.2017	1566.4907	1688.8160
3002.1778	3022.6288	3059.9487
3069.3513	3101.7708	3127.6175
3136.0135	3180.5896	3222.0309
3474.3465	3606.5718	3670.0898

TS6

Cartesian coordinates

O	-0.513201	1.850265	0.234697
C	0.733020	1.842224	-0.146736
H	1.510785	1.964379	0.635854
H	0.979980	2.387748	-1.075352
C	-2.252492	-0.797070	-0.400968
N	-1.170647	-0.679783	0.588966
H	-3.226719	-0.586732	0.043962
H	-2.257316	-1.796988	-0.836316
H	-2.058669	-0.062933	-1.181642
H	-1.061171	0.326729	0.841500
H	-1.338427	-1.247409	1.411398
H	-0.073522	-0.862259	0.042049
C	2.106438	-1.193023	0.196418
O	1.011115	-0.730665	-0.560843
H	3.021795	-0.679207	-0.112845
H	2.247152	-2.265693	0.031946
H	1.968996	-1.020000	1.273919
H	0.976540	0.531262	-0.480352

Vibrational frequencies

-1210.0113	69.1262	95.2585
113.5265	121.9493	144.6708
167.9400	176.8844	211.8117
344.5674	442.2057	519.6796
556.9470	660.2299	887.5590
1012.6190	1075.6385	1080.7293
1104.0699	1132.3862	1180.8147
1197.9695	1221.9425	1298.8182
1320.9286	1348.8874	1363.8854
1468.3737	1475.5389	1505.9071
1509.0575	1511.7175	1518.5960
1526.5611	1531.3352	1630.1218
1683.5220	1806.2369	2872.4598
2957.9672	2994.4841	3067.7269
3071.1551	3101.2712	3110.6850
3150.6048	3174.0056	3591.7205

P6**Cartesian coordinates**

O	-0.963409	1.915979	0.169428
C	0.334838	2.180043	-0.102210
H	0.939351	2.332469	0.806891
H	0.482761	2.990453	-0.829365
C	-2.147348	-1.220939	-0.391774
N	-1.098607	-1.006314	0.608559
H	-3.165634	-1.148030	0.009008

H	-2.022873	-2.205406	-0.847726
H	-2.038757	-0.471910	-1.177819
H	-1.180106	-0.063994	0.982069
H	-1.201412	-1.655489	1.379060
H	0.509925	-0.951156	-0.239268
C	2.380346	-0.897338	0.276463
O	1.362216	-0.737526	-0.679830
H	3.338381	-0.697362	-0.208120
H	2.413507	-1.918437	0.679795
H	2.276680	-0.201445	1.123304
H	0.740954	1.236283	-0.549406

Vibrational frequencies

33.2396	56.7988	70.4919
81.8638	96.6339	108.6827
129.5328	150.8236	171.6577
200.1370	246.6499	271.4251
450.7191	901.8783	918.8480
965.6867	1042.2466	1060.3726
1084.2380	1111.5139	1153.4595
1171.3179	1186.0954	1203.5153
1361.9856	1369.4545	1392.3026
1468.4106	1488.9518	1501.0958
1501.7400	1507.2455	1521.6699
1525.2109	1554.2633	1667.5216
2760.3991	2969.0479	2976.4612
3021.7356	3031.4782	3038.8479
3101.2594	3111.0952	3138.3183
3416.9881	3515.3334	3611.4160

R7

Cartesian coordinates

O	-0.273140	1.719880	0.631164
C	-1.152105	2.024191	-0.352740
H	-0.798247	2.007834	-1.379695
H	-1.944402	2.699269	-0.054326
C	2.632891	-0.456151	0.006384
O	1.377277	-0.076557	-0.513139
H	3.358024	0.311057	-0.269520
H	2.969905	-1.411257	-0.414359
H	2.621855	-0.541466	1.100983
H	0.462925	1.209189	0.233663
C	-1.883286	-1.539605	-0.387534
N	-0.799500	-1.351973	0.581024
H	-2.859550	-1.733434	0.072993
H	-1.640882	-2.372768	-1.050693
H	-1.965492	-0.634020	-0.991775

H	-0.740543	-2.141820	1.212176
H	0.696786	-0.721660	-0.209002
H	-0.981982	-0.524310	1.141525

Vibrational frequencies

50.9783	63.2854	77.3629
97.7202	110.5978	116.0586
119.3723	141.3224	178.9094
248.3438	267.5297	299.4998
457.7931	621.9996	827.9486
927.3538	993.2764	1074.6559
1083.6693	1114.6373	1136.5100
1173.0065	1188.2183	1202.9575
1258.8960	1362.7959	1464.7935
1483.3686	1491.0541	1497.4493
1502.8965	1506.4452	1513.0326
1525.1137	1550.1535	1669.3321
3001.1163	3020.1292	3060.2909
3098.5188	3117.0365	3124.3347
3135.2137	3253.3902	3359.3018
3509.4828	3527.3391	3615.9942

TS7

Cartesian coordinates

O	0.915396	1.573786	0.308860
C	-0.120536	2.164950	-0.242487
H	-0.294131	2.034066	-1.322982
H	-0.420332	3.136081	0.165051
C	2.060141	-1.431391	0.094384
O	1.011965	-0.692667	-0.479387
H	3.014246	-1.196815	-0.391524
H	1.873971	-2.502812	-0.037142
H	2.174110	-1.229837	1.169644
H	1.100307	0.386676	-0.199955
C	-2.416148	-0.974193	-0.215788
N	-1.295436	-0.342024	0.494035
H	-3.366316	-0.539313	0.095444
H	-2.423286	-2.046733	-0.022842
H	-2.276568	-0.808423	-1.283211
H	-1.351802	-0.454258	1.501325
H	-0.300104	-0.691653	0.127608
H	-1.221674	0.702042	0.287898

Vibrational frequencies

-502.4634	59.9112	72.3923
126.6068	134.7274	150.9148
167.4936	183.7921	207.9531
305.5610	355.3340	445.9284

661.7369	813.1016	887.3183
992.1059	1051.8128	1077.6120
1126.3487	1191.8206	1199.1621
1208.9459	1248.8371	1323.0731
1337.7208	1424.3572	1464.2912
1494.6780	1504.5147	1512.2652
1516.0285	1520.9001	1545.1117
1638.5204	1669.2380	1698.1129
1834.2391	2107.1363	2717.7478
2960.4714	2993.5943	3056.6743
3076.3092	3079.6125	3081.6351
3164.9526	3174.5762	3573.6759

P7

Cartesian coordinates

O	1.079803	1.777954	0.087186
C	-0.189111	2.196670	-0.049280
H	-0.517176	2.263124	-1.100619
H	-0.428226	3.108370	0.515769
C	2.222302	-1.423127	0.241884
O	1.218460	-0.910160	-0.608262
H	3.228184	-1.174883	-0.118046
H	2.124391	-2.510212	0.252000
H	2.123805	-1.054736	1.271214
H	1.291195	0.056544	-0.590846
C	-2.637418	-0.889895	-0.287833
N	-1.520758	-0.514595	0.572501
H	-3.561884	-0.443167	0.086467
H	-2.793733	-1.973291	-0.378125
H	-2.463447	-0.494393	-1.291286
H	-1.653463	-0.863444	1.513504
H	-0.644651	-0.895722	0.214419
H	-0.820431	1.339732	0.358019

Vibrational frequencies

29.1891	34.8131	66.5938
76.2384	103.1824	115.9559
123.3590	150.9049	180.7537
200.3534	249.4837	303.5092
505.7900	720.9612	930.0756
961.1857	1027.9217	1094.8940
1101.9292	1108.3414	1137.1505
1185.2382	1186.6350	1200.5998
1351.3852	1363.3423	1391.7088
1464.6536	1466.3449	1493.5603
1499.2710	1504.1882	1518.4405
1523.4326	1525.8008	1698.1787

2512.2246	2955.4280	3003.7252
3005.8528	3036.5179	3060.5054
3084.6180	3121.0842	3121.7358
3463.9398	3606.8995	3691.7548

R8

Cartesian coordinates

O	0.068898	1.727410	-0.679443
C	0.011310	2.014915	0.636712
H	-0.448097	2.968570	0.867150
H	0.797421	1.627777	1.282901
C	2.271106	-0.994158	0.208819
O	1.151663	-0.732660	-0.607948
H	3.147680	-0.548809	-0.264484
H	2.449855	-2.071040	0.314641
H	2.164802	-0.559702	1.212259
H	0.578000	0.895800	-0.790650
H	0.336229	-1.022580	-0.132848
C	-2.245120	-0.758386	-0.397126
N	-1.260958	-0.981114	0.668222
H	-3.257853	-0.558108	-0.028047
H	-2.279144	-1.633430	-1.049351
H	-1.917427	0.096430	-0.990505
H	-1.558888	-1.726366	1.286057
H	-1.174135	-0.132966	1.224012

Vibrational frequencies

63.2789	85.1446	92.1919
105.2162	114.6375	121.8057
140.0557	166.4560	187.8535
256.9972	281.2314	307.8201
443.1713	693.7183	876.5310
947.7801	992.1405	1055.4085
1078.3350	1110.8746	1140.9603
1174.3696	1188.8945	1206.3294
1271.1680	1362.7247	1468.3073
1481.6061	1492.2733	1499.2518
1501.4582	1509.8462	1515.2265
1529.1866	1558.8544	1655.8165
2997.2239	3024.0344	3057.1303
3096.6759	3104.5183	3122.9571
3144.9548	3237.2785	3333.8958
3490.6806	3498.9331	3606.4100

TS8

Cartesian coordinates

O	0.065587	1.418977	-0.717424
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C	-0.106964	1.906524	0.494233
H	-0.701296	2.819568	0.589089
H	0.702049	1.789425	1.232099
C	2.290568	-0.771509	0.186353
O	1.063692	-0.751475	-0.498197
H	2.975705	-0.018599	-0.219366
H	2.764366	-1.752646	0.077548
H	2.173422	-0.566801	1.262623
H	0.719184	0.307346	-0.674203
H	-0.139378	-0.968317	0.252948
C	-2.161262	-0.796102	-0.383386
N	-1.152660	-0.774554	0.695776
H	-3.150715	-0.567509	0.012407
H	-2.165307	-1.775974	-0.859189
H	-1.859782	-0.033828	-1.101169
H	-1.377913	-1.399640	1.461993
H	-1.039995	0.215358	1.036563

Vibrational frequencies

-600.4664	75.6845	116.9184
127.3385	144.7849	163.8871
185.7934	215.3856	235.2418
281.7822	347.5609	461.8174
639.9773	789.7120	854.0741
1003.4657	1049.7471	1057.6428
1120.6781	1191.8062	1197.9998
1202.9889	1265.8033	1328.8463
1344.7050	1442.7307	1477.8336
1488.3885	1504.7124	1508.5083
1512.7372	1523.8482	1542.0761
1616.7131	1634.4324	1697.3369
1779.5359	2068.8447	2935.3131
2970.8142	2975.4705	3049.5091
3079.0851	3083.9323	3094.0907
3172.9140	3180.9974	3581.4167

I8

Cartesian coordinates

O	-0.124588	1.390631	-0.728287
C	-0.433629	1.839227	0.458565
H	-1.228662	2.595371	0.538271
H	0.366313	1.947330	1.214363
C	2.504413	-0.506033	0.189312
O	1.258768	-0.715277	-0.434848
H	3.192222	0.034182	-0.470846
H	2.948227	-1.477853	0.419591
H	2.412282	0.064711	1.124038

H	0.850862	0.186941	-0.662564
H	-0.164672	-1.047477	0.401487
C	-2.081544	-0.972912	-0.421212
N	-1.146221	-0.824091	0.713349
H	-3.093899	-0.737990	-0.094435
H	-2.038588	-1.988104	-0.813817
H	-1.759995	-0.253482	-1.174298
H	-1.411460	-1.369461	1.526509
H	-1.057970	0.249948	0.943347

Vibrational frequencies

57.0503	98.9924	113.1393
127.4363	157.3322	168.6969
199.9348	209.4864	229.5870
333.3795	355.2004	370.7985
607.5883	920.6599	996.0495
1039.6191	1052.3212	1108.0524
1139.9825	1176.5768	1193.9871
1209.5448	1276.0252	1326.0644
1344.6886	1449.1394	1485.8762
1499.1787	1504.0351	1507.6973
1518.0552	1521.7633	1551.2460
1586.2768	1634.8540	1698.7393
2205.1631	2776.0886	2914.4919
2961.4794	3005.7101	3016.3161
3062.4903	3072.7534	3105.9118
3170.6516	3172.5956	3579.8890

TS9

Cartesian coordinates

O	-0.104425	1.462225	-0.729745
C	-0.520074	1.751532	0.469462
H	-1.355428	2.465495	0.566565
H	0.234186	1.854817	1.275301
C	2.575973	-0.481463	0.179688
O	1.304325	-0.707137	-0.382628
H	3.278576	-0.082830	-0.561893
H	2.969368	-1.435572	0.538392
H	2.539265	0.218100	1.025798
H	0.916461	0.171130	-0.647121
C	-2.064209	-1.009027	-0.467377
N	-1.211618	-0.816358	0.715711
H	-3.096288	-0.759811	-0.220508
H	-2.009428	-2.034604	-0.834734
H	-1.702762	-0.319905	-1.232032
H	-0.236338	-1.092953	0.503013
H	-1.556484	-1.289124	1.543167

H -1.049142 0.412798 0.842427

Vibrational frequencies

-547.8941	57.2576	92.3570
110.2772	116.4889	141.9233
164.5406	194.0990	217.4070
302.6939	372.9334	415.8395
573.1430	646.4295	994.3323
1020.8897	1055.8406	1064.3793
1067.9937	1115.0763	1170.4674
1195.2119	1217.4947	1262.8584
1335.9151	1351.1358	1470.2995
1492.2571	1499.3950	1503.3365
1507.6304	1518.0055	1524.5774
1527.2508	1561.7406	1611.4721
1671.3492	2884.6130	2977.9082
2999.0973	3059.4712	3066.0307
3107.2001	3154.5914	3158.9154
3166.4103	3258.6841	3592.1235

P9

Cartesian coordinates

O	0.027575	1.610693	-0.747503
C	-0.244816	1.859289	0.541986
H	-0.862805	2.752091	0.712414
H	0.644035	1.838065	1.195364
C	2.515344	-0.688294	0.209509
O	1.286032	-0.867719	-0.456633
H	3.272016	-0.231191	-0.440030
H	2.877962	-1.672749	0.510456
H	2.415887	-0.069980	1.112629
H	0.973964	0.004173	-0.746486
C	-2.183554	-0.856138	-0.491586
N	-1.428740	-0.888432	0.756320
H	-3.214553	-0.555531	-0.291902
H	-2.196764	-1.811213	-1.031059
H	-1.740328	-0.104711	-1.153137
H	-0.484625	-1.227370	0.578718
H	-1.871539	-1.479788	1.447048
H	-0.842771	0.944304	0.885388

Vibrational frequencies

31.2886	75.5315	76.4864
96.1088	112.6174	132.3173
166.6868	175.9170	191.6651
208.7664	248.8597	336.9840
491.4997	763.9817	921.1738
989.3335	1015.7411	1091.7621

1106.8390	1118.0387	1140.9444
1184.4974	1186.0569	1200.6597
1352.7204	1366.7341	1388.7329
1460.3563	1470.4401	1492.8903
1499.8567	1502.8697	1520.7901
1521.4236	1526.6175	1675.4144
2443.6304	2953.4910	2994.5127
3014.4354	3034.5827	3052.2618
3078.7431	3118.7733	3121.1282
3485.7425	3622.1007	3675.9328

R10

Cartesian coordinates

O	0.031789	1.642824	-0.647235
C	0.843767	2.149725	0.305249
H	0.486283	2.165962	1.332544
H	1.533229	2.910557	-0.039836
C	-2.708149	-0.713493	-0.118119
N	-1.484436	-0.278834	0.552832
H	-3.498398	0.025202	0.033628
H	-3.079006	-1.689472	0.219908
H	-2.520331	-0.777016	-1.192074
H	-0.629617	1.047004	-0.205213
H	-1.622326	-0.231128	1.554878
H	-0.716132	-0.931524	0.367716
C	2.261280	-1.213440	0.374174
N	1.121667	-1.293958	-0.538497
H	3.231311	-1.078238	-0.123065
H	2.312950	-2.120446	0.982237
H	2.111903	-0.363041	1.043482
H	1.271310	-2.016306	-1.232119
H	1.022508	-0.411361	-1.032374

Vibrational frequencies

40.3390	58.4170	74.1517
86.2375	86.5265	123.6376
139.2248	159.4503	176.0760
221.9187	255.8016	300.6665
429.2295	538.2966	612.4049
921.7984	963.2189	992.7045
1012.6352	1088.7370	1091.9792
1123.3173	1150.9162	1194.2203
1210.8782	1267.0474	1365.0793
1382.7833	1461.2901	1467.1698
1494.1033	1503.2879	1507.0399
1524.1535	1527.0392	1560.4244
1677.8132	1701.1191	3003.6904

3013.3796	3081.3497	3093.1392
3099.4268	3122.3059	3127.8647
3211.6478	3243.0338	3397.4155
3522.8793	3599.1634	3614.1099

TS10

Cartesian coordinates

O	-0.762473	1.769577	-0.052126
C	0.481639	2.148688	0.040056
H	0.956143	2.219729	1.039918
H	0.850146	2.905673	-0.672007
C	-2.205355	-1.141738	-0.305738
N	-1.137078	-0.708915	0.597750
H	-3.199717	-0.918103	0.089910
H	-2.139690	-2.214354	-0.507691
H	-2.089483	-0.594386	-1.242549
H	-1.111545	0.359823	0.600490
H	-1.258610	-1.082832	1.531303
H	0.093155	-0.813109	0.023669
C	2.318253	-1.136977	0.214810
N	1.174885	-0.584128	-0.516500
H	3.266489	-0.865652	-0.253703
H	2.246340	-2.224487	0.273417
H	2.306049	-0.729223	1.226704
H	1.178456	-0.858468	-1.493484
H	1.170181	0.490239	-0.462485

Vibrational frequencies

-887.6400	36.6461	81.2899
107.4037	125.3655	133.1992
157.5226	160.7410	174.5783
298.7042	312.9955	385.1522
576.9875	679.6640	707.8728
898.1074	995.0335	1021.2072
1078.6126	1085.7940	1103.2743
1140.7801	1206.9932	1304.0419
1320.9372	1338.4680	1367.3596
1385.5468	1462.7023	1471.5582
1506.9809	1508.8744	1514.2962
1520.2706	1526.7475	1643.3832
1665.0914	1761.2999	1775.5149
2539.0414	2699.7193	2878.2840
2969.7058	3048.3687	3062.5300
3114.6935	3139.2355	3145.5149
3151.4909	3568.0833	3585.3967

P10

Cartesian coordinates

O	-1.090832	1.828354	0.129706
C	0.180984	2.210368	-0.065674
H	0.707353	2.498926	0.860238
H	0.310976	2.963375	-0.858630
C	-2.175315	-1.291996	-0.434551
N	-1.223914	-1.095560	0.658225
H	-3.223309	-1.109152	-0.162280
H	-2.094551	-2.313018	-0.816865
H	-1.921214	-0.607786	-1.246750
H	-1.270664	-0.126392	0.963133
H	-1.464890	-1.679668	1.449437
H	0.644509	-0.967156	-0.170109
C	2.644957	-0.811315	0.284965
N	1.496204	-0.568991	-0.578376
H	3.538806	-0.346310	-0.139350
H	2.866416	-1.873549	0.460861
H	2.465444	-0.344844	1.257245
H	1.634950	-0.982701	-1.491804
H	0.723042	1.270952	-0.410164

Vibrational frequencies

29.9683	40.1384	51.5168
80.9927	90.0717	118.8627
129.5612	151.3995	165.4956
203.5345	238.1901	295.6824
423.0233	542.2929	932.6918
947.7785	986.4524	1013.3794
1049.6699	1088.9217	1090.1713
1097.5284	1178.4619	1195.1138
1195.7242	1358.7830	1367.1870
1371.0878	1395.8403	1464.4658
1465.0805	1503.5587	1503.6888
1521.5152	1524.8485	1527.0366
1671.8972	1708.2165	2535.1023
2947.8261	2995.7923	3007.5777
3012.0053	3076.1105	3084.3969
3113.5311	3126.4294	3379.9619
3510.5941	3600.2212	3610.1041

R11**Cartesian coordinates**

O	0.363367	-2.159406	0.144780
C	0.524177	-1.574440	1.342844
H	-0.341617	-1.668994	-0.341597
H	1.136995	-2.135437	2.040087
H	-0.294327	-0.965350	1.725631

C	-2.785315	-0.655520	-0.354303
O	-1.493407	-0.611245	-0.925209
H	-3.145663	-1.682954	-0.419930
H	-3.482550	-0.009133	-0.898208
H	-2.779691	-0.357962	0.702474
C	2.709924	0.050196	-0.917824
O	2.045370	0.681314	0.168402
H	3.665980	-0.377171	-0.598000
H	2.904670	0.815194	-1.670093
H	2.095999	-0.741917	-1.356861
H	0.560291	1.494714	-0.252700
H	1.726752	-0.022044	0.763201
C	-0.837483	2.284899	0.851496
O	-0.370624	1.768657	-0.378595
H	-0.769256	1.546597	1.661981
H	-1.885272	2.561640	0.722898
H	-0.278317	3.178430	1.148622
H	-1.139461	0.299011	-0.835806

Vibrational frequencies

28.8195	54.6085	59.6095
71.7918	74.8333	93.1683
105.8653	111.6626	111.9999
125.5565	144.1733	149.9338
159.5278	204.1230	241.2293
292.4211	305.6840	354.0775
662.2914	788.7133	807.4082
918.8479	1003.4775	1083.6597
1097.8654	1108.1994	1132.0536
1145.7868	1151.3670	1174.9361
1189.2388	1189.7618	1190.4296
1285.5185	1439.3966	1480.8724
1484.5636	1487.7764	1490.5077
1492.4689	1497.3910	1499.2135
1502.3021	1510.0223	1513.6973
1524.1002	1532.7586	1569.1960
3002.7047	3006.8664	3029.8175
3071.3802	3073.5372	3086.8381
3099.8136	3126.0787	3132.2683
3141.7889	3225.5602	3344.1057
3478.6710	3536.6131	3578.4282

TS11

Cartesian coordinates

O	0.212236	-1.993482	0.052382
C	0.538923	-1.554076	1.241578
H	-0.763880	-1.166097	-0.511114

H	1.189956	-2.190049	1.855845
H	-0.224891	-1.000937	1.820820
C	-2.709268	-0.641022	-0.279795
O	-1.440763	-0.427860	-0.859987
H	-3.058390	-1.656078	-0.490371
H	-3.423653	0.064822	-0.710997
H	-2.693464	-0.504314	0.810103
C	2.541677	-0.032603	-0.902225
O	1.888291	0.528996	0.247907
H	3.587295	-0.220102	-0.658143
H	2.481093	0.693889	-1.712885
H	2.042548	-0.961856	-1.185243
H	0.904450	1.104717	-0.071089
H	1.486635	-0.281336	0.809693
C	-0.726503	2.275266	0.758664
O	-0.160954	1.602034	-0.361976
H	-0.874187	1.588329	1.598639
H	-1.684954	2.711243	0.472681
H	-0.048309	3.073431	1.060716
H	-0.779706	0.781438	-0.624591

Vibrational frequencies

-737.2339	31.3703	68.1630
89.3851	105.9965	124.8735
126.5401	132.6515	146.7729
149.2976	183.1199	189.8675
198.8298	229.1272	333.9988
415.3817	459.3315	550.6125
607.0065	976.8042	1022.3124
1055.5589	1084.4385	1125.0662
1144.9245	1168.2797	1169.7671
1177.8574	1189.5370	1200.5771
1205.7605	1226.0525	1341.5602
1353.9194	1460.7483	1467.2769
1473.4394	1478.2457	1498.9148
1499.8697	1502.2244	1506.4372
1512.4674	1520.3787	1527.8476
1582.3030	1616.1834	1726.2910
1789.2498	1954.3098	2126.0585
2293.3474	2913.2532	3010.2146
3036.8279	3045.7056	3060.9760
3081.5260	3114.2741	3127.1974
3155.1544	3158.8981	3160.8997

P11

Cartesian coordinates

O	0.248341	-2.145119	0.282765
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C	0.495814	-1.456648	1.414746
H	-0.924021	-1.156317	-0.664140
H	0.953311	-2.065374	2.206153
H	-0.369293	-0.878378	1.777554
C	-2.800477	-0.658921	-0.430643
O	-1.510462	-0.440055	-0.965820
H	-3.224911	-1.604964	-0.783268
H	-3.443326	0.153621	-0.771689
H	-2.797570	-0.662791	0.667199
C	2.455659	-0.150543	-1.080511
O	2.261678	0.581105	0.110772
H	3.479781	-0.527022	-1.086852
H	2.303980	0.474531	-1.966694
H	1.772853	-1.013400	-1.146207
H	1.469428	1.138499	-0.018396
H	1.266265	-0.679345	1.124172
C	-0.790324	2.290136	0.864728
O	-0.138128	1.792636	-0.283891
H	-0.882373	1.530069	1.652714
H	-1.791406	2.668035	0.626785
H	-0.196849	3.117311	1.256454
H	-0.671335	1.052845	-0.634311

Vibrational frequencies

34.3454	54.1049	57.3340
68.2011	83.8194	104.4165
110.1644	115.9235	119.3618
134.5884	140.2543	144.8649
195.9352	214.0356	242.7312
270.1797	281.8114	329.0565
746.3302	817.2423	932.5089
1010.9842	1092.0102	1096.5601
1101.0696	1111.7869	1138.6413
1146.0536	1164.5213	1172.9450
1188.2879	1188.7989	1193.1886
1368.9725	1378.1731	1466.3670
1481.7214	1484.3646	1488.6628
1495.1485	1500.2267	1501.5455
1503.2473	1509.1925	1518.1739
1523.2911	1525.2702	1548.0782
2612.8849	2967.9381	2971.7740
2999.3533	3007.5919	3049.4084
3061.7636	3064.0576	3074.0926
3127.1213	3129.5540	3132.1795
3507.9618	3579.7949	3627.5349

R12

Cartesian coordinates

O	0.230966	-2.186986	0.215197
C	0.458909	-1.590446	1.393653
H	1.033827	-2.179689	2.100744
H	-0.299806	-0.905372	1.774787
H	1.718890	-0.122222	0.757936
C	-2.826049	-0.584522	-0.257532
N	-1.555600	-0.580527	-0.986507
H	-3.254895	-1.588877	-0.263024
H	-3.568254	0.113391	-0.662399
H	-2.639095	-0.312596	0.783615
H	-1.711582	-0.795918	-1.964444
H	-0.441209	-1.637902	-0.291028
H	-1.132680	0.351135	-0.941424
C	2.633439	-0.142163	-0.959394
O	2.086773	0.548482	0.152895
H	3.539192	-0.690362	-0.678522
H	2.897517	0.603745	-1.710220
H	1.914843	-0.848655	-1.386705
H	0.683275	1.553349	-0.251457
C	-0.664174	2.396874	0.861054
O	-0.198503	1.946725	-0.391074
H	-0.741136	1.581815	1.595464
H	-1.659499	2.822176	0.717336
H	-0.016840	3.175443	1.282058

Vibrational frequencies

21.8636	43.5978	55.2363
66.1184	75.9979	89.9286
98.1699	119.0832	120.0324
123.2267	141.4675	150.1924
177.9915	202.8109	222.9914
268.0531	301.2556	342.8648
543.5856	664.7075	785.5768
852.2874	972.6526	1024.4383
1086.3938	1088.0815	1105.3569
1132.6250	1140.5679	1152.0715
1171.3061	1185.7436	1190.5981
1231.7615	1291.5139	1388.2677
1442.0073	1466.1637	1485.9609
1489.4178	1491.8720	1496.9956
1498.6731	1504.8267	1506.1854
1523.4867	1524.7352	1538.1335
1590.4506	1700.9024	2985.3115
2991.2131	3025.1453	3030.7645
3053.6360	3087.2885	3092.2890
3099.2919	3116.8950	3128.7614

3135.4920	3215.1330	3410.2648
3532.9261	3587.6647	3594.0192

TS12

Cartesian coordinates

O	0.638816	-2.074314	-0.148123
C	0.934721	-1.663047	1.053184
H	1.772224	-2.159761	1.571749
H	0.099327	-1.406649	1.738946
H	1.463512	-0.295818	0.813275
C	-2.635191	-0.948147	0.023827
N	-1.509677	-0.616778	-0.857403
H	-2.979911	-1.975722	-0.116843
H	-3.470833	-0.266554	-0.148848
H	-2.310769	-0.839002	1.059918
H	-1.776712	-0.706432	-1.831608
H	-0.709616	-1.281786	-0.670600
H	-0.970044	0.569775	-0.596723
C	2.520368	0.471726	-0.794602
O	1.752987	0.729435	0.382277
H	3.581978	0.573519	-0.564699
H	2.244639	1.200164	-1.559975
H	2.308754	-0.539166	-1.156438
H	0.733043	1.166439	0.072175
C	-1.086616	2.325306	0.622964
O	-0.390127	1.534591	-0.316179
H	-1.175731	1.826657	1.596957
H	-2.092476	2.545598	0.251511
H	-0.562749	3.273460	0.766982

Vibrational frequencies

-1184.8233	13.7196	65.9730
82.7941	92.7498	111.4310
122.4659	135.4467	137.4333
143.1366	153.8160	177.5058
206.7515	241.6846	336.5324
387.9777	430.9876	543.6276
592.2547	653.4201	901.9688
1005.2342	1039.2361	1066.7073
1089.8097	1098.5538	1123.6135
1169.4400	1181.4371	1189.4704
1200.3767	1215.1384	1265.0612
1305.3922	1327.4150	1350.6017
1376.0370	1458.5703	1471.1012
1499.2085	1501.3548	1504.0072
1508.8595	1514.3948	1517.7601
1520.2635	1526.9916	1542.0410

1617.6442	1636.5541	1693.3442
1724.9753	1797.7215	2831.1780
2892.0707	2974.6705	3012.0030
3045.4014	3057.5447	3081.8958
3115.1030	3128.7122	3129.9860
3143.4079	3146.5239	3577.6184

P12

Cartesian coordinates

O	0.466466	-2.210243	0.318009
C	0.628008	-1.458087	1.426639
H	1.107692	-1.998747	2.255121
H	-0.291391	-0.941709	1.748773
H	1.342779	-0.639726	1.128711
C	-2.850230	-0.688769	-0.332877
N	-1.582874	-0.500591	-1.040744
H	-3.335412	-1.650966	-0.536418
H	-3.545308	0.110266	-0.600265
H	-2.671490	-0.622826	0.742921
H	-1.724914	-0.564049	-2.041845
H	-0.925761	-1.235514	-0.778439
H	-0.737019	0.988449	-0.588716
C	2.444638	-0.009765	-1.128079
O	2.258624	0.714852	0.066220
H	3.486950	-0.330384	-1.174912
H	2.227698	0.601825	-2.011386
H	1.809519	-0.910083	-1.165740
H	1.418162	1.206419	-0.023558
C	-0.877028	2.213130	0.930209
O	-0.227060	1.757705	-0.234016
H	-0.903853	1.448683	1.719927
H	-1.906361	2.529843	0.721098
H	-0.327737	3.075105	1.312880

Vibrational frequencies

33.9695	53.7763	64.5105
71.7475	81.7390	100.0576
106.6101	117.5785	121.1220
141.0857	154.3561	171.0138
188.6958	196.4707	225.2114
250.7840	280.6671	321.7649
485.1725	825.5548	968.4223
974.9461	1009.2956	1063.0237
1081.3951	1090.9399	1102.3089
1111.1656	1145.1628	1166.0764
1167.7569	1187.5628	1195.1642
1211.3201	1372.2706	1379.8747

1384.2959	1467.3825	1483.3233
1487.1695	1496.9849	1501.2963
1505.5255	1506.2132	1508.7309
1519.6468	1526.5893	1534.1777
1582.6891	1692.3362	2678.8589
2963.1427	2967.9642	2990.9249
3021.3090	3034.7261	3050.6482
3052.6318	3094.9129	3120.6174
3121.5004	3125.9606	3301.9722
3473.5655	3543.5915	3599.8650

R13

Cartesian coordinates

O	0.867085	-2.039692	0.400141
C	0.875416	-1.306672	1.525437
H	1.535438	-1.676855	2.301998
H	-0.045680	-0.797058	1.806997
C	-2.426512	-1.304789	-0.569345
O	-1.120593	-0.892904	-0.909906
H	-3.177250	-0.821108	-1.205242
H	-2.666772	-1.090972	0.480747
H	-2.494292	-2.383184	-0.721969
H	0.138442	-1.700491	-0.173247
C	2.326326	0.425045	-1.151897
O	2.038045	1.068514	0.077947
H	1.428852	-0.012148	-1.606969
H	3.069360	-0.368676	-1.027467
H	2.732008	1.180144	-1.827566
H	1.815399	0.372093	0.718772
C	-1.467888	2.075169	0.975286
N	-0.804765	1.740475	-0.285464
H	-1.167272	1.352450	1.737232
H	-2.551570	2.000877	0.857870
H	-1.228704	3.077354	1.350333
H	-1.042018	2.416813	-1.001297
H	-1.043584	0.085448	-0.750573
H	0.210648	1.762130	-0.163711

Vibrational frequencies

15.3351	53.5397	55.5416
66.8171	74.3017	84.5498
97.7019	105.3130	134.0350
134.9011	163.0494	166.5988
190.5675	203.2560	222.9844
252.7610	303.8075	340.3546
500.5129	692.8868	769.1947
944.8665	996.9208	1044.2277

1057.9485	1085.1224	1090.5791
1107.8189	1129.2817	1147.2345
1175.2144	1189.3108	1193.2060
1215.0348	1285.2734	1379.6080
1436.8678	1465.7092	1482.4756
1490.1966	1492.5828	1500.2021
1502.8070	1507.5178	1511.8565
1514.4384	1523.4418	1525.6066
1588.1559	1701.4336	2997.8536
3016.1704	3022.2085	3061.8561
3084.2883	3086.2559	3094.7734
3123.3717	3125.5736	3126.9123
3178.4507	3227.9123	3373.8464
3429.5236	3596.8223	3616.6310

TS13

Cartesian coordinates

O	0.015392	-2.042926	0.107428
C	0.401163	-1.512410	1.234716
H	0.995874	-2.144409	1.914938
H	-0.325888	-0.868886	1.774014
C	-2.868152	-0.490642	-0.213269
O	-1.644245	-0.340855	-0.893547
H	-3.559917	0.278615	-0.566192
H	-2.755643	-0.383642	0.875081
H	-3.318805	-1.469887	-0.411209
H	-1.029758	-1.072588	-0.585928
C	2.527572	-0.379002	-0.898188
O	1.988944	0.293284	0.235494
H	2.014463	-1.335543	-1.041328
H	3.596510	-0.545441	-0.752606
H	2.383491	0.235057	-1.793306
H	1.346456	-0.515391	0.821779
C	-0.397792	2.407828	0.811888
N	0.084539	1.742594	-0.407404
H	-0.570424	1.644606	1.571731
H	-1.330918	2.949050	0.640954
H	0.358327	3.099960	1.184435
H	0.251952	2.413326	-1.148973
H	-0.629082	1.054837	-0.725201
H	1.124114	1.031510	-0.112245

Vibrational frequencies

-1029.8773	36.9678	57.2072
70.9140	82.2252	101.4421
110.0890	119.8424	132.4609
154.1278	162.2525	179.9647

184.2611	259.0021	284.7059
341.5301	447.0197	487.8556
605.7313	634.1996	928.2338
1010.5774	1067.7731	1071.8542
1085.9067	1098.5515	1108.5123
1119.5824	1165.2062	1191.4760
1192.6808	1203.2885	1218.7716
1278.9798	1319.3109	1348.5209
1390.3987	1472.1643	1487.0750
1496.2605	1498.3403	1499.8294
1506.6098	1510.4625	1515.4294
1520.2005	1523.9632	1532.2457
1579.6944	1644.2899	1685.0133
1791.0388	2856.1985	2972.7281
2982.7966	3019.6917	3026.6984
3057.3435	3059.6616	3099.3550
3103.8738	3124.2580	3137.8888
3153.2833	3164.6886	3584.5012

P13

Cartesian coordinates

O	0.070332	-2.183529	0.193705
C	0.340072	-1.560854	1.356751
H	0.760757	-2.225617	2.123909
H	-0.498883	-0.958323	1.741685
C	-2.863917	-0.502621	-0.313829
O	-1.649919	-0.372644	-1.019383
H	-3.543438	0.273583	-0.670272
H	-2.732932	-0.371736	0.769630
H	-3.336814	-1.476193	-0.488973
H	-1.061873	-1.093603	-0.738990
C	2.481041	-0.359763	-1.005366
O	2.272900	0.379352	0.175344
H	1.732954	-1.160983	-1.126096
H	3.468230	-0.823166	-0.955186
H	2.439533	0.278499	-1.895909
H	1.152139	-0.808884	1.107987
C	-0.527715	2.402070	0.912238
N	0.054149	1.918308	-0.339797
H	-0.621588	1.564412	1.607676
H	-1.518764	2.858330	0.795783
H	0.137475	3.135359	1.373467
H	0.156690	2.680579	-0.998866
H	-0.571548	1.226301	-0.757204
H	1.535624	1.014852	-0.006148

Vibrational frequencies

33.7503	57.6199	63.5378
80.2733	90.5734	100.8267
108.1908	131.1678	134.4418
158.8675	163.9893	187.7590
197.7688	218.8394	241.0265
256.8291	285.7759	326.2575
501.3482	777.1896	964.5956
1004.8410	1011.3283	1061.8613
1090.8576	1102.4587	1106.5266
1112.7220	1146.2007	1156.5937
1175.8213	1193.4123	1195.5551
1223.5031	1369.6441	1377.4520
1388.9697	1463.0552	1469.8595
1480.6214	1500.8349	1501.6317
1506.0469	1508.5228	1515.3158
1518.4557	1526.0153	1529.1188
1568.5278	1689.0059	2585.0731
2963.9386	2969.2694	2996.2082
3016.2845	3044.6079	3049.4389
3057.6960	3096.1062	3121.1466
3125.0835	3129.8393	3276.8164
3449.7270	3596.9408	3653.6522

R14

Cartesian coordinates

O	-0.183572	-1.966383	0.478997
C	-0.792643	-1.787938	1.674289
H	-0.511589	-2.504449	2.435788
H	-1.782130	-1.338876	1.682698
C	-2.433623	0.280715	-1.487584
O	-1.119257	-0.021124	-1.071645
H	-2.441809	1.094427	-2.220960
H	-3.077484	0.560002	-0.644470
H	-2.849721	-0.611059	-1.958590
H	-0.588664	-1.346747	-0.168051
C	2.299671	-0.312613	-1.427045
N	2.161820	-0.108425	0.019019
H	2.830798	-1.233876	-1.693806
H	2.830635	0.534469	-1.866793
H	1.301956	-0.348586	-1.868837
H	3.070809	-0.078345	0.464362
H	1.055509	1.252478	0.237860
H	1.646450	-0.890280	0.418454
C	-0.170975	1.891917	1.622628
O	0.248617	1.826518	0.273500
H	-0.284528	0.893145	2.065069

H	-1.138224	2.398140	1.652303
H	0.533672	2.470821	2.231435
H	-0.709304	0.763142	-0.640147

Vibrational frequencies

30.5473	61.1345	62.4761
78.1265	79.4791	96.3186
106.9517	111.6376	132.1066
135.0690	150.3590	153.7382
179.9309	187.3425	232.1781
253.5234	303.4991	310.3950
477.4006	626.6436	872.0167
963.9167	975.1050	990.9835
1055.5428	1081.2054	1097.5716
1114.0398	1135.2821	1163.1578
1180.8134	1188.3328	1195.5643
1214.4506	1259.4657	1372.3518
1470.6903	1482.0989	1487.0335
1490.4555	1497.8053	1500.3416
1501.5404	1503.8515	1514.1112
1515.4928	1528.5483	1540.2313
1582.8779	1679.4487	2997.3745
3011.4904	3022.7579	3063.4365
3075.5481	3101.8507	3113.8946
3113.9987	3128.6246	3138.1000
3250.3081	3257.8638	3387.5871
3458.4188	3506.9832	3609.4812

TS14

Cartesian coordinates

O	1.210175	-1.648152	0.588745
C	1.319218	-0.922417	1.697048
H	2.173446	-1.151691	2.331540
H	0.397075	-0.592317	2.184709
C	-1.845896	-1.829214	-0.801083
O	-0.825650	-0.921334	-0.520487
H	-2.381820	-1.561917	-1.723734
H	-2.594141	-1.888745	0.006408
H	-1.443202	-2.842373	-0.942509
H	0.274267	-1.410335	0.111226
C	1.750553	0.640055	-1.520110
N	1.425767	1.321318	-0.243817
H	2.747399	0.205649	-1.468015
H	1.690261	1.362505	-2.333533
H	1.006199	-0.143691	-1.658648
H	1.983508	2.156909	-0.098876
H	0.346957	1.548054	-0.222319

H	1.578891	0.668229	0.561953
C	-1.721206	1.699944	1.033383
O	-1.133077	1.464412	-0.224103
H	-1.079204	1.365934	1.863116
H	-2.677900	1.174163	1.122509
H	-1.909785	2.770518	1.155053
H	-1.119916	0.400264	-0.390825

Vibrational frequencies

-197.2003	52.7548	72.9801
93.3998	105.5904	114.7085
119.6786	133.4502	154.5753
160.6974	185.2305	190.0410
208.5500	252.2243	279.5387
365.2455	384.6937	449.9665
588.8675	848.7672	1001.6094
1040.3473	1060.0178	1092.6318
1122.2856	1143.0139	1173.2133
1183.9089	1191.7227	1193.4809
1278.5859	1312.8701	1327.5610
1333.9887	1365.0110	1438.4581
1471.9352	1473.3259	1493.5760
1502.7356	1507.9182	1510.9066
1511.8618	1516.4594	1531.5405
1549.7713	1611.9997	1628.5772
1645.0166	1717.4315	1771.1089
2043.6477	2271.3395	2959.0723
2988.5582	2995.7874	3005.4553
3029.1240	3050.7313	3063.4992
3078.6994	3100.9796	3171.4609
3175.6852	3182.1544	3574.7742

II4

Cartesian coordinates

O	0.805804	-1.742425	0.737437
C	1.188642	-0.935292	1.688752
H	2.069441	-1.222593	2.283632
H	0.418103	-0.392532	2.269220
C	-2.284926	-1.637919	-0.581577
O	-1.150841	-0.807469	-0.533532
H	-3.027898	-1.178956	-1.238948
H	-2.737564	-1.772452	0.409379
H	-2.037856	-2.627611	-0.983276
H	-0.412118	-1.245545	0.025186
C	1.938360	0.024839	-1.487833
N	1.762648	0.908418	-0.314795
H	2.761692	-0.661653	-1.299308

H	2.131651	0.621055	-2.380173
H	1.021755	-0.548641	-1.607110
H	2.534941	1.557348	-0.201162
H	0.856943	1.430250	-0.381943
H	1.665840	0.280587	0.606100
C	-1.313448	2.186408	0.878878
O	-0.821115	1.776334	-0.382465
H	-0.859564	1.618068	1.701211
H	-2.400604	2.068356	0.936926
H	-1.077846	3.244460	1.009577
H	-1.088015	0.831205	-0.506579

Vibrational frequencies

37.4769	61.2648	71.4058
83.0844	88.0155	99.7450
110.9484	130.3929	134.2627
141.3129	151.9712	171.0615
217.7344	244.9942	306.9200
334.5051	364.4527	400.5010
611.0197	951.9402	983.6374
1018.2532	1050.3992	1059.9259
1096.4922	1125.5685	1144.8842
1155.7951	1183.0894	1190.3482
1193.6246	1220.4683	1286.8458
1335.7680	1354.8871	1469.3672
1484.7823	1487.8477	1496.4863
1498.7235	1500.7149	1505.9462
1510.0592	1514.0604	1518.7398
1540.0176	1569.9446	1618.3151
1657.6574	1702.1674	1939.5432
2625.0558	2906.3186	2996.7608
3003.4716	3004.6998	3043.8949
3062.8204	3075.5703	3079.0516
3103.0641	3120.5935	3170.4643
3191.9658	3336.5842	3571.4085

TS15

Cartesian coordinates

O	0.773150	-1.805429	0.837151
C	1.222232	-0.869826	1.622714
H	2.123311	-1.099313	2.217679
H	0.482478	-0.261712	2.182360
C	-2.355651	-1.612668	-0.581901
O	-1.195895	-0.819024	-0.496215
H	-3.078070	-1.097369	-1.218869
H	-2.815345	-1.773903	0.401287
H	-2.140638	-2.590320	-1.028650

H	-0.498942	-1.281047	0.058202
C	1.934705	-0.026830	-1.505756
N	1.847654	0.867047	-0.341509
H	2.727172	-0.757517	-1.343518
H	2.125135	0.531933	-2.424500
H	0.987474	-0.557914	-1.591034
H	2.672989	1.445195	-0.230517
H	0.996834	1.451857	-0.392894
H	1.651117	0.111398	0.697054
C	-1.312481	2.241933	0.853036
O	-0.787595	1.802045	-0.381761
H	-0.902168	1.678682	1.701903
H	-2.404747	2.154892	0.879131
H	-1.053025	3.295295	0.976592
H	-1.057264	0.864122	-0.495626

Vibrational frequencies

-479.6322	32.5573	59.5932
69.7479	83.7868	89.9719
96.8912	109.2416	118.1387
126.8267	135.6474	146.8292
187.6304	248.6019	274.4184
310.4365	381.0500	430.4765
500.3484	657.6533	932.3869
1002.1506	1035.8366	1059.6247
1068.4226	1087.4475	1104.1566
1124.9548	1150.5154	1178.1117
1188.0896	1190.4535	1219.5197
1257.5366	1345.7394	1350.4605
1479.2300	1486.5212	1488.9010
1489.1222	1498.7278	1499.9159
1501.4651	1508.0615	1510.0466
1512.5461	1521.6916	1531.7334
1539.2212	1585.0552	1684.7863
2872.8053	2965.6624	2991.1618
3001.9116	3039.2247	3062.1379
3064.3720	3066.6016	3113.2193
3118.3020	3146.8893	3170.9938
3257.2288	3457.8338	3588.2491

P15

Cartesian coordinates

O	1.560401	-1.046661	1.147532
C	1.613324	0.168774	1.682435
H	2.568946	0.413415	2.171388
H	0.741902	0.443409	2.302851
C	-0.923772	-2.543499	-0.745404

O	-0.920283	-1.454863	0.153583
H	-1.899399	-2.571448	-1.232911
H	-0.770139	-3.494990	-0.224376
H	-0.152802	-2.440756	-1.519914
H	-0.045703	-1.406495	0.590599
C	1.532690	0.505839	-1.685832
N	1.161989	1.607213	-0.806671
H	2.614543	0.491210	-1.831108
H	1.044129	0.547208	-2.666158
H	1.252131	-0.434593	-1.202963
H	1.562471	2.487403	-1.102833
H	0.143872	1.688182	-0.748349
H	1.530341	0.906357	0.771151
C	-2.211615	1.560275	0.791791
O	-1.669256	1.091279	-0.422462
H	-1.481552	1.529473	1.612874
H	-3.092311	0.981686	1.094537
H	-2.518168	2.598021	0.645757
H	-1.462832	0.145055	-0.301017

Vibrational frequencies

39.0105	45.6266	60.4606
70.4844	74.5584	85.9415
94.4644	117.1280	131.5427
135.8169	146.9279	163.0091
187.6146	228.9944	256.3399
266.3299	308.5467	372.9716
551.1049	796.8091	905.4868
954.5712	1027.3178	1054.5349
1095.9628	1104.5138	1111.4502
1146.1025	1158.4578	1167.7373
1188.8290	1192.2262	1198.3489
1224.4560	1344.2096	1374.1031
1385.6366	1465.7719	1482.4857
1492.1647	1493.3680	1497.9356
1499.9743	1500.9460	1511.2105
1515.8012	1527.5329	1532.5603
1540.6751	1690.2567	2118.0234
2939.4742	2998.6885	3010.9821
3019.6856	3030.7960	3058.3731
3073.7189	3104.2975	3122.2267
3134.1693	3137.1602	3420.1996
3492.4699	3589.8295	3620.9785

R16

Cartesian coordinates

O	-2.217797	0.410060	-0.670854
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C	-2.603301	0.404971	0.617130
H	-3.553128	-0.083071	0.806204
H	-2.294210	1.233464	1.252901
C	0.409933	2.314732	0.617503
N	0.079520	1.850831	-0.731042
H	-0.332718	3.040205	0.958088
H	1.403374	2.773331	0.696618
H	0.379343	1.459555	1.296488
H	0.116166	2.618938	-1.390614
H	-1.400027	0.977454	-0.759199
C	-0.743377	-2.559334	-0.379234
N	-0.177648	-1.726541	0.688517
H	-1.529160	-3.242347	-0.035084
H	0.051260	-3.146225	-0.845677
H	-1.172645	-1.898318	-1.132276
H	1.178246	-0.870865	-0.090272
H	-0.898603	-1.085549	1.021220
H	0.100740	-2.300716	1.475977
C	3.015224	-0.300212	0.252799
O	1.888640	-0.393258	-0.581540
H	2.803410	0.234074	1.190858
H	3.791712	0.253068	-0.280473
H	3.424162	-1.287661	0.507215
H	0.781349	1.159278	-1.004337

Vibrational frequencies

31.3501	52.7130	69.3040
77.5741	85.7449	90.5866
94.8467	113.3523	117.5921
128.8725	141.9244	170.7730
199.0924	208.4568	214.1812
276.5222	293.7905	310.6918
487.1502	519.2805	701.6127
927.9552	973.1337	989.9332
1013.7917	1048.0106	1077.9881
1084.9120	1106.3546	1117.4614
1159.6042	1163.4467	1186.7272
1213.5354	1232.3729	1282.7924
1366.7308	1390.3297	1463.8649
1465.7406	1489.0384	1496.1377
1503.2312	1504.2515	1507.4191
1512.7589	1525.0514	1530.9716
1562.4904	1575.8836	1666.8673
1673.1170	2985.0516	3017.0260
3026.5384	3036.7722	3076.8638
3095.3105	3104.3783	3107.8899
3128.9214	3132.0968	3155.1735

3228.4896	3334.5891	3442.1435
3451.5578	3587.8484	3594.7121

TS16

Cartesian coordinates

O	1.123617	-1.710657	-0.426676
C	1.430632	-1.778128	0.845095
H	2.435998	-2.133029	1.117951
H	0.645503	-2.046604	1.574908
C	-2.217261	-1.550626	0.223995
N	-1.344709	-0.950417	-0.790266
H	-2.222985	-2.641124	0.157217
H	-3.239839	-1.179921	0.126161
H	-1.840657	-1.270802	1.208977
H	-1.685315	-1.140203	-1.726125
H	-0.341419	-1.348829	-0.691645
C	2.368189	1.117745	-0.666928
N	1.521606	1.087641	0.542042
H	3.424986	1.089417	-0.399092
H	2.150530	2.017722	-1.242088
H	2.120781	0.223376	-1.238429
H	0.451767	1.286361	0.239845
H	1.552583	0.103927	0.948133
H	1.824996	1.760731	1.237948
C	-1.806574	2.119444	0.419879
O	-0.837153	1.417616	-0.298188
H	-1.536005	2.245273	1.481547
H	-2.776797	1.599210	0.401251
H	-1.971306	3.122346	0.002356
H	-1.172728	0.245317	-0.594683

Vibrational frequencies

-725.3206	27.3067	60.7180
77.2559	89.1162	102.2686
118.6018	135.8637	141.8303
149.0970	161.3169	173.2846
190.0940	192.3220	278.1510
299.4494	400.4064	459.7821
620.5554	655.7495	676.0367
858.8283	1008.1705	1015.3284
1060.1367	1070.9094	1087.3810
1106.5629	1129.5993	1187.3980
1198.9175	1203.1074	1289.9755
1330.3353	1341.9967	1351.2493
1404.9846	1454.6443	1465.9964
1477.6945	1493.2205	1502.9302
1504.3141	1508.1068	1519.9946

1520.5876	1526.1670	1595.9833
1610.5655	1661.9147	1726.5256
1737.8631	1790.0832	1901.9018
2444.5955	2719.7999	2922.6606
2957.8169	3002.6330	3007.3001
3025.6620	3057.4871	3067.2270
3130.3484	3147.8429	3156.4254
3170.4099	3573.8581	3579.0552

II6

Cartesian coordinates

O	1.303458	-1.681123	-0.378221
C	1.549594	-1.587774	0.896065
H	2.542223	-1.906846	1.264660
H	0.734420	-1.804235	1.616276
C	-2.167143	-1.713499	0.209780
N	-1.385279	-1.058391	-0.839573
H	-2.109209	-2.808019	0.179031
H	-3.218849	-1.420975	0.143646
H	-1.790626	-1.390396	1.183454
H	-1.724616	-1.337489	-1.752826
H	-0.397121	-1.370232	-0.764635
C	2.393687	1.157199	-0.723754
N	1.591397	1.125223	0.515119
H	3.452353	1.086122	-0.475051
H	2.198420	2.073822	-1.280290
H	2.110260	0.276101	-1.299430
H	0.587618	1.330975	0.296910
H	1.620597	0.052708	0.912575
H	1.925826	1.783782	1.211050
C	-2.057294	2.012509	0.461458
O	-0.982521	1.517985	-0.302281
H	-2.170913	1.484165	1.418344
H	-3.004726	1.933891	-0.084975
H	-1.879499	3.069996	0.671897
H	-1.199542	0.573308	-0.586737

Vibrational frequencies

9.9112	47.8767	58.7491
76.8653	92.3261	107.9648
111.3269	121.8875	130.0464
146.6579	150.7352	176.5144
202.6713	218.2130	291.5830
314.4727	343.4618	366.8314
569.8540	627.2545	954.2150
982.9770	1008.0564	1054.7699
1059.4207	1071.8258	1090.7807

1111.8988	1145.6396	1177.2252
1193.9579	1203.2068	1254.2690
1274.8008	1334.4757	1349.7853
1402.6888	1405.2339	1455.3879
1491.4672	1497.7506	1500.1044
1502.4228	1507.8695	1516.4425
1516.7396	1520.3938	1527.5764
1605.1329	1622.4654	1718.0918
1722.1860	1750.7360	2852.2710
2873.4656	2941.3145	2990.5592
3023.4139	3051.2048	3063.6238
3076.1637	3089.1466	3109.9431
3118.7000	3166.9200	3168.9228
3171.8016	3571.0048	3580.5127

TS17

Cartesian coordinates

O	1.295634	-1.765807	-0.289459
C	1.514106	-1.527940	0.969654
H	2.482830	-1.845412	1.400243
H	0.673793	-1.643100	1.686277
C	-2.233354	-1.688166	0.133743
N	-1.367597	-1.036360	-0.849662
H	-2.249318	-2.781284	0.048069
H	-3.259114	-1.320054	0.042427
H	-1.877856	-1.440454	1.136743
H	-1.666553	-1.275008	-1.788273
H	-0.399448	-1.388317	-0.734798
C	2.393345	1.090078	-0.797770
N	1.642281	1.125364	0.469352
H	3.459078	0.995714	-0.589423
H	2.205548	1.988762	-1.386313
H	2.067272	0.198730	-1.334456
H	0.644214	1.366380	0.287281
H	2.033081	1.783183	1.135337
H	1.634226	0.002518	0.897664
C	-2.031515	2.016459	0.509502
O	-0.968758	1.554203	-0.290147
H	-2.108761	1.472638	1.461419
H	-2.992650	1.928651	-0.011553
H	-1.866653	3.073712	0.730892
H	-1.172981	0.610556	-0.573293

Vibrational frequencies

-182.4422	13.8991	47.9233
60.1765	74.2361	92.3565
110.0594	118.7157	120.0961

133.6465	139.1398	171.0179
178.3098	223.2744	285.2333
314.9116	347.7295	386.8535
563.7385	641.0507	814.3143
982.0575	1007.6642	1039.2321
1065.3339	1067.9175	1070.6449
1088.4576	1115.2365	1131.1703
1176.0209	1192.0107	1209.8422
1250.9424	1299.6740	1342.3448
1357.0904	1399.1057	1457.2506
1473.9348	1492.9670	1499.4936
1502.2113	1505.3674	1516.2501
1518.3629	1519.9389	1521.6140
1561.4218	1605.5487	1618.0757
1711.8017	1722.5880	2860.9629
2928.7501	2938.3154	3001.0809
3026.2419	3055.8237	3069.4726
3090.6813	3109.2518	3123.4282
3131.1444	3162.9796	3167.9492
3209.6959	3574.8991	3579.8418

P17

Cartesian coordinates

O	-0.784664	2.147896	0.282450
C	-0.899774	1.431978	1.402494
H	-1.543247	1.888111	2.171656
H	0.058930	1.078648	1.823876
C	2.685738	1.045660	-0.328024
N	1.451444	0.684298	-1.026765
H	3.007022	2.080901	-0.496633
H	3.494729	0.379111	-0.636463
H	2.539087	0.909559	0.745997
H	1.563202	0.817858	-2.024983
H	0.692987	1.297718	-0.722556
C	-2.472886	-0.238168	-1.125153
N	-2.076157	-0.953528	0.080013
H	-3.470713	0.186035	-0.993961
H	-2.473127	-0.858519	-2.029960
H	-1.785633	0.599619	-1.284605
H	-1.205943	-1.468849	-0.071817
H	-2.793476	-1.593838	0.393203
H	-1.439099	0.458686	1.084729
C	1.254333	-2.028762	0.970240
O	0.676851	-1.885176	-0.304613
H	0.875156	-1.286274	1.688702
H	2.348826	-1.943762	0.937726

H	1.006931	-3.022411	1.350640
H	0.955400	-1.003995	-0.648319

Vibrational frequencies

33.3815	56.2067	62.1112
64.6941	83.4896	91.6485
101.7836	107.8156	135.8651
145.0268	168.2441	174.3417
190.5753	210.4112	228.5268
254.8970	278.6744	336.2228
505.9760	519.9193	922.5709
954.0787	984.7404	1026.9098
1038.6952	1062.8573	1086.7676
1097.6700	1110.8852	1138.8704
1151.3763	1183.0743	1186.9840
1204.8898	1215.1377	1356.3521
1378.1675	1382.3604	1386.1442
1465.4651	1466.6295	1484.2051
1498.3758	1501.0575	1505.9175
1507.2606	1520.1366	1524.5510
1527.3803	1568.4319	1699.0465
1699.9935	2308.3175	2932.0072
2983.5057	3006.2478	3014.4365
3022.1630	3038.1680	3080.4472
3095.4064	3114.1052	3119.5727
3126.9472	3353.6084	3438.8127
3442.8445	3593.7061	3617.0733

R18

Cartesian coordinates

O	-0.351555	-1.669281	1.147230
C	0.898901	-2.024946	0.823374
H	1.095035	-2.309107	-0.212035
H	1.448747	-2.526180	1.613489
C	-2.918681	-0.380294	-0.854228
N	-1.470190	-0.526846	-1.009793
H	-3.405315	-1.354833	-0.934952
H	-3.373693	0.296578	-1.587532
H	-3.126757	0.011639	0.143602
H	-1.249010	-0.892896	-1.928251
H	-0.806823	-1.322810	0.321465
C	2.559467	0.138593	-1.265330
O	2.402346	0.486482	0.092627
H	3.063411	0.969477	-1.762076
H	1.594036	-0.026534	-1.764124
H	3.175353	-0.760319	-1.392127
H	1.990032	-0.276361	0.535891

C	-0.803000	1.824991	1.336147
N	-0.215188	1.953127	0.001423
H	-0.696025	0.789292	1.667149
H	-1.871955	2.052723	1.293496
H	-0.346856	2.474790	2.094423
H	0.770686	1.697807	0.046128
H	-0.271025	2.910891	-0.321881
H	-1.018634	0.394212	-0.912705

Vibrational frequencies

42.9255	57.8128	69.6980
80.9838	87.4386	96.2414
111.2353	121.6879	132.0497
138.1341	152.5515	164.4280
188.6151	203.6911	214.9483
247.2159	311.2523	365.5017
462.2184	570.8611	694.2374
799.7562	953.4593	993.4721
1020.2677	1037.9645	1084.7787
1088.6579	1099.5686	1125.9022
1145.2419	1173.0332	1189.8296
1202.0214	1240.3654	1294.3322
1379.4487	1404.7222	1438.5764
1463.5285	1469.9182	1490.5821
1496.0613	1504.2899	1506.7182
1514.7070	1517.3807	1523.5870
1529.0506	1591.2179	1691.6106
1709.8364	2989.5112	2998.3935
3011.5753	3029.0025	3055.3783
3083.3885	3086.3004	3099.6784
3123.1054	3130.4539	3133.7443
3213.7449	3308.6211	3479.0345
3583.2671	3587.9437	3603.6937

TS18

Cartesian coordinates

O	-0.346777	-1.413758	1.045381
C	0.873167	-1.862600	0.890069
H	1.099611	-2.480834	0.000605
H	1.432088	-2.161230	1.790574
C	-3.030636	-0.393009	-0.815394
N	-1.579588	-0.380509	-1.007326
H	-3.464293	-1.383531	-0.980842
H	-3.521980	0.319458	-1.483654
H	-3.246528	-0.104696	0.215110
H	-1.329180	-0.715755	-1.930532
H	-1.101212	-0.988860	-0.261638

C	2.916110	0.090408	-1.151773
O	2.204683	0.478515	0.001641
H	3.300365	0.990536	-1.637125
H	2.283145	-0.450697	-1.868755
H	3.768561	-0.551241	-0.900013
H	1.834832	-0.360255	0.419023
C	-0.700803	1.651095	1.371772
N	-0.306363	1.646140	-0.053336
H	-0.616829	0.618335	1.723088
H	-1.733983	1.990451	1.463695
H	-0.050547	2.304267	1.955679
H	0.684625	1.336688	-0.124698
H	-0.396731	2.564143	-0.475105
H	-0.950564	0.780386	-0.624999

Vibrational frequencies

-716.5441	24.9978	61.2114
71.0978	88.7312	93.8205
112.0853	115.8969	126.1249
134.6434	153.7750	184.9151
207.8814	255.3433	269.5893
311.5650	328.5883	397.2773
616.7029	648.3447	713.6553
896.4637	945.8774	1012.2641
1021.3618	1056.9541	1089.2548
1103.7125	1106.2593	1136.3753
1151.6056	1187.5957	1201.8671
1313.7473	1329.1557	1354.5489
1371.7252	1390.1575	1470.0907
1480.0221	1482.9950	1495.2712
1502.2636	1507.9181	1511.0697
1518.2099	1523.2053	1533.8035
1546.3967	1694.0761	1727.6319
1766.9713	1777.5572	2578.1036
2897.3077	2926.7456	2992.3318
3001.8985	3035.7764	3039.6635
3058.5292	3105.1296	3110.9527
3129.0771	3131.6504	3142.3018
3155.1406	3576.5372	3578.9841

II8

Cartesian coordinates

O	-0.249737	-1.206201	1.081114
C	0.942079	-1.740632	1.113927
H	1.179262	-2.549197	0.397133
H	1.431968	-1.866012	2.094775
C	-3.153833	-0.459626	-0.677615

N	-1.739076	-0.437923	-1.047620
H	-3.598122	-1.461154	-0.714793
H	-3.735595	0.198668	-1.329303
H	-3.253224	-0.096042	0.347567
H	-1.603917	-0.849037	-1.963655
H	-1.187798	-0.984672	-0.348975
C	2.793607	-0.067585	-1.292731
O	2.242698	0.415126	-0.085855
H	3.099262	0.788156	-1.899425
H	2.072252	-0.666623	-1.864532
H	3.678056	-0.686061	-1.104666
H	1.916153	-0.393612	0.438384
C	-0.599346	1.748087	1.298659
N	-0.189379	1.600403	-0.118545
H	-0.579706	0.737585	1.718418
H	-1.603282	2.170850	1.345046
H	0.103083	2.399330	1.818330
H	0.780641	1.185169	-0.161907
H	-0.192216	2.487026	-0.612967
H	-0.846368	0.895407	-0.611792

Vibrational frequencies

20.2572	45.6757	68.1320
79.7467	89.6820	92.7677
116.4158	124.8929	133.4369
158.7144	165.6324	217.2730
251.0227	263.4235	296.8986
320.8085	327.8635	357.3458
565.3664	647.1133	909.8729
981.1115	998.8738	1015.8925
1047.3681	1077.2115	1089.2948
1100.2576	1111.1950	1155.0683
1188.8414	1200.0652	1252.2575
1321.2282	1357.3576	1363.8697
1391.8288	1459.0992	1464.4290
1479.8220	1495.8015	1501.5067
1504.5738	1505.9619	1518.0455
1524.5899	1537.2031	1548.4972
1671.2600	1708.7964	1722.4869
1747.5546	2445.2848	2722.3774
2894.3798	2918.8233	2967.9860
3013.1240	3018.9485	3031.7331
3068.1339	3074.9269	3092.0856
3110.9898	3121.2719	3138.7213
3162.4698	3569.2907	3584.8340

TS19

Cartesian coordinates

O	-0.145511	1.476689	-1.060089
C	1.121321	1.767555	-0.974913
H	1.415313	2.544904	-0.240723
H	1.684860	1.852848	-1.923001
C	-3.116397	0.358024	0.606717
N	-1.720336	0.359247	1.041705
H	-3.605825	1.337667	0.676881
H	-3.696716	-0.356934	1.196459
H	-3.159984	0.042510	-0.438211
H	-1.647192	0.704922	1.991036
H	-1.175736	0.985456	0.434328
C	2.315806	-0.090509	1.511779
O	2.080801	-0.391469	0.156523
H	3.289830	-0.475329	1.829627
H	1.542267	-0.530311	2.158652
H	2.303981	0.994194	1.675378
H	1.694267	0.672771	-0.432558
C	-0.428609	-1.644459	-1.475807
N	-0.032139	-1.664354	-0.055113
H	-0.472418	-0.597126	-1.783161
H	-1.403231	-2.114849	-1.624755
H	0.319551	-2.167226	-2.073356
H	1.061989	-1.083603	0.060525
H	-0.009012	-2.608834	0.313039
H	-0.709670	-1.090735	0.495564

Vibrational frequencies

-1047.1264	20.3761	37.6749
54.3669	75.0333	87.3378
125.5221	129.5192	151.1137
157.0034	170.3195	180.8506
205.4840	242.4611	263.5052
293.2026	466.9434	504.4629
542.9752	615.5003	652.2726
921.2547	980.9535	1019.1625
1058.7394	1070.6604	1089.4396
1093.2028	1103.1593	1140.2637
1180.6382	1194.5949	1215.2050
1220.3078	1273.7092	1336.1397
1352.1257	1382.1504	1389.0220
1455.2569	1464.2590	1477.3345
1494.8882	1504.8174	1509.6067
1513.4686	1520.9672	1525.4767
1528.7555	1541.5641	1655.7630
1694.1849	1707.0999	1783.7551
2875.7752	2944.9152	2986.5660

3012.1879	3042.3209	3049.5510
3071.6811	3081.7564	3083.8792
3120.6238	3131.3798	3145.9479
3341.9554	3580.4389	3589.6718

P19

Cartesian coordinates

O	0.078889	1.890022	0.823980
C	-1.251644	2.081166	0.731876
H	-1.551935	2.680181	-0.142502
H	-1.711261	2.449910	1.660519
C	3.028478	0.271423	-0.724962
N	1.647199	0.273946	-1.202554
H	3.577887	1.202800	-0.917202
H	3.578422	-0.551084	-1.189517
H	3.030069	0.100121	0.354046
H	1.615772	0.457056	-2.197886
H	1.125374	1.013690	-0.737491
C	-2.186532	-0.533114	-1.520186
O	-2.278109	-0.677438	-0.123206
H	-2.967702	0.157378	-1.847358
H	-2.338875	-1.487665	-2.041339
H	-1.212349	-0.127966	-1.831181
H	-1.687613	1.056241	0.547363
C	0.664169	-1.345404	1.757591
N	0.172653	-1.786069	0.451145
H	0.552229	-0.260848	1.828326
H	1.719294	-1.589230	1.940410
H	0.066821	-1.795908	2.554038
H	-1.478007	-1.185857	0.157999
H	0.315232	-2.781767	0.332843
H	0.694612	-1.297286	-0.283306

Vibrational frequencies

35.5868	56.3252	64.4079
72.1038	77.1586	95.5629
100.6345	109.2336	114.7720
133.7153	149.2957	155.9029
178.5994	203.8473	209.0464
218.5078	302.0895	310.5813
440.9625	532.0343	927.1419
956.5282	989.8720	1012.4499
1017.1765	1066.3726	1075.4331
1089.9151	1091.8394	1107.0305
1163.4255	1169.7819	1189.6307
1194.9701	1224.4748	1369.2725
1371.8132	1375.4228	1393.2907

1462.2753	1471.5461	1488.6531
1501.5731	1506.3035	1509.9203
1514.2995	1523.6374	1524.2490
1536.8613	1574.5106	1685.0944
1693.9655	2650.1783	2970.4363
2990.0904	3008.3726	3009.9300
3035.7683	3042.8703	3087.7914
3090.7752	3109.0375	3127.3865
3128.5086	3306.5351	3385.4214
3504.3838	3594.1774	3606.3388

R20

Cartesian coordinates

O	0.144002	-1.272854	1.350619
C	0.014968	-0.523980	2.468436
H	0.903981	-0.036355	2.860074
H	-0.778744	-0.830373	3.138864
C	-2.765720	-0.873190	-0.813770
O	-1.396424	-0.541753	-0.841337
H	-2.923645	-1.957739	-0.765004
H	-3.215886	-0.505911	-1.737816
H	-3.287670	-0.406327	0.031418
H	-0.978561	-0.870030	-0.027803
C	1.952307	-1.114627	-1.461058
N	2.066747	-0.352061	-0.213313
H	2.306083	-2.136699	-1.307203
H	2.512795	-0.674707	-2.294499
H	0.897316	-1.161072	-1.739765
H	1.684819	0.591381	-0.365723
H	0.969149	-0.976730	0.842033
H	3.035150	-0.268769	0.071187
C	-0.231461	2.602478	0.470097
N	0.248622	1.935085	-0.738936
H	-0.347459	1.856635	1.261753
H	-1.193910	3.118840	0.348700
H	0.505565	3.335331	0.809618
H	0.325872	2.594913	-1.503094
H	-0.423631	1.219208	-1.013473

Vibrational frequencies

20.3350	49.7779	63.5412
72.8384	82.7778	92.9419
105.3212	113.5310	123.7615
135.6663	159.0318	174.8992
192.2744	195.9438	223.0626
233.2004	260.2962	337.3998
471.8563	587.1491	610.8711

742.1448	957.6875	993.9699
1035.5036	1046.8105	1081.8934
1089.9864	1111.7824	1135.1659
1161.2043	1184.4050	1185.9275
1206.6423	1243.1329	1263.4177
1377.5411	1397.1717	1468.4434
1469.8002	1473.6543	1489.5747
1495.2024	1499.7419	1508.5024
1514.8577	1524.2805	1526.9333
1532.4370	1610.9058	1686.4535
1695.7800	2832.2524	2995.2386
3002.8253	3022.4796	3058.9924
3072.1769	3097.7871	3109.1577
3113.9338	3120.6008	3133.3847
3245.6077	3323.3606	3479.4100
3594.9996	3601.4392	3659.2697

TS20

Cartesian coordinates

O	-0.948998	-1.446469	0.878336
C	-0.269982	-1.168161	1.971577
H	-0.068170	-1.985470	2.677974
H	-0.388426	-0.175990	2.437478
C	-2.688404	1.042169	-0.538821
O	-1.363050	0.581564	-0.583032
H	-3.404188	0.246219	-0.781745
H	-2.809664	1.841419	-1.275996
H	-2.954396	1.446023	0.447824
H	-1.266215	-0.214464	0.045892
C	0.750052	-1.739235	-1.538978
N	1.503728	-1.156577	-0.407113
H	0.446643	-2.752794	-1.287241
H	1.369461	-1.729576	-2.436789
H	-0.140059	-1.128738	-1.681205
H	1.612126	-0.096807	-0.538494
H	0.940897	-1.257966	0.481573
H	2.409317	-1.595147	-0.274372
C	1.587279	2.071045	0.841334
N	1.292762	1.565632	-0.502989
H	1.266757	1.323450	1.571588
H	1.079964	3.014024	1.073683
H	2.663562	2.220478	0.958658
H	1.614240	2.213761	-1.211553
H	0.275431	1.452536	-0.609663

Vibrational frequencies

-173.8218	42.3837	72.6328
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78.0210	85.6586	92.2045
112.8945	125.7697	139.7192
144.9932	158.4396	185.2689
205.8509	215.2120	293.5149
312.3962	342.7845	363.1070
511.3524	640.1363	836.0062
958.1171	995.6102	1032.0521
1044.3498	1077.6679	1089.6932
1125.6981	1139.0627	1173.9172
1188.1600	1211.8467	1240.0261
1266.2199	1321.8243	1343.3254
1380.9424	1468.1248	1474.4343
1485.5264	1496.2234	1500.9900
1504.8828	1511.1966	1514.2362
1517.7741	1528.2352	1559.4528
1608.9679	1685.4807	1697.5892
1737.5255	2591.2117	2711.6329
2912.4800	2953.8943	2996.3399
3023.2191	3025.5966	3045.8976
3075.2935	3088.6728	3095.2409
3121.8275	3170.0788	3189.1007
3334.9826	3575.7529	3595.6458

I20

Cartesian coordinates

O	-1.029038	-1.593605	0.821503
C	-0.094512	-1.477670	1.723719
H	0.173863	-2.372220	2.309135
H	-0.022888	-0.535379	2.301282
C	-2.750023	0.973458	-0.483749
O	-1.405861	0.567942	-0.475209
H	-3.412296	0.184130	-0.862142
H	-2.850714	1.842336	-1.140665
H	-3.101869	1.260889	0.516461
H	-1.317244	-0.269860	0.088067
C	0.855197	-1.618602	-1.541207
N	1.641534	-1.046488	-0.427928
H	0.616180	-2.656963	-1.319564
H	1.416401	-1.543679	-2.474016
H	-0.072977	-1.054162	-1.609938
H	1.667943	0.013492	-0.503940
H	1.122405	-1.257291	0.530990
H	2.582093	-1.425694	-0.384107
C	1.428183	2.226175	0.911318
N	1.199795	1.688057	-0.431700
H	1.114951	1.479765	1.644946

H	0.873646	3.149712	1.114086
H	2.492442	2.423325	1.063532
H	1.478596	2.358113	-1.138133
H	0.196287	1.497640	-0.549433

Vibrational frequencies

37.6360	59.6666	64.2093
76.0124	83.5837	97.4436
117.2292	126.2179	133.1328
138.3810	165.4329	167.8178
210.0417	235.2279	297.8551
327.1226	348.5834	366.1856
549.2804	671.3284	943.1597
990.0102	1003.1650	1045.7902
1062.3866	1085.2568	1091.0879
1100.7589	1125.4595	1172.2700
1188.7058	1210.4855	1235.9174
1300.0943	1332.9682	1359.0572
1384.5537	1466.0854	1470.4989
1486.2944	1495.7566	1505.2266
1505.6924	1510.7449	1514.2696
1519.1085	1526.4666	1580.0747
1612.6112	1672.5221	1685.7618
1709.3373	2029.4488	2760.2429
2812.6123	2909.4229	2980.1271
2999.2584	3025.2497	3047.0458
3070.9216	3091.4708	3093.6361
3125.2570	3164.5362	3184.5584
3351.2619	3569.7245	3594.6348

TS21

Cartesian coordinates

O	-0.512396	-1.904226	0.910773
C	0.459494	-1.424772	1.630654
H	1.056394	-2.144849	2.219049
H	0.280456	-0.475339	2.176688
C	-2.959060	0.062328	-0.496559
O	-1.554895	0.079501	-0.435293
H	-3.338919	-0.869283	-0.934933
H	-3.286310	0.891847	-1.128686
H	-3.417481	0.187186	0.493436
H	-1.243852	-0.688445	0.116514
C	1.336800	-1.261054	-1.549056
N	1.941002	-0.520543	-0.434007
H	1.417592	-2.332694	-1.364188
H	1.811305	-1.012983	-2.501866
H	0.279331	-0.999893	-1.588659

H	1.686106	0.488867	-0.485743
H	1.348846	-0.956849	0.661060
H	2.946256	-0.640493	-0.382938
C	0.632457	2.650985	0.889432
N	0.609231	2.003887	-0.422032
H	0.587777	1.881368	1.663639
H	-0.200873	3.344319	1.059836
H	1.567503	3.201626	1.021370
H	0.638621	2.697358	-1.159586
H	-0.264202	1.477734	-0.523388

Vibrational frequencies

-492.0226	35.4538	56.0195
65.7583	81.6381	88.1965
98.7344	114.3950	122.2755
124.8321	136.6047	158.7055
185.5873	228.7344	264.6342
307.4439	365.5064	425.8281
503.8620	541.6947	695.3328
978.9937	984.7983	1001.0190
1050.9124	1070.0817	1082.8849
1091.3020	1101.4840	1122.7175
1168.2141	1187.4442	1218.1570
1221.3522	1264.5637	1346.0166
1350.2784	1382.4870	1465.3188
1479.6418	1488.6817	1493.8047
1497.0012	1501.7847	1506.1607
1510.5163	1512.4080	1519.9686
1525.1211	1536.7206	1577.5439
1683.9012	1700.0432	2870.4892
2954.2952	2994.4874	3012.8473
3052.1380	3052.4707	3086.4727
3096.3613	3102.4741	3122.0059
3138.1155	3162.7024	3181.8320
3413.2657	3585.5899	3594.9146

P2I

Cartesian coordinates

O	-1.772268	-0.766432	1.123638
C	-0.775013	-1.476442	1.634009
H	-1.074266	-2.433310	2.091138
H	-0.074417	-0.909556	2.273294
C	-1.809347	2.211835	-0.628596
O	-0.807875	1.586750	0.140173
H	-2.184219	1.560522	-1.430214
H	-1.374996	3.101905	-1.088261
H	-2.661200	2.525872	-0.013399

H	-1.199755	0.805291	0.576199
C	-0.397528	-1.449021	-1.725891
N	0.696520	-1.840917	-0.846590
H	-1.176422	-2.215026	-1.724204
H	-0.085350	-1.266409	-2.761550
H	-0.833795	-0.528123	-1.333405
H	1.387819	-1.081975	-0.788851
H	-0.104958	-1.769484	0.707934
H	1.137141	-2.703667	-1.138274
C	2.640436	0.848548	0.896566
N	2.004416	0.771448	-0.416768
H	2.063899	0.249683	1.606140
H	2.716788	1.865512	1.303658
H	3.646059	0.422235	0.850549
H	2.531012	1.310702	-1.093188
H	1.069960	1.180046	-0.361078

Vibrational frequencies

43.5450	47.8181	58.5383
67.0459	76.3570	82.5061
97.0741	109.0147	119.3340
128.9120	139.5076	153.0922
161.0334	215.2692	227.6962
256.7773	283.4949	369.3560
481.8457	602.4968	825.0279
951.3927	964.3137	1029.3843
1047.2849	1060.0931	1092.1022
1096.0120	1111.2490	1153.7818
1165.6727	1189.6445	1192.7366
1205.4719	1230.3089	1343.9825
1377.4446	1382.4754	1388.8091
1462.1877	1464.5343	1490.1677
1495.1049	1498.6999	1503.0339
1503.7924	1514.3394	1523.5235
1525.0664	1535.1433	1681.6810
1702.8561	2056.8515	2929.9923
2996.0534	3005.3059	3007.7786
3019.2359	3055.3552	3082.6241
3099.7370	3115.2111	3117.0427
3141.2290	3327.6655	3449.5898
3538.5051	3597.6082	3610.8093

R22

Cartesian coordinates

O	0.372971	-2.175841	0.307588
C	0.357033	-1.661105	1.548622
H	0.884078	-2.246476	2.294019

H	-0.504714	-1.066438	1.850808
C	-2.681038	-0.756484	-0.478236
N	-1.352215	-0.613556	-1.075566
H	-3.021354	-1.791123	-0.563696
H	-3.440589	-0.103093	-0.925302
H	-2.618081	-0.519367	0.586279
H	-1.392705	-0.816357	-2.067951
H	-0.243076	-1.634676	-0.265258
C	2.460230	-0.067225	-1.113022
N	2.233235	0.643914	0.144900
H	2.995577	-1.018167	-1.003493
H	3.021724	0.573259	-1.798388
H	1.495240	-0.285438	-1.575014
H	3.117251	0.910213	0.561754
H	1.776101	0.013358	0.803850
C	-0.914392	2.250986	1.044768
N	-0.357960	2.087396	-0.295463
H	-0.753724	1.325205	1.603863
H	-1.993456	2.420928	0.988677
H	-0.469965	3.070568	1.626252
H	-0.434523	2.949999	-0.820018
H	-1.028888	0.359214	-0.970490
H	0.634923	1.843815	-0.216487

Vibrational frequencies

35.2496	53.7646	67.3455
73.1527	86.1133	92.3023
103.5011	105.9521	117.1085
129.9065	156.5853	168.1732
187.3291	206.0579	220.0836
233.1325	278.7328	308.8440
404.2404	515.2630	599.8247
686.4097	942.8821	959.7502
975.4668	1014.3965	1018.5798
1050.7149	1087.0020	1088.9013
1093.4612	1125.0376	1157.4951
1201.7593	1203.2450	1238.3523
1284.4747	1372.3476	1383.0548
1403.4398	1458.0850	1461.1546
1478.5968	1491.8894	1501.3173
1507.9020	1511.2620	1517.0484
1526.2423	1529.3585	1582.3617
1675.6066	1696.7983	1712.9320
3002.6438	3016.8595	3024.6978
3062.6089	3079.9857	3095.6556
3097.4916	3115.5329	3119.6997
3129.8089	3131.4452	3227.8404

3301.6933	3379.5495	3453.9345
3580.8148	3593.0751	3593.6230

TS22

Cartesian coordinates

O	0.223325	-1.703235	0.200841
C	0.220221	-1.413817	1.479762
H	0.958529	-1.908002	2.130496
H	-0.743507	-1.204600	1.983060
C	-2.977709	-0.512662	-0.307468
N	-1.696834	-0.417673	-1.008780
H	-3.406954	-1.518972	-0.350008
H	-3.707687	0.192496	-0.716647
H	-2.819598	-0.268794	0.745300
H	-1.801032	-0.686345	-1.981013
H	-0.970180	-1.071428	-0.550979
C	2.833368	-0.423256	-0.922693
N	2.291527	0.518706	0.063157
H	3.721855	-0.957586	-0.565367
H	3.096198	0.102545	-1.845561
H	2.053799	-1.159658	-1.119736
H	3.029389	1.078543	0.474419
H	1.846053	-0.020346	0.813506
C	-0.596732	2.020422	0.958355
N	-0.226107	1.647053	-0.419052
H	-0.428357	1.139471	1.584009
H	-1.648293	2.308524	0.999671
H	0.019987	2.844571	1.321600
H	-0.279667	2.440331	-1.049647
H	-0.929910	0.774658	-0.777935
H	0.767784	1.279745	-0.396913

Vibrational frequencies

-367.8233	36.1515	66.9375
80.9052	97.0710	116.8219
123.4121	139.6974	146.4293
159.6511	173.0492	182.7011
198.9864	205.1834	231.3076
251.7193	322.3851	389.1899
498.8548	637.6408	721.3876
798.2717	914.5612	980.4523
1007.6044	1029.3589	1054.0748
1072.4687	1084.4094	1089.9898
1110.2605	1162.7624	1192.3516
1217.4234	1317.3523	1338.0386
1350.5048	1369.1709	1382.9383
1425.7768	1447.3809	1466.6536

1480.2973	1506.7419	1506.9465
1511.5507	1517.4414	1523.7049
1528.6999	1533.2731	1651.1495
1690.0730	1740.5005	1755.9176
1776.2920	2502.1405	2828.0005
2896.4909	2983.7782	3017.7097
3030.9038	3040.2904	3080.2847
3092.0535	3123.5900	3127.8954
3143.4058	3146.5351	3376.4553
3569.9828	3572.0277	3583.8441

I22

Cartesian coordinates

O	0.083440	-1.589876	0.373031
C	-0.442508	-1.493081	1.576370
H	0.229440	-1.523458	2.449749
H	-1.439379	-1.924984	1.753881
C	-2.940007	-0.241285	-0.730564
N	-1.583897	-0.212707	-1.280393
H	-3.467139	-1.183415	-0.922220
H	-3.542242	0.577318	-1.136673
H	-2.874288	-0.117474	0.352844
H	-1.596517	-0.429486	-2.270156
H	-1.000705	-0.927592	-0.787894
C	3.065109	-0.268018	-1.026292
N	2.242319	0.032741	0.143235
H	3.645278	-1.192968	-0.925173
H	3.760131	0.550875	-1.234859
H	2.414265	-0.384293	-1.896680
H	2.819044	0.099255	0.973706
H	1.540809	-0.734329	0.295050
C	-0.498920	1.881237	1.203850
N	0.061971	1.643117	-0.142739
H	-0.643461	0.895509	1.667310
H	-1.455186	2.399607	1.123498
H	0.194622	2.478157	1.797500
H	0.208485	2.509496	-0.651181
H	-0.608192	1.001015	-0.701180
H	1.002720	1.110591	-0.052680

Vibrational frequencies

29.6596	68.9895	81.0460
92.0672	104.5796	113.5620
126.9864	138.5426	148.3192
162.7425	167.8794	189.1907
204.2244	253.6548	263.4844
298.0707	325.0883	357.9117

557.2271	626.2112	704.2113
752.7940	999.9925	1000.8704
1015.3616	1055.6676	1078.5769
1086.6776	1096.4680	1113.3082
1118.3298	1189.4633	1257.2634
1265.0069	1322.7985	1335.0423
1365.5523	1398.3074	1412.9763
1460.1917	1463.8495	1469.5428
1502.3095	1504.3623	1508.8775
1511.6902	1524.9267	1525.1111
1530.4481	1685.7758	1712.3087
1721.7435	1733.1655	1764.7341
2353.5778	2495.0821	2918.0533
2958.0460	2972.3488	3001.5667
3016.4633	3023.4095	3063.4671
3082.1312	3083.4732	3109.8283
3112.2857	3120.1862	3152.1555
3566.2049	3580.7014	3582.2147

TS23

Cartesian coordinates

O	0.261199	-1.765813	0.098031
C	0.418339	-1.551059	1.376064
H	1.074849	-2.224847	1.953921
H	-0.436979	-1.164432	1.967201
C	-3.034912	-0.460511	-0.157955
N	-1.845552	-0.401607	-1.004706
H	-3.506044	-1.451221	-0.125266
H	-3.786280	0.262910	-0.490229
H	-2.754143	-0.203595	0.866768
H	-2.071029	-0.705979	-1.944581
H	-1.114370	-1.046387	-0.628239
C	2.701862	-0.347877	-0.972081
N	2.154028	0.463679	0.126072
H	3.626876	-0.850235	-0.678957
H	2.899106	0.279428	-1.845275
H	1.949309	-1.104166	-1.197418
H	2.865218	1.042821	0.559670
H	1.741277	-0.178148	0.847415
C	-0.531552	2.078366	0.934077
N	-0.060692	1.669346	-0.398654
H	-0.480213	1.203954	1.586388
H	-1.560225	2.443818	0.905350
H	0.114133	2.858772	1.342325
H	-0.039737	2.457048	-1.037829
H	-0.736298	0.946490	-0.774279

H 1.068046 1.126836 -0.230829

Vibrational frequencies

-851.4938	38.1694	51.2768
90.0972	99.6931	117.4427
127.0033	141.9446	158.9394
165.9363	172.8666	177.0006
186.7638	203.2517	260.7226
285.5345	294.6157	333.1185
547.9189	581.3352	613.5168
753.6953	847.9139	996.2178
1007.5418	1014.3255	1061.4025
1079.2115	1083.5785	1095.6774
1104.9950	1123.4531	1189.1400
1249.3915	1291.5007	1325.0504
1341.6590	1364.1492	1390.9768
1434.4936	1444.1236	1460.5794
1468.7229	1502.9932	1504.1320
1507.7024	1514.9315	1521.2162
1528.3792	1536.3105	1631.5508
1699.2303	1735.8766	1763.4141
1778.8519	2822.7182	2866.4201
2948.3397	2950.4588	3010.4088
3047.1395	3052.8429	3060.5308
3080.4004	3111.3350	3122.2068
3137.3665	3142.7156	3156.7076
3567.8547	3569.1873	3578.2679

I23

Cartesian coordinates

O	0.589309	-1.967412	0.108737
C	0.746392	-1.496249	1.309642
H	1.433463	-2.023543	1.998376
H	-0.135163	-1.066631	1.833261
C	-2.813454	-0.914050	-0.098177
N	-1.689600	-0.672916	-1.000385
H	-3.109282	-1.969051	-0.021613
H	-3.688703	-0.336946	-0.412424
H	-2.541369	-0.579332	0.906349
H	-1.918624	-1.008022	-1.929031
H	-0.874771	-1.218992	-0.674030
C	2.659517	-0.027717	-0.963088
N	2.013156	0.651006	0.174155
H	3.582748	-0.501566	-0.629863
H	2.874967	0.679782	-1.765375
H	1.974374	-0.808130	-1.293332
H	2.653585	1.248594	0.686833

H	1.569932	-0.158059	0.856147
C	-0.983808	2.198354	0.874824
N	-0.401687	1.900189	-0.435958
H	-0.802368	1.348309	1.538476
H	-2.065619	2.375588	0.846560
H	-0.504387	3.076726	1.315984
H	-0.545665	2.676553	-1.070984
H	-0.893694	1.074382	-0.821972
H	1.171136	1.219653	-0.137145

Vibrational frequencies

33.3811	50.5808	76.3486
86.3974	107.0542	112.2802
125.3518	134.7732	143.3074
148.5787	154.6745	173.9156
197.4099	231.3385	268.5424
292.6460	338.0791	362.4978
517.8443	590.9995	683.5762
962.3825	990.5080	993.0984
1005.5967	1052.3328	1062.6393
1072.4018	1086.6793	1092.1179
1103.8581	1204.3842	1231.3684
1252.5000	1254.4684	1326.9510
1353.3870	1395.7580	1400.2379
1414.1426	1460.7323	1465.7338
1493.4910	1499.6186	1501.8234
1507.2506	1515.7001	1524.1468
1525.7251	1528.0905	1636.0860
1700.5175	1718.7786	1720.0937
1731.8783	2761.3636	2845.2560
2923.0161	3002.1666	3018.5641
3064.1522	3070.1278	3084.9779
3107.7787	3113.7508	3154.3304
3169.3647	3199.6838	3257.6602
3567.6990	3577.1445	3583.6696

TS24

Cartesian coordinates

O	0.649190	-2.004656	0.149077
C	0.804403	-1.452005	1.313891
H	1.501166	-1.926474	2.031648
H	-0.086774	-1.014960	1.816161
C	-2.770887	-0.990022	-0.114728
N	-1.637649	-0.727926	-0.999692
H	-3.019108	-2.054426	-0.007141
H	-3.663054	-0.465930	-0.470652
H	-2.541591	-0.606694	0.883196

H	-1.845288	-1.072875	-1.929861
H	-0.819519	-1.259041	-0.660886
C	2.624618	0.042094	-0.988825
N	2.000813	0.694779	0.172976
H	3.541644	-0.459318	-0.679233
H	2.847104	0.766314	-1.774717
H	1.927278	-0.717205	-1.341825
H	2.650993	1.278653	0.688551
H	1.549189	-0.169794	0.860493
C	-1.076987	2.197984	0.869969
N	-0.459016	1.911707	-0.426200
H	-0.878184	1.360928	1.544942
H	-2.163873	2.337132	0.820170
H	-0.637297	3.095781	1.313295
H	-0.621308	2.676363	-1.070885
H	-0.909258	1.065373	-0.815313
H	1.158444	1.265194	-0.111983

Vibrational frequencies

-151.9848	34.6019	53.5091
76.4228	89.8097	104.9608
123.1312	128.3524	133.9497
140.3499	151.4203	183.5454
229.0097	252.2496	266.4114
282.3756	345.5102	382.6084
512.9075	590.4354	691.9572
866.4993	986.8682	991.8119
1007.6113	1047.4129	1050.9611
1066.5561	1084.7757	1092.2798
1093.1499	1105.5667	1210.2887
1231.3575	1247.8030	1314.5526
1346.6249	1356.7756	1396.0458
1414.0724	1460.2099	1465.7897
1477.2641	1499.1017	1500.4891
1514.4087	1519.0445	1520.5272
1526.3185	1535.0217	1579.9703
1631.3186	1703.3299	1716.2162
1726.3015	2839.5703	2863.5164
2919.0231	3009.6417	3021.9205
3066.3113	3078.7734	3088.9520
3114.8581	3119.9063	3154.6705
3169.6493	3227.1654	3270.7841
3571.8865	3575.1430	3582.0859

P24

Cartesian coordinates

O	0.789920	-2.181124	0.279709
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C	0.874853	-1.451061	1.391855
H	1.497570	-1.896505	2.185050
H	-0.094914	-1.093669	1.784418
C	-2.682875	-1.078453	-0.249979
N	-1.515062	-0.801307	-1.082942
H	-3.000381	-2.130146	-0.245012
H	-3.529276	-0.469733	-0.579737
H	-2.461699	-0.793080	0.781874
H	-1.701779	-1.063095	-2.043450
H	-0.728167	-1.368163	-0.765792
C	2.482621	0.203146	-1.110734
N	2.108150	0.917743	0.101277
H	3.459308	-0.268561	-0.980813
H	2.518974	0.836645	-2.006303
H	1.758359	-0.598750	-1.289625
H	2.854228	1.513550	0.435110
H	1.426382	-0.481052	1.078355
C	-1.233041	2.102941	0.999203
N	-0.626935	2.004762	-0.325262
H	-0.870431	1.275471	1.615630
H	-2.331824	2.065816	1.002684
H	-0.924537	3.030729	1.488832
H	-0.933398	2.771711	-0.911227
H	-0.932363	1.129669	-0.765395
H	1.262170	1.480331	-0.055862

Vibrational frequencies

29.8865	51.8873	66.4245
68.5629	83.3330	84.2909
96.9104	116.6464	117.9200
126.3667	144.3955	159.6618
174.4419	214.9817	222.3421
236.7476	261.5240	337.8756
451.3113	503.1844	582.6286
948.6744	959.9921	970.9231
1022.2031	1037.0918	1044.3758
1054.1176	1090.3885	1094.7238
1100.3806	1139.5065	1193.0526
1201.9376	1209.2956	1211.3581
1354.6262	1379.0429	1382.4923
1389.7342	1395.1819	1460.3710
1466.0923	1468.2134	1497.3730
1501.6477	1503.0586	1515.7549
1522.9308	1524.5920	1526.8389
1697.1604	1700.1530	1707.8583
2282.7501	2925.2595	2993.2928
2995.5371	3002.6692	3008.4889

3073.5620	3075.8609	3078.5662
3109.7113	3113.4553	3116.8169
3325.2428	3373.3296	3465.8238
3592.0364	3596.1036	3611.4133

R25

Cartesian coordinates

N	0.654657	0.000000	-0.098526
C	-0.726558	0.000000	0.085024
H	1.127152	-0.832370	0.220751
H	1.127152	0.832371	0.220750
H	-1.238779	0.929712	-0.130982
H	-1.238779	-0.929712	-0.130983

Vibrational frequencies

454.9564	634.1172	710.5559
958.1070	1248.9592	1334.1041
1491.5743	1664.6829	3150.8247
3263.6955	3582.1160	3684.9428

TS25

Cartesian coordinates

N	-0.749915	-0.126789	-0.098820
C	0.682370	0.031638	0.009957
H	-1.153585	0.803270	0.022275
H	-0.103491	-0.272253	0.961148
H	1.153316	1.007980	-0.076499
H	1.258948	-0.841301	-0.274928

Vibrational frequencies

-2000.4504	768.8196	898.3545
1014.4756	1118.8095	1241.1492
1346.2149	1475.9031	2394.6462
3106.7457	3227.6610	3486.4792

P25

Cartesian coordinates

N	-0.801749	-0.152890	0.000055
C	0.625623	0.012263	0.000071
H	-1.200895	0.791494	0.000003
H	0.967175	0.584239	0.877338
H	0.966700	0.579117	-0.880734
H	1.125527	-0.958198	0.002585

Vibrational frequencies

244.3432	957.3004	1025.4541
1078.4542	1346.8370	1404.2442
1483.1205	1497.1242	2969.1804
3014.5505	3119.2650	3437.2413

R26**Cartesian coordinates**

C	1.909186	0.229858	-0.444222
O	1.268713	-0.230357	0.718864
H	2.275730	-0.589989	-1.078208
H	2.770112	0.828058	-0.138238
H	1.257697	0.868619	-1.060010
N	-1.358631	-0.725183	-0.244381
C	-1.816984	0.589732	0.100232
H	0.476200	-0.706621	0.434001
H	-2.123812	-1.225790	-0.701810
H	-1.016128	1.136485	0.599618
H	-2.694679	0.545494	0.762685
H	-2.137626	1.145347	-0.794349

Vibrational frequencies

46.7934	84.6236	110.1125
119.0077	142.5006	163.1233
367.8579	826.4208	878.7137
987.2242	1045.4851	1096.7466
1153.3683	1169.1011	1349.4186
1376.0595	1407.5305	1468.4571
1500.6951	1518.2452	1520.3125
1668.4273	2936.6375	2973.2655
2994.9734	3036.4328	3077.4105
3122.1921	3529.2615	3621.7306

TS26**Cartesian coordinates**

C	1.969798	0.113480	0.432091
O	1.205007	-0.304316	-0.670575
H	2.396989	1.116734	0.294396
H	2.796387	-0.590272	0.550114
H	1.395014	0.115307	1.370578
H	0.433579	0.276685	-0.723410
N	-1.394143	0.717201	-0.162978
C	-1.850683	-0.598563	0.221327
H	-2.201547	1.336795	-0.207948
H	-1.101719	-1.373322	0.105673
H	-2.904539	-0.857981	0.182917
H	-1.409902	0.300680	1.012618

Vibrational frequencies

-2008.7010	37.3083	105.8010
121.1134	147.0024	171.4673
230.8838	722.3706	768.1328
910.5208	1018.2694	1111.5241

1123.1961	1133.8200	1189.3229
1236.7007	1335.5299	1457.5201
1468.7782	1494.7691	1500.3590
1523.1943	2386.5039	2981.1195
3027.8347	3116.9900	3120.1479
3249.6191	3519.3554	3741.6229

P26

Cartesian coordinates

C	1.804378	-0.575331	-0.043009
O	1.423838	0.771979	0.073116
H	1.383924	-1.205561	0.754540
H	2.893067	-0.622980	0.032180
H	1.515725	-1.016830	-1.008752
H	0.458765	0.798653	0.028397
N	-1.517095	0.605938	-0.058550
C	-1.815005	-0.757291	0.049904
H	-1.780363	1.020970	-0.941739
H	-1.704293	-1.198433	1.031806
H	-1.619012	-1.365240	-0.823615
H	-1.855098	1.167759	0.710734

Vibrational frequencies

19.9832	74.9329	91.2111
136.1436	156.9674	204.8920
442.5020	621.1177	705.2243
810.6087	960.8380	1112.9338
1135.4969	1184.8735	1226.9458
1335.5556	1463.2807	1482.9904
1495.6897	1496.6378	1519.9342
1662.1905	2975.2005	3018.8383
3108.0741	3158.3960	3276.1417
3568.0831	3667.6839	3738.8709

R27

Cartesian coordinates

N	1.457962	-0.451311	0.467775
C	2.072573	0.447525	-0.394651
H	2.042651	-1.208193	0.787464
H	3.088633	0.743391	-0.158076
H	1.424164	1.188999	-0.849076
H	0.528686	-0.756020	0.178076
C	-1.782108	0.602642	0.344014
N	-1.422147	-0.591503	-0.420269
H	-1.754678	0.366470	1.409602
H	-2.770584	1.017447	0.105644
H	-1.031215	1.376613	0.171626

H	-1.430351	-0.395405	-1.413839
H	-2.090805	-1.334609	-0.260138

Vibrational frequencies

35.2964	56.3371	72.7944
137.8722	202.9581	224.4743
364.7145	530.5774	645.8358
809.1462	889.9506	985.0961
998.0424	1084.8527	1183.7684
1262.6576	1350.1771	1356.0780
1470.8519	1486.1730	1504.1610
1523.0873	1672.3072	1689.2410
3007.0686	3097.6022	3129.6995
3132.4684	3237.6988	3440.7706
3549.9219	3630.5639	3653.9045

TS27

Cartesian coordinates

N	-1.531324	-0.547263	-0.473381
C	-1.522830	0.663543	0.178200
H	-2.190132	-1.170296	-0.008951
H	-2.319299	0.928267	0.879788
H	-1.186164	1.516424	-0.424912
H	0.130015	-0.881876	-0.150652
C	1.937518	0.248997	-0.297303
N	0.860870	-0.382871	0.463078
H	2.590936	-0.496276	-0.754550
H	2.528464	0.901365	0.347653
H	1.483594	0.849020	-1.086256
H	-0.013759	0.350389	0.753946
H	1.181394	-0.961314	1.230671

Vibrational frequencies

-859.5111	100.1060	135.3648
176.2507	366.3907	402.2582
549.3393	684.7651	787.5643
935.3662	988.5482	1044.9633
1079.2734	1108.6633	1240.3692
1289.7495	1327.3378	1350.5725
1473.7159	1492.9094	1502.5389
1515.6924	1545.4856	1670.8261
1738.5638	2683.2377	3007.1891
3064.1057	3093.3811	3140.8964
3161.4324	3497.7836	3589.9867

P27

Cartesian coordinates

N	1.705160	-0.606131	0.466348
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C	1.759199	0.653094	-0.222977
H	2.171242	-1.293014	-0.133857
H	2.720544	0.855260	-0.714005
H	1.518617	1.471376	0.460071
H	-0.525944	-0.915209	0.262204
C	-2.023701	0.470120	0.227207
N	-1.243148	-0.599457	-0.385343
H	-2.542376	0.196569	1.157996
H	-2.773371	0.830272	-0.482436
H	-1.363278	1.312173	0.451252
H	0.983343	0.637911	-1.007152
H	-1.835852	-1.395509	-0.586488

Vibrational frequencies

52.8655	53.9452	100.4894
126.3879	148.8072	190.9343
289.1097	421.9206	903.2066
977.4434	1005.3669	1033.9412
1083.5087	1092.9309	1185.2915
1341.7587	1367.7048	1405.1895
1466.3633	1477.6651	1502.7236
1504.9988	1525.7400	1683.1189
2967.5132	2985.7761	3035.6623
3074.0187	3104.4204	3112.1721
3449.3689	3505.8984	3607.3057

R28

Cartesian coordinates

N	-0.411295	1.831133	-0.652354
C	-0.850886	1.805611	0.656969
H	-1.119053	1.865329	-1.368370
H	-1.744328	2.377341	0.882746
H	-0.068279	1.794887	1.409870
C	2.558739	-0.387209	0.274812
O	1.448989	-0.419357	-0.595699
H	3.372129	0.125966	-0.240848
H	2.901831	-1.395913	0.535393
H	2.344675	0.156397	1.204800
H	0.369195	1.213267	-0.867147
H	0.711189	-0.854691	-0.134673
C	-1.853885	-1.496475	-0.336106
O	-0.904940	-1.155480	0.656630
H	-2.877430	-1.452300	0.052662
H	-1.648168	-2.519899	-0.651607
H	-1.779231	-0.839955	-1.212323
H	-1.059665	-0.221231	0.894481

Vibrational frequencies

37.9465	59.8064	86.5157
100.2353	112.8141	115.2212
120.6600	149.3691	201.5407
213.4557	249.6921	291.7729
564.6437	671.2145	765.8714
821.7235	894.6024	997.5094
1095.0755	1108.1143	1132.3743
1148.4233	1186.8243	1187.6597
1279.1734	1350.3954	1448.9527
1476.5465	1485.1460	1489.0100
1496.0641	1499.7345	1502.2397
1518.3254	1525.0083	1683.1873
3000.4507	3010.0409	3057.4945
3072.0026	3123.3506	3126.5420
3135.1256	3235.1810	3468.2304
3532.0228	3642.8382	3678.4108

TS28

Cartesian coordinates

N	0.113418	1.701934	-0.620733
C	-0.600921	1.746985	0.567603
H	-0.418653	1.954217	-1.445632
H	-1.441355	2.440413	0.591827
H	0.053406	1.841284	1.440580
C	2.290081	-0.691768	0.243565
O	1.105644	-0.546614	-0.493401
H	3.023953	0.071431	-0.047148
H	2.745923	-1.672439	0.060971
H	2.122203	-0.597436	1.327342
H	0.763055	0.738479	-0.677365
H	0.060340	-0.845805	0.142270
C	-1.907193	-1.228627	-0.339942
O	-0.970578	-0.879200	0.647422
H	-2.890386	-1.383959	0.112965
H	-1.604229	-2.151770	-0.845755
H	-1.999417	-0.446860	-1.113197
H	-0.981101	0.585872	0.738753

Vibrational frequencies

-1438.9686	67.0144	88.4581
99.8906	142.3443	153.1472
168.8653	198.4341	256.8390
336.0718	435.8765	543.2027
638.9478	681.9847	917.0672
1010.0910	1047.5501	1103.2722
1164.4716	1186.4787	1189.8823
1196.2037	1211.3021	1222.7242

1273.8842	1376.1303	1415.1288
1473.5179	1494.1312	1499.8211
1502.3472	1503.2676	1515.8311
1522.4406	1542.8437	1618.1582
1687.3023	1715.1446	1819.0808
2960.7264	2979.0444	3036.8204
3055.3438	3057.0652	3057.4994
3100.7928	3157.6906	3588.2946

P28

Cartesian coordinates

N	-0.190191	1.718834	0.743240
C	0.212350	2.026142	-0.596107
H	0.385024	2.241305	1.405157
H	0.735336	2.979436	-0.721229
H	-0.658536	1.985683	-1.258676
C	-2.374539	-0.870119	-0.219845
O	-1.142244	-0.878863	0.467855
H	-3.203796	-0.585479	0.438675
H	-2.560110	-1.881343	-0.584945
H	-2.365016	-0.190134	-1.082128
H	-0.954706	0.029588	0.771893
H	0.427093	-1.092212	-0.463539
C	2.146242	-0.987000	0.393228
O	1.343290	-0.967101	-0.762050
H	3.189324	-0.902923	0.081345
H	2.031428	-1.917529	0.963023
H	1.921990	-0.147643	1.070924
H	0.870616	1.202989	-0.933280

Vibrational frequencies

48.3161	64.6678	84.9146
95.0970	107.3725	113.0991
119.4622	132.9204	159.4098
206.3516	236.8798	241.3189
292.9175	724.3456	901.2821
1016.5068	1045.6434	1103.4616
1106.7123	1108.9056	1135.5983
1152.4950	1186.5177	1188.0372
1321.0630	1414.3277	1463.2954
1471.3258	1482.1470	1492.5645
1494.8237	1497.1727	1502.6322
1513.5674	1524.7536	1528.1313
2922.8228	2971.0933	3001.2415
3040.3674	3048.1936	3060.5924
3101.3074	3114.2812	3126.6586
3497.0735	3558.0276	3664.2307

R29**Cartesian coordinates**

N	0.252212	1.767786	0.703648
C	0.686952	1.859864	-0.604758
H	0.961996	1.846077	1.414866
H	1.506839	2.541674	-0.803468
H	-0.089759	1.789675	-1.360670
C	-2.628994	-0.406905	-0.331214
N	-1.480930	-0.639201	0.542291
H	-3.428137	0.082654	0.230548
H	-3.040206	-1.315283	-0.791643
H	-2.335105	0.271623	-1.135646
H	-0.442377	1.036187	0.884399
H	-1.729302	-1.275314	1.289838
H	-0.717754	-1.066206	0.018293
C	2.008442	-1.274555	0.372136
O	1.209756	-1.090673	-0.775395
H	3.014407	-0.855378	0.245422
H	2.106546	-2.348475	0.540879
H	1.554889	-0.822213	1.265400
H	1.162541	-0.130157	-0.933614

Vibrational frequencies

49.3890	58.8227	88.3287
90.4346	112.2166	128.3298
146.6231	152.5592	187.0298
205.8277	231.0433	290.3599
463.6599	568.0388	735.8204
785.3579	842.1548	957.6814
1001.9300	1041.7396	1091.9246
1100.3435	1129.0274	1186.8296
1195.5885	1278.5533	1359.2932
1376.4535	1451.0703	1467.4297
1484.7562	1488.7996	1497.2807
1504.7353	1519.4856	1525.1629
1693.4222	1702.7080	2993.1295
3005.8661	3050.5870	3086.6398
3120.7621	3122.1539	3123.7838
3231.4048	3360.5366	3479.3273
3570.3205	3604.4105	3664.6397

TS29**Cartesian coordinates**

N	0.007871	1.787737	0.637146
C	0.651672	1.667848	-0.585033
H	0.672830	2.064415	1.356091

H	1.578672	2.232265	-0.734128
H	-0.026939	1.774064	-1.441690
C	-2.388978	-0.559725	-0.351195
N	-1.231895	-0.543647	0.553241
H	-3.256055	-0.091113	0.116194
H	-2.635194	-1.582793	-0.637856
H	-2.125928	0.001066	-1.247803
H	-0.914347	0.481871	0.775565
H	-1.407122	-1.057062	1.409714
H	-0.293836	-0.899306	0.037011
C	1.980796	-1.216655	0.290847
O	0.970961	-0.930210	-0.631795
H	2.953190	-1.348297	-0.201186
H	1.763599	-2.145151	0.838582
H	2.095435	-0.413345	1.041955
H	0.935237	0.367626	-0.718515

Vibrational frequencies

-1065.2348	75.5208	90.2631
117.2300	135.3903	159.7022
175.9077	189.9181	253.3222
346.6395	410.5356	450.3795
553.6874	706.5222	735.0954
1010.0127	1040.0178	1055.2493
1065.4343	1080.6827	1101.9436
1188.4819	1194.6304	1208.1989
1238.3011	1331.2228	1351.3668
1394.9170	1459.6182	1485.7748
1493.7210	1497.7310	1509.4601
1512.2619	1517.0505	1549.4559
1655.3342	1711.7144	1742.1111
1916.6393	2330.1777	2937.3929
3006.4850	3008.5258	3041.0188
3071.0037	3085.2989	3152.9241
3163.9312	3520.0093	3581.8306

P29

Cartesian coordinates

N	0.185239	1.875054	0.782051
C	0.418812	1.978036	-0.629261
H	1.052770	2.122736	1.263908
H	1.130299	2.759577	-0.922321
H	-0.528302	2.124490	-1.156618
C	-2.452489	-0.565272	-0.313428
N	-1.310439	-0.754875	0.579673
H	-3.330274	-0.115641	0.168236
H	-2.749279	-1.525452	-0.741324

H	-2.152422	0.081085	-1.141311
H	-1.021026	0.141597	0.972363
H	-1.559081	-1.363030	1.350293
H	0.231025	-1.171030	-0.347155
C	2.041979	-1.202520	0.310421
O	1.124481	-1.193695	-0.751164
H	3.050546	-1.243047	-0.107312
H	1.914355	-2.073022	0.969167
H	1.969651	-0.297443	0.936046
H	0.822481	1.006030	-0.973125

Vibrational frequencies

56.9904	80.8573	92.2490
95.3979	98.4794	121.1428
129.9994	147.8071	164.8445
184.1111	213.2283	264.9292
311.7638	470.9521	913.9049
960.2899	998.8616	1037.0233
1042.7983	1090.3526	1095.4748
1115.7253	1150.4422	1186.6612
1201.6343	1332.3238	1374.1679
1415.9152	1467.9051	1476.4721
1487.0686	1497.3265	1499.9871
1508.0712	1510.3631	1524.2234
1553.9051	1689.4468	2917.7055
2962.1905	3012.3920	3019.0217
3037.7835	3093.0380	3097.6572
3106.3304	3127.7584	3445.0137
3469.2656	3477.8135	3601.6979

R30

Cartesian coordinates

N	-0.017381	1.868051	-0.663730
C	-0.372539	2.060512	0.659664
H	-0.727800	2.055307	-1.352854
H	-1.044050	2.885498	0.870425
H	0.405374	1.853549	1.387796
C	2.379318	-0.753112	0.278669
O	1.322550	-0.755221	-0.651381
H	2.182894	-0.092238	1.135517
H	3.276567	-0.391173	-0.227196
H	2.590496	-1.759451	0.664281
H	0.545727	1.042886	-0.863700
H	0.507468	-1.030619	-0.177018
C	-2.142681	-1.131909	-0.377276
N	-1.111322	-1.054455	0.657364
H	-3.159439	-0.938577	-0.013150

H	-2.123748	-2.119054	-0.844045
H	-1.912146	-0.395952	-1.150336
H	-1.099484	-0.112098	1.050362
H	-1.305935	-1.704427	1.409188

Vibrational frequencies

40.0612	63.7917	65.9562
87.1918	106.8122	118.6437
127.3865	156.2527	173.4713
209.2125	257.1505	275.6674
458.9983	539.2775	739.7732
781.1349	924.7109	958.0904
997.3770	1046.7527	1087.5702
1110.8860	1157.4655	1186.5253
1202.2836	1273.9353	1347.1544
1370.0821	1460.8279	1483.1096
1490.6403	1499.6727	1502.6098
1507.0232	1523.1970	1553.5318
1665.3675	1689.6057	2984.0384
3016.6267	3037.4709	3096.8107
3115.6203	3127.5863	3131.7915
3235.7105	3406.5011	3450.4389
3478.1185	3600.8285	3675.1312

TS30

Cartesian coordinates

N	0.201432	1.531689	-0.663115
C	-0.393976	1.904590	0.517918
H	-0.277698	1.919963	-1.468101
H	-1.051762	2.776632	0.535682
H	0.248163	1.824765	1.401926
C	2.404193	-0.707644	0.211595
O	1.159123	-0.765119	-0.435398
H	2.834969	0.298816	0.134045
H	3.109249	-1.416155	-0.238556
H	2.323729	-0.951202	1.282017
H	0.835391	0.256357	-0.651531
H	-0.182106	-0.978797	0.356780
C	-2.120747	-1.021375	-0.427632
N	-1.184656	-0.752867	0.675076
H	-3.131829	-0.726419	-0.146763
H	-2.100735	-2.076647	-0.698848
H	-1.791005	-0.423392	-1.276304
H	-1.110525	0.346164	0.825486
H	-1.433087	-1.234306	1.532339

Vibrational frequencies

-331.1176	29.9690	58.9002
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97.7206	133.4468	143.9518
167.9117	190.1404	222.2499
335.4343	351.3589	395.3681
640.1229	676.3364	895.5301
998.2295	1013.0089	1065.4429
1070.1558	1088.0432	1151.4630
1187.6041	1204.0634	1260.2397
1289.8217	1331.8538	1385.5045
1450.9887	1464.5781	1491.8180
1498.1849	1504.1489	1508.0436
1514.0042	1544.6672	1600.8529
1645.6379	1652.5895	1764.5151
2099.2268	2623.7458	2977.0116
3022.6963	3035.8733	3065.9250
3074.7312	3110.7459	3162.6075
3173.4229	3561.2957	3582.2318

P30

Cartesian coordinates

N	0.331915	1.651698	-0.733358
C	0.032252	1.979970	0.626258
H	-0.267736	2.195617	-1.355557
H	-0.432163	2.959774	0.780643
H	0.938178	1.893254	1.235279
C	2.271386	-0.952790	0.315731
O	1.255721	-1.011313	-0.658347
H	3.126520	-0.349028	-0.014142
H	2.625450	-1.970000	0.495301
H	1.909117	-0.544804	1.270986
H	1.017167	-0.092774	-0.879285
H	-0.545772	-1.193556	0.364453
C	-2.361108	-0.693401	-0.402407
N	-1.446533	-0.874948	0.718703
H	-3.330995	-0.341073	-0.040789
H	-2.529125	-1.592586	-1.011698
H	-1.958513	0.078636	-1.065711
H	-0.652140	1.187610	0.999135
H	-1.798613	-1.580483	1.353260

Vibrational frequencies

32.2249	72.3359	78.3715
85.3052	113.7060	119.6670
144.4787	147.2000	176.5445
198.4549	210.8350	248.4748
304.2806	445.7584	816.7582
934.1386	1016.8038	1025.7398
1040.0927	1095.2652	1105.6239

1110.7713	1142.9654	1187.0059
1193.0719	1322.9133	1380.7348
1416.0853	1462.0317	1469.2405
1484.2622	1491.4009	1499.5360
1501.0089	1511.5890	1526.6043
1527.4438	1691.8657	2859.0396
2985.3999	2996.5346	3040.3890
3043.3253	3068.1547	3096.2011
3105.9134	3113.9209	3481.8198
3492.4635	3595.3382	3610.0156

R3I

Cartesian coordinates

C	-1.837926	-1.740259	0.254958
O	-0.752050	-1.374796	-0.565893
H	-1.879218	-1.151151	1.181324
H	-1.715399	-2.791746	0.522291
H	-2.800344	-1.630813	-0.261494
H	-0.841383	-0.426709	-0.761730
N	-0.631802	1.507063	-0.533336
C	-1.550568	1.980677	0.403503
H	-0.576427	2.053765	-1.380846
H	-1.491893	1.549024	1.394731
H	-2.510251	2.321597	0.035440
H	1.875078	0.011716	1.566091
C	2.943286	-0.163645	-0.172168
N	1.697332	0.014143	0.569262
H	3.491498	-1.082912	0.074719
H	3.606093	0.686131	0.009060
H	2.722419	-0.185290	-1.241749
H	1.054943	-0.751131	0.369605
H	0.293813	1.286803	-0.149539

Vibrational frequencies

19.6225	42.6141	72.0012
81.6697	94.4075	115.0897
135.4470	164.1439	167.0034
206.7691	232.4561	266.0777
472.5771	549.5556	595.9149
790.6074	901.7367	959.3614
1001.6191	1052.3941	1092.9857
1107.7371	1143.6111	1186.4738
1195.4444	1241.2481	1353.0602
1374.6071	1467.4434	1473.3656
1483.2359	1494.5482	1498.3593
1506.1141	1523.4020	1526.1657
1689.6693	1697.6391	2995.1215

3004.4179	3047.6731	3084.8300
3115.9527	3122.4142	3149.8562
3265.1242	3353.4414	3485.8069
3604.9174	3631.5169	3635.1950

TS3I

Cartesian coordinates

C	2.014536	-1.216821	-0.239969
O	2.505169	-0.063468	0.362293
H	1.373162	-1.821875	0.428532
H	2.859179	-1.850003	-0.525953
H	1.439977	-1.011883	-1.162715
H	1.729566	0.499977	0.581983
N	0.121834	1.308498	0.603145
C	-0.244511	1.682806	-0.665650
H	-0.310615	1.914760	1.294580
H	0.458400	1.395402	-1.454477
H	-0.740973	2.639846	-0.843145
H	-1.181449	0.281986	-0.838104
C	-2.745716	-0.756898	0.272134
N	-1.379430	-0.683206	-0.251464
H	-3.448718	-0.947506	-0.538503
H	-2.978019	0.206097	0.726978
H	-2.832764	-1.539904	1.025996
H	-1.068638	-1.521481	-0.729620
H	-0.683145	-0.369242	0.475246

Vibrational frequencies

-524.3160	53.4229	65.1605
78.9035	111.7041	148.2691
175.0278	201.9705	208.9885
268.0072	359.4157	388.4692
522.0071	721.7402	828.3633
892.3174	957.1487	989.9966
1048.8538	1080.0864	1117.7742
1141.2710	1147.4440	1195.8021
1265.0485	1324.5159	1336.7067
1359.7769	1473.0478	1481.9236
1493.9056	1500.8990	1506.9504
1514.3120	1520.6318	1551.5537
1555.2386	1668.0285	1891.3998
2913.9341	2942.0045	2983.1404
3035.2746	3075.7066	3088.4057
3118.5156	3159.5498	3170.4252
3407.2115	3532.1426	3591.0771

P3I

Cartesian coordinates

C	-1.911401	-1.384706	0.190998
O	-2.515293	-0.239813	-0.354522
H	-1.461285	-2.032781	-0.577105
H	-2.686190	-1.963274	0.698314
H	-1.134278	-1.140943	0.931070
H	-1.812008	0.286654	-0.760352
N	-0.211798	1.408033	-0.683794
C	-0.185200	1.771109	0.702634
H	0.553262	1.884009	-1.165943
H	-1.155095	1.549398	1.153520
H	0.098230	2.813959	0.889104
H	0.562032	1.121628	1.193837
C	2.892727	-0.447976	-0.259318
N	1.651119	-0.921849	0.342452
H	3.707522	-0.545346	0.461888
H	2.797161	0.617015	-0.490624
H	3.191422	-0.965614	-1.181959
H	1.724119	-1.901959	0.585696
H	0.885442	-0.838089	-0.317763

Vibrational frequencies

30.3095	46.4208	60.5694
77.1885	104.6714	115.2867
125.4760	134.0362	163.7066
181.5160	187.9337	228.3689
314.1144	386.5608	739.7229
887.0657	985.0214	995.8260
1033.2312	1092.9637	1096.7294
1113.0311	1136.5060	1181.1872
1191.0191	1328.3134	1357.8799
1399.8149	1462.2545	1467.0512
1474.1025	1496.9812	1500.2423
1502.9289	1505.0313	1524.4659
1527.3296	1678.1593	2945.4081
2970.4200	2994.3955	3017.0843
3044.8529	3075.2352	3110.8670
3115.5374	3118.8456	3481.2898
3536.7453	3622.2868	3726.3062

R32**Cartesian coordinates**

N	-0.048996	1.824090	-0.689556
C	-0.423371	2.052599	0.622957
H	-0.765636	1.963770	-1.384296
H	-1.117430	2.866609	0.802540
H	0.348452	1.883884	1.367319

C	2.541072	-0.640606	0.342001
N	1.424815	-0.771193	-0.589347
H	3.388631	-0.160790	-0.154193
H	2.890247	-1.589829	0.772424
H	2.240305	0.008220	1.168627
H	0.530816	0.994718	-0.852181
H	1.670232	-1.388347	-1.353458
H	0.610875	-1.166647	-0.111325
C	-2.181038	-1.101038	-0.420547
N	-1.284655	-1.084553	0.731939
H	-3.179761	-0.683693	-0.231022
H	-2.303603	-2.125599	-0.781421
H	-1.722751	-0.520375	-1.224926
H	-1.164062	-0.119612	1.042016
H	-1.684446	-1.606444	1.502179

Vibrational frequencies

30.3298	48.3055	83.3023
88.5751	102.3518	130.5266
135.1250	150.9432	164.3506
220.3965	227.4388	262.9471
415.1729	522.2983	555.9277
734.3697	832.0175	932.8830
959.7617	1002.0345	1011.9648
1056.8991	1091.5310	1094.7801
1194.5460	1198.3981	1273.8287
1356.1291	1370.6854	1384.2069
1459.1723	1464.4508	1486.5329
1503.7369	1504.0212	1523.8866
1525.6881	1671.0529	1698.2765
1706.3977	2996.1957	2998.4477
3079.1505	3080.6075	3116.0852
3119.5096	3125.5101	3232.5774
3356.1299	3416.2425	3448.7510
3598.0193	3598.2785	3661.5721

TS32

Cartesian coordinates

N	0.075060	1.644159	0.712908
C	0.499591	1.897539	-0.572595
H	0.744334	2.013876	1.382151
H	1.247085	2.674635	-0.760514
H	-0.284815	1.865263	-1.338896
C	-2.412497	-0.528303	-0.303904
N	-1.231783	-0.681218	0.545768
H	-3.234505	-0.023398	0.212096
H	-2.768770	-1.496568	-0.666934

H	-2.138953	0.083037	-1.166719
H	-0.839639	0.299067	0.818355
H	-1.441622	-1.220029	1.378084
H	-0.098982	-1.001797	-0.139765
C	2.046918	-1.137541	0.340648
N	1.008475	-0.918131	-0.672690
H	3.047461	-0.979400	-0.066380
H	1.978180	-2.146959	0.751255
H	1.870141	-0.409272	1.133457
H	1.009954	0.128378	-0.924467
H	1.143788	-1.490681	-1.498516

Vibrational frequencies

-961.2655	89.7039	114.0637
140.4458	147.2036	156.9079
177.3905	192.8575	220.7868
294.9644	316.4365	379.2908
585.5739	648.0130	664.8152
747.8830	866.5721	1007.1207
1016.2482	1052.1547	1076.4224
1094.2358	1113.9616	1134.0071
1273.0492	1316.8173	1330.8076
1339.3581	1355.0170	1379.2451
1460.1516	1468.0249	1496.1589
1505.9729	1513.3078	1520.4740
1521.9069	1611.4163	1718.2143
1763.3964	1785.5574	2349.9517
2560.8317	3004.0088	3037.1091
3059.0710	3082.7789	3102.6188
3126.1705	3136.6172	3157.2365
3523.8279	3577.1823	3577.8146

P32

Cartesian coordinates

N	-0.016989	1.845320	0.773063
C	0.183390	1.996868	-0.637266
H	0.827186	2.177332	1.245921
H	0.792589	2.863342	-0.924646
H	-0.780813	2.035171	-1.152799
C	-2.428654	-0.733482	-0.359430
N	-1.381695	-0.918176	0.640863
H	-3.297930	-0.156144	-0.014064
H	-2.785330	-1.706683	-0.707081
H	-2.005568	-0.216772	-1.224967
H	-1.066392	-0.008305	0.977028
H	-1.739929	-1.429873	1.437658
H	0.413057	-1.270038	-0.378385

C	2.269039	-0.945701	0.382356
N	1.343209	-1.043833	-0.738055
H	3.264528	-0.663638	0.027349
H	2.370494	-1.861772	0.983203
H	1.924484	-0.153622	1.054764
H	0.701558	1.081625	-0.997034
H	1.627738	-1.779908	-1.371996

Vibrational frequencies

27.9792	67.7616	81.2155
83.8619	91.8220	114.6712
140.9688	150.9537	167.5936
178.8557	213.6213	221.2202
339.5957	419.1752	523.9651
937.4655	942.6723	1001.5134
1018.3243	1035.3458	1040.1632
1093.2504	1097.3241	1099.0519
1194.3528	1195.3168	1333.7911
1376.6111	1386.6861	1418.0558
1459.9990	1464.2407	1479.8440
1500.7707	1501.2453	1509.4720
1524.2601	1526.0805	1689.3490
1697.3282	2856.8186	2984.4856
2996.0341	3027.7668	3063.2581
3077.9553	3093.0579	3102.5589
3114.3531	3423.1796	3464.7639
3468.9697	3599.3511	3601.6685

R33

Cartesian coordinates

N	-1.182826	-1.899392	-0.816797
C	-1.769765	-0.864586	-1.515259
H	-1.778899	-2.420527	-0.194005
H	-2.791828	-1.019540	-1.845757
H	-1.111372	-0.329703	-2.193160
C	2.616823	-1.458575	0.528195
O	1.280012	-1.031266	0.400944
H	3.101604	-1.017902	1.407459
H	3.214585	-1.214482	-0.359510
H	2.613402	-2.543450	0.648349
H	-0.244657	-1.737997	-0.450839
C	-1.627804	0.329670	1.785292
O	-1.632301	1.162407	0.635665
H	-2.590563	-0.178619	1.909497
H	-1.464814	0.970889	2.652593
H	-0.826251	-0.416333	1.740264
H	0.028251	1.661482	0.337921

H	-1.828492	0.590340	-0.135078
C	1.130871	2.046483	-1.229671
O	0.981179	1.647735	0.117491
H	0.538267	1.424428	-1.912372
H	2.184385	1.939840	-1.493436
H	0.844160	3.094207	-1.372589
H	1.260144	-0.055845	0.334093

Vibrational frequencies

26.9640	57.5318	60.9601
69.8382	84.7317	92.3239
111.0733	112.1169	126.3603
134.0654	144.3456	164.5088
194.7035	212.9403	229.3678
255.9676	287.6048	298.0459
562.5847	725.7456	782.5755
838.5803	849.7887	895.8973
1007.4971	1083.4871	1101.0725
1114.4855	1132.1055	1149.6107
1162.3671	1188.5679	1194.7111
1208.7497	1285.5754	1350.6363
1455.5118	1484.2618	1485.2884
1486.6837	1490.4845	1490.9252
1501.4735	1504.9585	1509.1944
1519.2675	1529.3188	1535.9289
1550.0603	1698.7971	3006.4105
3015.6273	3021.6576	3065.9416
3077.7081	3089.2780	3125.3478
3130.4747	3131.9845	3138.3186
3237.4091	3423.7555	3468.1647
3509.0107	3569.3334	3676.5222

TS33

Cartesian coordinates

N	0.650373	-1.921900	0.696371
C	1.363417	-1.012331	1.437364
H	1.184473	-2.649118	0.240682
H	2.289116	-1.375893	1.884331
H	0.735664	-0.440283	2.125618
C	-2.535323	-1.142710	-0.632729
O	-1.205937	-0.747832	-0.494694
H	-2.713538	-1.662827	-1.586021
H	-3.215742	-0.278164	-0.606667
H	-2.850106	-1.822712	0.175023
H	-0.275060	-1.532125	0.191199
C	1.838502	0.266489	-1.553450
O	1.757775	0.913757	-0.285077

H	2.728689	-0.365789	-1.565995
H	1.931482	1.023566	-2.334500
H	0.941658	-0.335657	-1.734175
H	0.765648	1.309966	-0.209964
H	1.678145	-0.032831	0.606564
C	-1.109446	2.029121	1.045544
O	-0.597839	1.551959	-0.174166
H	-1.019690	1.285419	1.851138
H	-2.169823	2.286971	0.945492
H	-0.568226	2.930888	1.346880
H	-0.970199	0.525399	-0.353081

Vibrational frequencies

-1007.0797	37.0139	59.1953
69.1171	77.2936	92.4671
101.9347	109.7022	130.4363
141.0801	153.8010	185.9031
193.3414	269.8436	372.5848
416.5929	440.6088	500.7555
624.3815	701.3685	985.5639
1012.6444	1065.9033	1098.8118
1110.7768	1128.3434	1162.8235
1169.9477	1184.6090	1189.6722
1199.8266	1201.7736	1218.6065
1274.1573	1297.2433	1384.6917
1426.5547	1448.3440	1470.7356
1481.3767	1492.9685	1496.7727
1497.8260	1501.3424	1512.4481
1516.9130	1518.4774	1522.1801
1536.6379	1649.1770	1680.4288
1743.4937	2007.7371	2091.2817
2962.2140	2993.6515	3005.0284
3015.9908	3035.1826	3059.3577
3065.9071	3096.4684	3121.4621
3133.9335	3160.7419	3623.8995

P33

Cartesian coordinates

N	0.000050	-2.148827	0.299780
C	0.370773	-1.445387	1.486879
H	0.615550	-2.954315	0.179743
H	0.631511	-2.102133	2.325914
H	-0.425594	-0.756692	1.779484
C	-2.888059	-0.455415	-0.477985
O	-1.597339	-0.355493	-1.040958
H	-3.439389	-1.310588	-0.885311
H	-3.435179	0.455102	-0.728327

H	-2.856507	-0.551433	0.615658
H	-1.073151	-1.125308	-0.737351
C	2.544875	-0.193319	-1.116896
O	2.439470	0.501556	0.102153
H	3.503363	-0.716686	-1.127456
H	2.512305	0.481894	-1.980716
H	1.742901	-0.939284	-1.242228
H	1.630129	1.039859	0.046164
H	1.262691	-0.828089	1.257702
C	-0.699510	2.297055	0.873860
O	-0.019031	1.691006	-0.200847
H	-0.964439	1.576474	1.659960
H	-1.615847	2.799436	0.541112
H	-0.038335	3.047514	1.310039
H	-0.603635	1.011878	-0.590778

Vibrational frequencies

34.5118	55.2784	72.3893
76.6583	93.1631	101.7239
110.8853	116.2878	122.7512
129.8835	136.6164	146.8102
168.0591	187.5882	223.8622
272.5045	281.3341	310.4373
407.9039	737.4659	811.2514
930.9038	1005.3171	1046.3636
1101.0182	1106.8432	1113.0913
1115.0712	1137.2316	1147.3941
1162.9118	1183.6554	1186.1075
1187.6293	1336.3283	1419.8189
1478.3905	1481.7702	1484.4078
1488.0382	1488.6863	1495.8293
1498.8272	1499.7193	1505.6426
1506.7433	1513.1267	1527.5361
1529.4762	1549.9092	2898.5299
2971.7544	3000.2083	3006.3338
3042.7750	3047.1973	3058.7482
3067.8693	3118.3668	3119.2139
3127.3511	3128.7986	3477.4555
3500.5750	3557.9658	3634.5091

R34

Cartesian coordinates

C	3.265567	-0.318598	0.643996
O	2.884051	-0.054684	-0.684077
H	2.547371	0.082772	1.374571
H	4.227154	0.168624	0.816802
H	3.388441	-1.392176	0.840201

H	2.078874	-0.558778	-0.859238
N	0.161795	-1.238588	-0.795219
C	-0.070527	-1.657927	0.507517
H	-0.133600	-1.874898	-1.520102
H	0.261905	-0.972893	1.281603
H	0.016834	-2.719189	0.707881
C	-3.445229	-0.373918	-0.234630
O	-2.556349	0.062197	0.778593
H	-2.921335	-0.577216	-1.176976
H	-4.165608	0.426571	-0.404736
H	-3.992047	-1.273323	0.068991
H	-1.914998	-0.651328	0.925099
H	-1.360441	1.274399	-0.013793
C	0.413484	2.075835	0.239302
O	-0.593776	1.489030	-0.567416
H	0.467078	1.604751	1.229507
H	0.241559	3.149311	0.375310
H	1.371393	1.921358	-0.259643
H	-0.096314	-0.262563	-0.972867

Vibrational frequencies

40.5637	52.7883	70.9154
77.8806	103.2267	105.4461
109.5090	114.5633	119.6579
143.4071	149.2272	173.4769
184.8417	186.3975	208.4513
239.7407	260.9698	320.4896
555.6338	607.6569	696.5077
779.4617	805.2200	916.9245
1037.4332	1087.3716	1096.0405
1108.2397	1127.3275	1136.6998
1159.0127	1191.6346	1195.9337
1201.8873	1259.6705	1364.9382
1432.9357	1447.6380	1456.0086
1485.4194	1495.7217	1502.3673
1502.9201	1507.2288	1512.3436
1516.2321	1518.5714	1520.9250
1531.3079	1675.8712	2985.7670
3009.2389	3016.1399	3038.7034
3071.5494	3078.3894	3118.3814
3137.7210	3138.6182	3141.5454
3250.3918	3366.8383	3648.8305
3653.7441	3702.8436	3756.1958

TS34

Cartesian coordinates

C	3.121790	-0.374113	0.726594
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O	2.799723	0.016510	-0.584345
H	2.404891	0.011614	1.468769
H	4.105128	0.034835	0.968946
H	3.169847	-1.465610	0.839385
H	1.964203	-0.425097	-0.817193
N	0.182783	-1.090340	-0.880295
C	-0.253352	-1.704772	0.273802
H	-0.109941	-1.602685	-1.706377
H	0.306757	-1.425447	1.172368
H	-0.516483	-2.764372	0.238175
C	-3.339085	-0.246015	-0.039005
O	-2.167989	0.022257	0.726108
H	-3.084395	-0.724822	-0.990544
H	-3.851666	0.695873	-0.237667
H	-3.997513	-0.899695	0.534229
H	-1.451705	-0.874644	0.642333
H	-1.485247	0.760784	0.159966
C	0.351731	2.079702	0.178091
O	-0.589421	1.283189	-0.543107
H	0.280512	1.881546	1.253168
H	0.137175	3.133247	-0.005442
H	1.360719	1.839006	-0.162826
H	-0.136782	0.353393	-0.821368

Vibrational frequencies

-1340.8354	38.0982	62.8339
81.4347	96.2897	108.9436
127.6394	143.7387	156.7540
167.8820	172.7607	183.2971
194.2310	238.0463	264.1939
371.7476	417.5234	506.7685
588.0998	738.2030	803.1200
985.8106	1043.7529	1056.7610
1092.4344	1110.9391	1130.4243
1142.6715	1170.3630	1192.3097
1193.5127	1195.5270	1213.3955
1243.6105	1293.0947	1353.1298
1397.7597	1476.5360	1478.3703
1491.4828	1493.8053	1496.4293
1503.5992	1506.9926	1513.2172
1521.4554	1524.3521	1527.2775
1549.0327	1588.6037	1663.4334
1797.1395	2048.9199	2972.6578
3032.1172	3035.4722	3036.1141
3044.2375	3114.8528	3117.2584
3124.9727	3126.6290	3150.5362
3153.8745	3555.0481	3604.4244

P34**Cartesian coordinates**

C	2.831781	0.988191	-0.089668
O	1.561663	0.713512	-0.643238
H	2.990927	0.462993	0.860715
H	2.891325	2.061626	0.097061
H	3.637682	0.713765	-0.779888
H	1.473552	-0.257856	-0.740622
N	1.116681	-1.992011	-0.388858
C	0.632343	-2.179590	0.942786
H	0.915392	-2.825784	-0.942351
H	1.084059	-1.446148	1.615051
H	0.782155	-3.194501	1.330408
C	-2.099638	-0.869907	-1.003910
O	-2.184384	-0.833368	0.399264
H	-1.062918	-0.990223	-1.357352
H	-2.507799	0.037315	-1.468633
H	-2.683742	-1.722558	-1.357096
H	-0.457973	-1.978176	0.942094
H	-1.712871	-0.028120	0.679467
C	-1.203334	2.554249	0.108969
O	-0.654582	1.416322	0.739974
H	-0.578468	3.442044	0.263869
H	-2.182631	2.743995	0.551887
H	-1.332792	2.404830	-0.970267
H	0.178855	1.191488	0.280598

Vibrational frequencies

19.7078	45.2083	50.3708
75.1461	80.3734	89.3619
98.3682	101.6757	106.5238
129.8963	135.4350	144.5830
151.7972	168.9071	210.9697
239.0200	266.5086	303.9611
404.5028	813.3626	866.0011
938.2130	1002.5351	1047.8067
1100.3198	1107.9586	1110.7585
1113.3440	1139.1543	1147.5487
1163.7749	1188.4706	1188.7076
1189.3866	1335.0216	1415.7576
1471.5453	1478.6769	1481.0181
1488.1850	1491.8835	1495.6627
1497.4560	1500.0682	1500.6767
1505.7612	1507.2845	1522.4548
1524.9973	1542.9608	2897.5996
2970.9751	3005.9149	3008.3429

3033.3621	3039.8039	3064.1261
3069.0478	3110.3258	3112.1643
3122.8154	3126.2688	3455.2946
3498.1927	3546.6857	3618.3687

R35

Cartesian coordinates

N	0.822108	-2.153830	0.402309
C	1.117322	-1.379428	1.504768
H	1.595147	-2.620247	-0.044542
H	1.907676	-1.734889	2.158154
H	0.262266	-0.908409	1.981623
C	-2.525060	-1.225436	-0.330736
N	-1.343428	-0.834973	-1.099952
H	-2.722470	-2.291389	-0.468073
H	-3.435854	-0.670132	-0.590626
H	-2.327984	-1.067017	0.732484
H	-1.509401	-0.979454	-2.088771
H	0.106910	-1.786754	-0.238979
C	2.224413	0.501728	-1.234128
O	1.848331	1.060561	0.009910
H	3.179775	-0.031015	-1.161130
H	2.342701	1.322641	-1.942959
H	1.462082	-0.187413	-1.617187
H	0.224978	1.781655	-0.148655
H	1.729116	0.318875	0.638742
C	-1.261425	2.006907	1.076405
O	-0.731058	1.954106	-0.227853
H	-1.108167	1.067470	1.627041
H	-2.336135	2.181555	0.994960
H	-0.825135	2.823638	1.664683
H	-1.165962	0.162548	-0.967572

Vibrational frequencies

45.1744	59.6712	61.7147
82.7062	83.7062	100.5848
116.8182	123.0411	130.2429
146.2636	158.6477	166.8585
181.8631	195.4647	209.9424
248.9921	275.8713	307.8293
481.2570	575.4885	718.0393
820.9743	852.7894	863.3247
979.8610	1012.4153	1053.5239
1089.2400	1093.7113	1106.3443
1135.2154	1153.0479	1183.8859
1194.7859	1213.2857	1285.5151
1355.6012	1388.7553	1458.7562

1472.4364	1485.3963	1488.4305
1490.1671	1498.3422	1503.0762
1505.6829	1509.6336	1526.3724
1531.8715	1539.6566	1700.3412
1705.9230	2996.6535	3012.4118
3015.4021	3053.8602	3076.6929
3091.3731	3121.0054	3123.3423
3124.7631	3133.8707	3230.3761
3291.9293	3433.8585	3459.7848
3590.2309	3609.0903	3668.9050

TS35

Cartesian coordinates

N	0.232680	-2.140376	0.403917
C	0.789043	-1.353984	1.415878
H	0.851265	-2.907803	0.155660
H	1.478544	-1.860655	2.100061
H	0.018384	-0.805249	1.972849
C	-2.765944	-0.633711	-0.279716
N	-1.437648	-0.538613	-0.904494
H	-3.208668	-1.612223	-0.467016
H	-3.425761	0.146908	-0.659307
H	-2.645309	-0.504036	0.795398
H	-1.485128	-0.653625	-1.911692
H	-0.771643	-1.299315	-0.476499
C	2.232454	-0.027980	-1.176605
O	1.946538	0.633155	0.004909
H	3.313782	-0.150312	-1.332422
H	1.828712	0.502965	-2.055384
H	1.785518	-1.047985	-1.198320
H	0.795347	1.261298	-0.150521
H	1.409067	-0.461172	0.894681
C	-0.613219	2.319750	0.891203
O	-0.223265	1.662065	-0.285683
H	-0.707587	1.631593	1.746795
H	-1.581735	2.809442	0.740503
H	0.113541	3.091740	1.169411
H	-0.973731	0.425138	-0.678534

Vibrational frequencies

-470.5565	31.4847	60.1018
77.8495	87.9120	122.2447
127.7237	146.1892	156.9758
174.7237	179.9588	185.2143
198.3596	260.4220	334.6941
363.9790	395.1213	465.2041
635.1658	674.3683	981.5468

1006.9903	1041.2668	1061.0851
1075.6384	1087.0821	1112.5951
1140.1165	1183.4866	1186.5161
1195.8629	1199.4585	1228.0746
1286.0745	1333.1548	1344.3975
1383.5879	1425.6893	1443.3386
1469.2958	1492.3015	1496.2970
1499.9703	1503.4369	1504.8613
1511.2855	1513.9836	1518.7589
1522.5615	1669.5118	1718.5513
1746.4242	1785.2833	1813.5755
2187.7802	2371.6877	2851.8440
2964.3271	2973.4072	3011.5880
3015.7392	3045.8517	3075.8751
3079.5857	3085.8959	3160.1780
3167.2794	3542.7077	3574.2798

P35

Cartesian coordinates

N	0.234035	-2.265312	0.361661
C	0.459018	-1.423884	1.498378
H	0.987458	-2.955718	0.327651
H	0.736247	-1.979390	2.404429
H	-0.425032	-0.812354	1.696628
C	-2.927977	-0.514567	-0.408846
N	-1.632027	-0.408029	-1.078914
H	-3.502501	-1.406841	-0.687040
H	-3.534081	0.367355	-0.629380
H	-2.768553	-0.543535	0.671685
H	-1.753677	-0.401725	-2.084686
H	-1.052292	-1.215846	-0.841230
C	2.479110	-0.095931	-1.165032
O	2.426587	0.635788	0.034055
H	3.451883	-0.589888	-1.220434
H	2.372605	0.547500	-2.048083
H	1.696822	-0.871282	-1.214589
H	1.586622	1.129808	0.019772
H	1.293299	-0.733875	1.270815
C	-0.763180	2.252671	0.939902
O	-0.091612	1.694218	-0.163058
H	-0.929843	1.521053	1.743533
H	-1.734276	2.676527	0.653582
H	-0.147512	3.059653	1.341748
H	-0.652851	0.972168	-0.538017

Vibrational frequencies

33.3690	36.2838	58.3873
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72.2869	78.6155	84.2737
99.2395	103.4543	111.6019
124.9906	147.2886	164.0692
172.7874	185.7007	207.7562
229.3198	244.3384	302.7960
380.8380	495.3293	794.9504
950.7810	977.1198	996.5927
1032.5154	1061.4596	1088.5601
1095.8712	1109.5462	1114.7630
1142.7559	1162.0551	1186.2661
1189.3875	1211.2980	1336.3488
1379.6170	1418.5166	1468.4901
1481.8077	1482.8877	1488.4268
1495.5535	1500.4170	1501.7409
1504.2354	1506.8158	1511.6032
1522.2425	1536.1681	1579.5533
1696.8364	2924.6923	2969.2295
2993.7660	3018.2256	3030.1026
3037.3060	3048.7842	3093.3529
3108.4826	3111.9555	3124.0535
3127.3486	3306.2157	3435.5693
3475.3890	3592.9904	3608.1729

R36

Cartesian coordinates

N	-1.155195	-1.879627	-0.805258
C	-1.658959	-0.872822	-1.603562
H	-1.818533	-2.364107	-0.221847
H	-2.640277	-1.038999	-2.036436
H	-0.929756	-0.361091	-2.224188
C	2.538772	-1.525106	0.612516
O	1.215235	-1.049637	0.605481
H	3.111718	-1.129598	1.461558
H	3.076148	-1.276211	-0.312864
H	2.510518	-2.612928	0.703674
H	-0.259480	-1.703108	-0.347687
C	-1.831212	0.407061	1.656239
O	-1.847480	1.232589	0.506710
H	-0.943129	-0.235964	1.689962
H	-2.727372	-0.223473	1.713733
H	-1.824146	1.061191	2.530359
H	-1.917100	0.641782	-0.268107
C	1.416197	1.910981	-1.255207
N	1.054746	1.649539	0.137287
H	0.920726	1.175961	-1.893178
H	2.493526	1.786836	-1.388695

H	1.137504	2.911074	-1.609369
H	0.045265	1.749581	0.266837
H	1.509276	2.311381	0.754406
H	1.227430	-0.066010	0.500198

Vibrational frequencies

25.5496	44.8380	56.8757
67.8381	74.3027	91.4966
94.7686	101.8864	119.7667
127.5772	145.5878	157.9466
170.3745	191.7580	211.6472
236.0559	262.6680	301.3925
511.6949	558.9338	751.3955
794.6812	833.0389	918.4186
1002.8323	1020.7693	1053.0808
1089.6549	1091.3528	1118.3498
1134.1356	1165.7445	1186.4254
1198.1533	1210.5559	1283.4853
1349.4858	1376.8192	1454.1077
1465.2549	1486.4711	1489.4679
1491.5560	1499.0642	1503.6537
1507.0725	1512.0599	1523.0649
1527.0746	1575.4744	1697.7133
1703.2168	2990.6876	3005.8365
3018.6140	3045.1589	3069.5435
3093.7595	3112.3182	3118.0767
3122.9987	3126.5279	3229.5595
3282.7481	3429.3267	3433.8634
3519.2680	3600.9047	3671.6898

TS36

Cartesian coordinates

N	-0.060365	-2.023531	0.152082
C	0.582798	-1.498529	1.252206
H	0.432916	-2.830489	-0.216650
H	1.212991	-2.167817	1.849904
H	-0.075289	-0.888139	1.885631
C	-2.894506	-0.507694	-0.227120
O	-1.676625	-0.366471	-0.917680
H	-3.728987	-0.625857	-0.927562
H	-3.103982	0.370132	0.401227
H	-2.864522	-1.387627	0.426268
H	-1.034060	-1.113997	-0.575221
C	2.649115	-0.192543	-0.917292
O	2.031397	0.393975	0.200152
H	2.208312	-1.175043	-1.140668
H	3.724796	-0.321547	-0.752788

H	2.518008	0.434855	-1.809918
H	1.443494	-0.495098	0.772099
C	-0.518020	2.304598	0.868268
N	-0.058486	1.676730	-0.381789
H	-0.631950	1.520662	1.616442
H	-1.476483	2.805271	0.726143
H	0.224020	3.020335	1.221953
H	0.927261	1.134303	-0.176585
H	0.052296	2.360038	-1.123234
H	-0.751359	0.932601	-0.685239

Vibrational frequencies

-951.4248	33.2251	45.9222
64.9162	70.5809	86.0743
96.6726	117.6447	136.7970
155.8158	161.5805	172.5160
186.2015	250.4856	306.3163
373.7255	400.5544	483.5876
526.6988	644.3022	703.6962
1004.6762	1024.2451	1036.0013
1072.1736	1079.5567	1095.5097
1113.9442	1175.8951	1178.7068
1185.0207	1188.2354	1233.9875
1278.4227	1297.1735	1325.0373
1364.4647	1390.7941	1447.8434
1477.8324	1479.4324	1492.3438
1494.6495	1497.6420	1508.2025
1511.0740	1512.6626	1520.6408
1568.2555	1610.1963	1660.3413
1682.8874	1731.1177	1825.3477
2284.9680	2814.4675	2983.3831
2989.4783	2990.8550	3036.9518
3046.9960	3063.9159	3067.4908
3071.7298	3077.1106	3156.5586
3165.9955	3552.1638	3579.7044

P36

Cartesian coordinates

N	-0.070359	-2.181574	0.208957
C	0.310501	-1.563855	1.440074
H	0.563949	-2.958122	0.015970
H	0.630703	-2.272658	2.213763
H	-0.506817	-0.943483	1.817246
C	-2.912811	-0.358764	-0.359368
O	-1.718406	-0.354398	-1.105449
H	-3.493770	-1.275933	-0.518128
H	-3.519381	0.487189	-0.689374

H	-2.733942	-0.248892	0.720152
H	-1.175844	-1.107015	-0.801024
C	2.550242	-0.305344	-1.054217
O	2.418864	0.417472	0.142530
H	1.682031	-0.957074	-1.247961
H	3.440288	-0.934986	-0.980137
H	2.672372	0.350804	-1.926760
H	1.166968	-0.888689	1.235051
C	-0.539040	2.306769	0.972674
N	0.071471	1.855727	-0.276955
H	-0.604520	1.461922	1.662435
H	-1.547397	2.724235	0.853381
H	0.092175	3.063020	1.444890
H	1.644405	1.014201	0.024796
H	0.157311	2.630785	-0.923741
H	-0.533322	1.158191	-0.716197

Vibrational frequencies

35.2526	53.7124	63.8366
71.3918	88.7985	89.6853
92.2244	108.0485	119.1845
132.2575	133.1574	147.6785
158.3195	177.7641	204.9024
221.5129	265.6273	289.3129
405.3413	477.9258	836.5755
949.7282	995.2461	1006.9452
1044.7903	1052.7534	1091.9114
1107.6254	1111.9893	1113.7669
1144.2933	1154.9384	1187.9111
1188.5566	1219.5981	1336.5439
1388.5804	1419.4935	1463.0614
1481.8790	1483.0115	1488.3384
1492.6980	1496.0120	1498.9306
1502.4385	1508.3255	1510.1480
1523.5069	1530.1436	1566.1311
1693.8398	2879.6879	2961.1458
2989.1813	3010.5761	3025.1758
3035.1747	3047.0139	3090.5911
3102.6342	3103.6104	3114.1131
3124.7871	3380.7369	3443.1218
3494.1957	3557.9403	3594.3496

R37

Cartesian coordinates

N	1.238120	-1.939285	0.697655
C	1.827814	-1.038692	1.565552
H	1.831333	-2.318337	-0.023265

H	2.855217	-1.238186	1.851461
H	1.173453	-0.619083	2.322620
C	-2.575649	-1.480581	-0.592382
O	-1.266385	-0.989953	-0.423031
H	-3.068367	-1.034137	-1.464701
H	-3.201510	-1.300701	0.291220
H	-2.512262	-2.558864	-0.750267
H	0.298950	-1.718104	0.369384
C	1.511967	0.430904	-1.875149
N	1.545044	1.266320	-0.670558
H	2.458769	-0.085157	-2.078990
H	1.264584	1.048616	-2.741526
H	0.722640	-0.314717	-1.762065
H	2.241923	1.995998	-0.762217
H	-0.124875	1.700016	-0.284753
H	1.813191	0.690032	0.132326
C	-1.086424	1.930611	1.397394
O	-1.069135	1.668492	0.010889
H	-0.371012	1.302345	1.944149
H	-2.088726	1.716463	1.773929
H	-0.860170	2.982437	1.610967
H	-1.297370	-0.019630	-0.293307

Vibrational frequencies

22.0462	52.3407	57.5476
77.6902	83.4442	93.9550
105.0425	108.8979	120.4739
136.7975	142.1964	166.2494
180.0530	197.7031	239.8505
253.3958	285.4396	304.7992
489.8939	548.6935	752.5147
801.9903	868.4088	971.3599
993.2301	996.6568	1051.0286
1082.0848	1103.6477	1116.6159
1152.4606	1170.3958	1186.0372
1193.9380	1221.9965	1277.1339
1343.8163	1373.9142	1472.8485
1481.7740	1484.5900	1489.4395
1492.4129	1503.9328	1505.5756
1512.8415	1521.1953	1532.2979
1542.0851	1579.0063	1674.0941
1694.0320	3004.7129	3007.0360
3017.2222	3063.2198	3064.0096
3099.4583	3120.6886	3123.5312
3131.3702	3141.1883	3238.7861
3276.3783	3390.9026	3459.6303
3509.4601	3589.8575	3670.1141

TS37**Cartesian coordinates**

N	0.750450	-1.731267	0.846745
C	1.405433	-0.854601	1.674090
H	1.357200	-2.467809	0.505471
H	2.300133	-1.197690	2.199877
H	0.749845	-0.230280	2.289316
C	-2.157280	-1.651042	-0.658559
O	-1.021384	-0.834711	-0.628087
H	-2.289147	-2.129261	-1.639108
H	-3.070948	-1.078812	-0.445154
H	-2.084772	-2.447773	0.096071
H	-0.239089	-1.286335	0.075358
C	1.824611	0.269447	-1.594626
N	1.696495	1.039632	-0.340440
H	2.735871	-0.327958	-1.561829
H	1.852373	0.943912	-2.450968
H	0.953113	-0.382213	-1.665151
H	2.417625	1.747489	-0.244949
H	0.742825	1.480697	-0.289946
H	1.737863	0.332966	0.541101
C	-1.506046	1.944790	1.005214
O	-0.928521	1.688691	-0.257125
H	-1.122882	1.266643	1.779106
H	-2.596499	1.840151	0.969576
H	-1.273470	2.973043	1.292222
H	-1.099729	0.721259	-0.470147

Vibrational frequencies

-538.8099	54.1288	64.6789
91.0928	101.4707	109.1143
120.5247	132.6695	136.4594
147.0249	151.6731	179.0636
193.9307	232.8273	308.8135
323.6963	350.3190	392.1581
600.8826	689.3061	720.0875
942.0485	1003.4369	1030.8512
1050.4880	1068.6160	1081.5923
1101.6939	1142.0329	1170.9589
1188.3978	1195.5006	1205.9513
1283.1757	1307.2838	1339.5785
1344.8247	1449.9960	1472.4721
1483.0211	1496.1693	1497.4087
1500.5635	1504.4517	1511.2720
1512.8869	1519.7652	1530.5721
1574.9117	1585.0669	1655.1110

1696.1226	1712.0838	1827.5756
2906.9310	2971.5684	2996.8649
3029.0669	3031.1930	3035.3589
3061.2069	3068.0195	3080.3352
3112.8461	3117.6074	3159.4147
3165.9252	3568.8358	3569.3715

P37

Cartesian coordinates

N	0.374283	-2.106951	0.669460
C	1.145089	-1.414101	1.648096
H	0.944352	-2.840401	0.246355
H	1.879945	-2.034690	2.174385
H	0.485934	-0.916617	2.365115
C	-2.763251	-0.982205	-0.755366
O	-1.446650	-0.497764	-0.626920
H	-2.795553	-1.926005	-1.313011
H	-3.340542	-0.239831	-1.309060
H	-3.243694	-1.135211	0.219328
H	-0.896130	-1.152650	-0.145675
C	1.914596	-0.023068	-1.647421
N	2.143812	0.773115	-0.445612
H	2.671332	-0.810071	-1.724675
H	1.926767	0.551068	-2.584365
H	0.935253	-0.502643	-1.573199
H	3.014458	1.284637	-0.515499
H	1.387145	1.448556	-0.343648
H	1.696375	-0.604926	1.107600
C	-0.772218	2.127376	1.277757
O	-0.557948	2.032916	-0.110335
H	-0.140306	1.429651	1.845967
H	-1.819593	1.938533	1.546342
H	-0.521054	3.143238	1.590718
H	-0.919862	1.174977	-0.393971

Vibrational frequencies

30.7003	40.8626	54.6461
63.5923	67.8105	78.8775
91.2346	98.2259	118.7563
135.5400	142.1498	147.5617
172.4562	184.5892	199.3443
219.3931	236.5451	301.9768
394.5147	467.6806	828.9740
879.1393	936.2492	1014.0556
1032.8497	1052.3017	1092.1762
1108.1085	1115.2825	1124.3196
1135.0719	1160.8077	1186.6520

1190.4020	1193.6420	1333.8651
1380.9910	1419.5970	1467.0886
1471.6348	1477.4125	1487.3902
1489.4170	1495.2934	1498.8740
1505.5744	1507.2956	1509.9060
1521.4509	1527.3328	1536.8676
1688.3099	2768.8415	2995.1362
3001.6648	3007.5468	3041.8661
3048.0543	3065.3229	3071.4963
3109.1443	3115.4567	3119.8799
3128.4087	3442.1739	3472.0481
3498.3891	3601.9644	3633.5248

R38

Cartesian coordinates

C	-3.183360	-0.124831	0.550988
O	-2.795178	0.158930	-0.777835
H	-2.332384	-0.445265	1.164485
H	-3.909217	-0.939668	0.512754
H	-3.667701	0.735079	1.033572
H	-2.127050	0.853110	-0.733111
N	-0.145349	1.482670	-0.494517
C	0.466101	2.400384	0.351278
H	0.134560	1.535661	-1.463155
H	0.231939	2.297230	1.404760
H	0.639123	3.396257	-0.039010
H	0.972586	-1.017089	0.828303
C	-0.210347	-2.116734	-0.309309
O	0.010875	-1.137104	0.684805
H	-0.180465	-3.130767	0.107056
H	0.529403	-2.054403	-1.118971
H	-1.198885	-1.932763	-0.735259
H	-0.157376	0.522695	-0.137100
C	3.076622	-0.271882	-0.684947
N	2.608738	-0.166918	0.697460
H	2.248661	-0.022987	-1.352453
H	3.372827	-1.302009	-0.894655
H	3.919294	0.387134	-0.927315
H	3.356525	-0.377335	1.347213
H	2.304760	0.788634	0.878478

Vibrational frequencies

39.7576	47.4750	58.8518
79.2190	87.1907	97.2097
100.1227	110.5840	124.7049
135.2488	143.7146	151.6839
158.4747	179.5234	189.0838

234.0539	265.4270	291.4765
441.3104	570.1220	625.7683
714.8105	834.8145	930.8697
957.6098	1010.0357	1038.0882
1085.9823	1094.5167	1102.7561
1132.5815	1170.2836	1189.6944
1193.1165	1200.1229	1255.9635
1361.9818	1366.6770	1445.4864
1462.2879	1479.4460	1485.7312
1491.5101	1494.8954	1503.5137
1507.0483	1515.1237	1523.7578
1527.0799	1531.8586	1667.7053
1693.1531	2996.6430	2998.2835
3019.5403	3057.1626	3061.1461
3096.8963	3116.3167	3121.1236
3130.4818	3140.3997	3252.3599
3361.2856	3476.3125	3498.7042
3605.6033	3641.6106	3782.7929

TS38

Cartesian coordinates

C	-2.932753	-0.216689	-0.811259
O	-2.806327	-0.209133	0.590429
H	-2.068005	0.251911	-1.300201
H	-3.828721	0.352276	-1.072453
H	-3.051080	-1.233074	-1.215688
H	-1.956953	-0.638636	0.789411
N	-0.081920	-1.113890	0.812113
C	0.383810	-2.066777	-0.066011
H	0.213561	-1.294952	1.764728
H	-0.100728	-2.072117	-1.044271
H	0.671811	-3.048770	0.310320
H	1.453492	0.674565	-0.681356
C	-0.438874	2.226932	0.342497
O	0.125545	1.100578	-0.280299
H	-0.543836	3.040732	-0.382809
H	0.174341	2.594905	1.178945
H	-1.433733	1.973302	0.725445
H	-0.067232	0.145153	0.299382
C	3.242527	0.139213	0.315831
N	2.299140	-0.028139	-0.800912
H	2.676765	0.018667	1.238753
H	3.680633	1.136481	0.289263
H	4.029508	-0.613424	0.273504
H	2.742731	0.052717	-1.709591
H	1.804904	-0.973172	-0.709187

Vibrational frequencies

-712.6866	20.2783	49.8395
75.3229	85.6419	95.6746
117.9156	131.9276	147.8422
155.2479	170.0684	179.7164
187.3604	197.2718	235.9295
289.1368	356.2682	430.0151
640.6882	665.8855	743.6663
758.1244	875.0344	989.3634
1031.6760	1067.0939	1070.4900
1106.9943	1134.8660	1146.0313
1190.0803	1193.6615	1197.9339
1276.1886	1290.1762	1303.8541
1336.1377	1430.4079	1454.8516
1478.6710	1485.9480	1492.8475
1498.2022	1498.5031	1506.6133
1512.8305	1516.2881	1517.9427
1535.5368	1617.7161	1625.5773
1688.2737	1818.1583	2200.0562
2658.2942	2982.6909	2984.5545
3040.9720	3056.4335	3067.9067
3083.6564	3093.0556	3101.7037
3158.6409	3170.9697	3180.2275
3568.9993	3579.7268	3626.4332

P38**Cartesian coordinates**

C	3.026605	-0.201761	0.631600
O	2.687595	-0.081971	-0.732695
H	2.233032	0.183751	1.284991
H	3.928444	0.389272	0.802426
H	3.246884	-1.240339	0.916502
H	1.878132	-0.592549	-0.867891
N	0.105759	-1.475193	-0.751831
C	-0.413279	-2.208960	0.356730
H	-0.366792	-1.779145	-1.604516
H	0.270502	-2.146917	1.206400
H	-0.648622	-3.255111	0.127167
H	-1.946855	0.584394	1.070708
C	0.473911	2.324424	-0.183244
O	-0.020904	1.187956	0.501430
H	0.465141	3.161437	0.516753
H	-0.156894	2.588045	-1.042737
H	1.497075	2.155330	-0.532113
H	0.174725	0.409284	-0.036937
C	-3.012372	0.325020	-0.632729

N	-2.711281	-0.007332	0.754184
H	-2.128021	0.121877	-1.244442
H	-3.291124	1.374190	-0.804332
H	-3.823698	-0.307665	-1.002442
H	-3.513617	0.160834	1.347506
H	-1.362391	-1.709240	0.662460

Vibrational frequencies

9.7040	29.1313	64.7430
71.4192	79.8428	95.0084
104.8269	121.4009	132.8376
136.5453	141.4974	148.8005
156.8399	171.2344	176.8135
190.7206	217.8818	245.5116
379.3031	467.1401	625.7983
745.1755	926.3107	997.3350
1014.5303	1043.4440	1090.3002
1096.2092	1100.8461	1114.6536
1134.4236	1141.9734	1189.9138
1191.6369	1193.9229	1335.6711
1373.4121	1412.0967	1437.6598
1461.0781	1462.6508	1479.4031
1482.8594	1494.2011	1499.1055
1501.2731	1502.1412	1506.9657
1525.1115	1526.2959	1529.1693
1668.9865	2804.9389	2990.2154
2997.5793	3004.7607	3036.6339
3048.8594	3070.1927	3083.1753
3109.0923	3115.3591	3117.0101
3130.6048	3494.1930	3509.0751
3617.6616	3724.5539	3759.0956

R39

Cartesian coordinates

C	-3.513348	-0.208675	-0.592391
O	-2.527605	0.556358	0.063601
H	-3.090524	-1.083236	-1.104801
H	-3.982687	0.431628	-1.341043
H	-4.294158	-0.555763	0.096571
H	-2.067828	-0.015436	0.691339
N	-0.354112	-1.087797	1.208431
C	-0.319828	-1.968967	0.136478
H	-0.046720	-1.465397	2.091826
H	-0.662032	-1.559812	-0.809331
H	-0.532685	-3.011772	0.340783
C	0.946737	2.688791	0.259890
N	0.401099	1.383128	-0.090778

H	0.999996	3.395779	-0.578929
H	1.956829	2.566854	0.659676
H	0.335082	3.142073	1.043411
H	0.966294	0.928946	-0.803750
H	-0.551105	1.460927	-0.437659
H	0.027979	-0.151899	0.997697
C	3.087863	-0.640840	0.055685
O	2.263564	-0.833800	-1.073635
H	2.553719	-0.134151	0.871071
H	3.924035	-0.010338	-0.251747
H	3.495187	-1.585824	0.436449
H	1.543505	-1.422212	-0.802826

Vibrational frequencies

39.3944	49.6553	61.0397
75.7642	87.5225	89.3354
108.7673	122.8196	126.6622
137.3590	143.8840	160.1847
163.4343	168.0997	186.0786
201.8806	266.6281	318.9536
525.6100	581.3295	649.4557
704.7398	770.5145	923.6010
966.3029	1014.3611	1054.4227
1096.8123	1101.9066	1108.5505
1126.4087	1140.3489	1186.7875
1190.2332	1191.7725	1260.2168
1363.6937	1379.5548	1434.2683
1443.0336	1466.3554	1483.8585
1492.1262	1495.2418	1498.4588
1501.9736	1505.0342	1519.1955
1520.8629	1526.8067	1685.7215
1705.7755	2998.3895	2999.1115
3005.2875	3051.1990	3054.5166
3082.4366	3119.7990	3122.5460
3123.7061	3130.5171	3227.7761
3244.4061	3497.0652	3581.7418
3650.7787	3691.1635	3769.4930

TS39

Cartesian coordinates

C	-3.292620	-0.075592	-0.610234
O	-2.243586	0.520003	0.114760
H	-2.930786	-0.817445	-1.334915
H	-3.819262	0.709325	-1.157976
H	-4.013652	-0.569278	0.052906
H	-1.768911	-0.177334	0.640380
N	-0.519763	-1.281292	1.142583

C	-0.090525	-1.990907	0.036001
H	-0.141668	-1.691045	1.992467
H	-0.768552	-1.908079	-0.823276
H	0.257326	-3.020272	0.183762
C	0.900465	2.646932	0.249241
N	0.393669	1.278465	0.098557
H	1.020968	3.095732	-0.736280
H	1.871764	2.622405	0.743096
H	0.211544	3.253674	0.837974
H	1.081874	0.558084	-0.472287
H	-0.557233	1.238880	-0.298997
H	0.265285	0.783957	0.987977
C	2.944009	-0.685140	-0.107901
O	1.826102	-0.509789	-0.935157
H	2.665013	-1.115677	0.868954
H	3.444494	0.274537	0.083849
H	3.680024	-1.354049	-0.568699
H	0.956321	-1.317088	-0.526385

Vibrational frequencies

-1019.2162	19.8508	30.1344
63.1590	87.7786	99.1429
102.6091	120.5863	134.2108
160.9813	167.9055	206.6764
219.9887	234.5242	260.8838
310.4857	409.4752	457.8256
534.9600	638.4521	721.7935
965.5187	976.5063	1027.7668
1051.8599	1073.8049	1092.0535
1095.1893	1118.8325	1165.7611
1180.6843	1187.5011	1193.0326
1215.8512	1255.5571	1318.0075
1356.9099	1379.1687	1446.5309
1479.5957	1489.5599	1493.8999
1494.3853	1504.8366	1507.9859
1512.2997	1518.4061	1522.3038
1544.7330	1550.5152	1611.5277
1689.5839	1769.0147	1828.4797
2959.1987	2996.5378	3002.7974
3020.5446	3056.9556	3060.2683
3075.0792	3080.3176	3109.1805
3159.0156	3165.7715	3200.4154
3342.7242	3432.0388	3530.7235

P39

Cartesian coordinates

C	2.948082	-0.320991	-0.352229
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O	1.751329	-0.321570	-1.094618
H	2.774991	-0.172309	0.723673
H	3.568492	0.502418	-0.711995
H	3.511312	-1.253458	-0.482077
H	1.215009	-1.078869	-0.789772
N	0.135327	-2.169660	0.222266
C	-0.268414	-1.550031	1.444934
H	-0.462256	-2.978492	0.045318
H	0.516931	-0.878957	1.802677
H	-0.543649	-2.261225	2.233545
C	0.453009	2.368824	0.948388
N	-0.117820	1.830179	-0.285240
H	0.554890	1.561659	1.677920
H	-0.223734	3.110743	1.378544
H	1.438727	2.834595	0.819461
H	-1.665936	0.949228	0.027007
H	0.525980	1.146544	-0.690070
H	-0.234946	2.570246	-0.967254
C	-2.566737	-0.370404	-1.055776
O	-2.437690	0.348587	0.143372
H	-1.726989	-1.066176	-1.220649
H	-2.625577	0.288850	-1.932392
H	-3.489484	-0.953961	-1.010778
H	-1.161050	-0.924989	1.235727

Vibrational frequencies

34.1385	55.6738	58.5185
77.4048	83.3800	88.1264
104.8100	113.3776	125.4910
137.6295	139.4814	146.7287
177.9924	207.0492	214.5771
235.4316	264.7924	299.0849
396.7268	483.9908	843.2697
953.1238	998.0748	1006.0555
1043.6099	1060.4919	1093.3392
1106.8936	1111.3718	1113.7481
1142.8108	1151.5630	1181.8761
1194.1994	1224.3362	1333.0052
1392.6161	1415.5925	1470.2648
1480.4568	1482.8826	1485.0456
1491.8221	1497.1213	1498.6156
1505.8962	1507.6398	1517.7530
1528.3539	1535.4382	1566.6796
1697.7251	2881.4534	2965.1355
2992.5090	3010.6964	3028.6033
3041.0474	3052.0346	3091.7314
3106.0739	3109.4797	3120.1700

3125.9560	3387.4832	3442.4096
3494.2199	3551.0587	3591.9944

R40

Cartesian coordinates

N	0.851576	-2.108614	0.459721
C	1.109290	-1.293037	1.542105
H	1.644313	-2.572364	0.045623
H	1.879112	-1.621552	2.233311
H	0.239715	-0.804796	1.972182
C	-2.499985	-1.327432	-0.350757
N	-1.329372	-0.910544	-1.120623
H	-2.672916	-2.398700	-0.481820
H	-3.425905	-0.796371	-0.610833
H	-2.306799	-1.160049	0.712060
H	-1.483797	-1.077341	-2.107850
H	0.147851	-1.774090	-0.211561
C	2.253000	0.472794	-1.232762
O	2.063193	1.090666	0.021863
H	3.053931	-0.277042	-1.202227
H	2.544239	1.248515	-1.943895
H	1.337369	-0.011371	-1.596128
H	1.849029	0.381291	0.658723
C	-1.443057	1.991574	1.077599
N	-0.806096	1.932048	-0.234858
H	-1.237219	1.062432	1.615470
H	-2.527656	2.065880	0.962013
H	-1.108972	2.824476	1.711371
H	0.205450	1.852543	-0.127067
H	-0.990578	2.781603	-0.753840
H	-1.180952	0.097993	-0.997221

Vibrational frequencies

40.1321	48.3207	60.6127
76.9856	86.9970	102.6309
103.7227	120.6794	131.3558
146.2066	162.9787	183.5239
198.7313	200.1139	218.7206
224.2099	254.6761	296.1351
435.2591	540.0904	574.4059
755.9668	808.9569	855.2803
953.2248	981.2331	1012.8265
1032.3284	1068.4481	1091.3362
1095.4162	1099.2849	1140.7751
1196.2488	1198.7390	1218.5238
1285.0274	1354.8904	1381.3221
1399.4958	1459.9966	1469.6189

1473.7094	1492.3038	1496.4708
1500.2446	1505.8964	1509.8723
1525.4679	1529.5236	1532.8543
1702.2170	1707.0746	1711.5989
3005.2558	3005.7733	3006.6466
3061.9060	3083.3700	3086.0342
3119.3504	3120.2052	3122.3069
3126.5833	3232.4123	3287.6996
3363.0348	3462.0580	3520.0301
3584.9684	3600.2468	3665.3750

TS40

Cartesian coordinates

N	0.195742	-1.711043	0.555666
C	1.121193	-1.281607	1.482612
H	0.558811	-2.544831	0.097838
H	1.867686	-1.988923	1.863704
H	0.731656	-0.632240	2.276717
C	-3.136396	-0.573856	-0.385045
N	-1.791926	-0.454498	-0.946477
H	-3.529204	-1.596663	-0.419257
H	-3.840501	0.082099	-0.905740
H	-3.109159	-0.271700	0.664779
H	-1.770601	-0.813158	-1.894491
H	-1.104086	-1.021261	-0.371613
C	2.503478	-0.127133	-1.337246
O	2.203070	0.620916	-0.176747
H	3.488211	-0.601458	-1.258714
H	2.520152	0.547598	-2.198459
H	1.750831	-0.908279	-1.502115
H	1.965302	-0.073329	0.553083
C	-0.684005	1.765763	1.197855
N	-0.274998	1.618914	-0.213266
H	-0.740147	0.766285	1.626791
H	-1.661715	2.244935	1.254057
H	0.051658	2.352385	1.747016
H	0.723117	1.243322	-0.257580
H	-0.315056	2.502862	-0.710370
H	-0.938859	0.872416	-0.672184

Vibrational frequencies

-28.2047	38.9376	89.3660
93.9430	100.3998	113.4321
127.0914	140.1775	146.2284
160.9705	191.9785	197.5815
210.6524	233.8795	292.6149
310.0122	340.9770	357.3331

593.4859	673.3093	681.9919
890.6442	1000.2991	1009.2029
1051.5928	1062.9386	1069.5689
1084.1289	1087.1374	1100.5355
1120.5441	1171.9962	1190.2594
1278.8981	1293.6036	1324.5998
1356.8881	1374.4767	1404.9426
1458.8121	1461.2114	1467.6368
1493.2632	1496.0022	1503.3442
1509.7286	1515.9193	1521.0387
1526.2627	1562.3952	1663.4354
1716.9531	1734.4899	1747.5454
2188.3746	2404.5263	2733.7449
2802.2487	2991.4403	3010.5784
3023.8214	3061.3946	3073.1337
3076.2284	3084.4611	3093.7464
3115.6336	3164.1524	3179.9893
3499.0837	3572.9565	3574.5785

I40

Cartesian coordinates

N	0.194166	-1.468979	0.976857
C	1.316062	-0.997906	1.627880
H	0.367142	-2.436349	0.708669
H	2.038249	-1.711793	2.039721
H	1.152911	-0.146565	2.301633
C	-3.100432	-0.648845	-0.400277
N	-1.729275	-0.528382	-0.892829
H	-3.441131	-1.687224	-0.312400
H	-3.796987	-0.112720	-1.051245
H	-3.158281	-0.201856	0.595043
H	-1.624563	-1.010887	-1.777938
H	-1.062454	-0.963234	-0.206759
C	2.195629	-0.366838	-1.539972
O	2.176771	0.540449	-0.457009
H	3.197549	-0.783780	-1.691329
H	1.907528	0.161851	-2.454710
H	1.492070	-1.190122	-1.364505
H	2.055148	-0.039137	0.393790
C	-0.638870	1.749754	1.157317
N	-0.251800	1.630251	-0.265420
H	-0.694669	0.736558	1.557988
H	-1.611236	2.237083	1.233944
H	0.109054	2.322724	1.703672
H	0.740983	1.242210	-0.353932
H	-0.304057	2.519033	-0.752439

H -0.907386 0.893388 -0.713073

Vibrational frequencies

24.5640	72.9786	89.0616
96.6085	100.3571	123.7364
129.0989	138.6197	147.9218
175.3354	194.5844	206.9611
230.6792	280.3162	293.3676
317.5794	338.4609	357.8975
586.2165	659.4327	676.6143
895.2945	1000.5626	1003.5496
1044.4808	1060.2487	1070.4840
1086.5945	1088.3586	1100.9708
1122.0770	1181.5647	1190.2191
1270.9698	1281.4174	1324.9589
1361.0489	1366.1645	1398.5340
1461.8309	1465.7049	1468.7965
1496.4600	1497.4748	1503.9656
1509.7122	1513.9353	1523.9013
1539.3319	1559.9429	1653.7432
1708.4435	1717.4122	1752.2537
2333.9688	2469.3450	2705.2815
2944.6824	2995.2521	3009.6230
3025.3731	3065.8419	3067.4076
3074.7333	3084.8546	3086.5017
3118.3796	3160.1631	3169.3746
3491.4770	3574.9901	3579.9477

TS41

Cartesian coordinates

N	0.230514	-1.605622	0.941015
C	1.415835	-1.115737	1.456411
H	0.409141	-2.534130	0.559612
H	2.210268	-1.826981	1.715942
H	1.289808	-0.358990	2.243532
C	-3.103689	-0.604091	-0.373945
N	-1.734702	-0.471681	-0.869734
H	-3.454990	-1.641963	-0.325651
H	-3.797081	-0.036406	-1.000720
H	-3.155059	-0.193975	0.637556
H	-1.643528	-0.907820	-1.780036
H	-1.077726	-0.957547	-0.222879
C	2.020563	-0.228767	-1.628109
O	2.073424	0.540598	-0.454170
H	2.991954	-0.249204	-2.134926
H	1.281340	0.180128	-2.333931
H	1.720632	-1.261817	-1.401888

H	1.927731	-0.198596	0.419122
C	-0.536923	1.699425	1.284195
N	-0.197779	1.680820	-0.153490
H	-0.598384	0.661484	1.614609
H	-1.496070	2.194602	1.440928
H	0.241957	2.215052	1.844992
H	0.819736	1.250322	-0.299046
H	-0.248063	2.604417	-0.569951
H	-0.870012	1.007029	-0.629752

Vibrational frequencies

-599.5700	32.7294	72.0176
79.9557	86.2764	97.9300
125.1976	141.5154	148.7689
164.2140	169.5504	189.3907
229.0187	271.3164	278.8783
320.1477	373.0905	441.6375
585.0315	640.8623	662.3893
719.1735	997.7932	1004.5174
1018.8162	1058.4585	1069.5343
1088.4019	1092.2988	1104.6851
1115.8344	1184.1080	1193.3362
1251.4949	1263.6196	1305.4733
1319.8666	1363.5078	1374.5486
1396.7162	1461.5918	1465.4961
1486.2653	1492.6786	1500.5963
1504.2752	1510.6499	1512.3653
1524.8386	1533.9676	1582.7745
1658.3801	1713.7435	1717.3792
1763.2636	2051.1437	2746.6145
2975.4464	2978.6660	3017.5766
3029.4569	3050.6915	3062.7764
3064.2860	3082.5959	3110.2364
3118.2446	3154.6130	3165.0354
3485.6455	3578.5814	3580.1781

P41

Cartesian coordinates

N	0.161264	-2.319349	0.314636
C	0.406773	-1.521071	1.478014
H	0.943428	-2.970651	0.214621
H	0.751429	-2.103308	2.343582
H	-0.492345	-0.960953	1.748662
C	-2.965314	-0.422385	-0.312098
N	-1.749659	-0.426931	-1.121559
H	-3.569680	-1.336378	-0.390839
H	-3.595617	0.426393	-0.590788

H	-2.695141	-0.292987	0.739351
H	-1.980903	-0.541792	-2.100925
H	-1.159630	-1.215917	-0.853650
C	2.468551	-0.221589	-1.135238
O	2.417823	0.531471	0.048185
H	3.372000	-0.836489	-1.113602
H	2.514784	0.411846	-2.032444
H	1.599388	-0.891425	-1.243357
H	1.204216	-0.788810	1.244557
C	-0.583004	2.295513	1.033168
N	0.004134	1.883074	-0.239992
H	-0.578202	1.445208	1.719442
H	-1.616435	2.659221	0.954190
H	0.022734	3.082536	1.488856
H	1.618624	1.103121	-0.020176
H	0.026690	2.666095	-0.882796
H	-0.580131	1.152152	-0.664845

Vibrational frequencies

25.9647	38.3718	54.5464
69.5523	77.8846	80.7239
90.6119	114.0569	123.4715
129.1847	136.2472	148.5416
155.2799	172.5944	193.0868
215.5574	223.2220	290.5208
385.3206	454.2791	540.7372
947.2800	953.2182	994.7969
1001.4369	1023.5437	1038.6358
1064.8191	1090.7843	1094.8479
1096.5359	1114.2529	1155.3879
1190.0265	1197.8494	1224.1273
1340.9824	1376.2644	1397.2913
1421.5592	1461.3389	1466.3586
1486.2904	1487.5973	1497.2852
1499.0955	1503.5313	1505.3223
1509.9149	1523.5730	1524.9014
1567.9334	1698.2413	1709.3162
2911.2060	2961.6182	3001.9118
3004.4673	3017.7295	3023.6661
3078.0357	3086.3366	3097.4449
3098.3303	3112.5655	3121.5379
3330.7692	3396.4230	3452.0548
3471.4108	3586.3148	3596.3803

R42

Cartesian coordinates

N	-2.598944	0.461981	-0.393780
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C	-2.651403	0.205776	0.964723
H	-2.994215	-0.245765	-0.992567
H	-3.528143	-0.316282	1.333217
H	-2.221879	0.968779	1.605621
C	0.282424	2.236182	0.342921
N	0.075416	1.632986	-0.972990
H	-0.524357	2.940310	0.564239
H	1.240018	2.762557	0.453554
H	0.247868	1.446419	1.097567
H	0.144312	2.339329	-1.695881
H	-1.723320	0.863615	-0.748450
C	-0.569020	-2.298760	-0.681023
N	-0.091354	-1.717170	0.575591
H	-1.537696	-2.806992	-0.593325
H	0.166775	-3.012471	-1.057922
H	-0.663853	-1.501256	-1.420284
H	1.404156	-0.885163	0.035318
H	-0.809762	-1.084965	0.937542
H	0.034169	-2.444533	1.270240
C	3.103105	-0.052102	0.528598
O	2.138053	-0.417339	-0.424927
H	2.706122	0.635064	1.290160
H	3.919110	0.457563	0.010971
H	3.527387	-0.925060	1.043549
H	0.822434	0.956411	-1.127201

Vibrational frequencies

38.1089	58.7872	88.9919
94.9921	108.5612	109.8985
116.9283	124.6364	126.1121
145.1745	157.5169	180.8132
184.0579	193.4816	211.8188
242.8641	276.6241	297.5506
471.0463	503.8255	566.6574
747.4966	861.5092	928.8235
976.2034	987.5923	1014.1569
1038.1800	1042.9425	1084.8116
1089.4948	1117.0426	1164.6286
1192.8870	1218.3931	1220.2241
1276.8095	1357.5065	1379.2838
1389.1419	1470.0786	1473.2172
1483.4276	1494.6934	1502.4403
1503.9822	1507.7247	1512.7196
1528.8056	1532.6403	1559.6117
1681.6361	1690.0498	1710.0722
2986.4505	3008.8676	3016.9041
3036.7385	3086.8352	3101.0883

3104.4448	3123.5988	3134.2822
3138.0053	3240.8551	3325.3846
3381.3889	3418.5000	3482.8048
3584.4785	3597.0887	3661.7274

TS42

Cartesian coordinates

N	1.159075	-1.836131	-0.351942
C	1.539434	-1.628132	0.953423
H	1.950709	-2.126599	-0.917090
H	2.462593	-2.080369	1.330640
H	0.722530	-1.647736	1.684479
C	-2.139991	-1.656732	0.189488
N	-1.323435	-0.983550	-0.824946
H	-2.058119	-2.743628	0.111190
H	-3.189725	-1.366116	0.108047
H	-1.774686	-1.359669	1.173894
H	-1.688445	-1.148550	-1.756409
H	-0.298604	-1.377440	-0.759208
C	2.264247	1.294485	-0.744583
N	1.512985	1.164567	0.512808
H	3.335172	1.185534	-0.567343
H	2.057520	2.257476	-1.212100
H	1.929173	0.488394	-1.396293
H	0.435181	1.320386	0.292387
H	1.624203	0.135098	0.871174
H	1.836073	1.817638	1.218946
C	-1.933153	2.038088	0.439271
O	-0.906529	1.381897	-0.235813
H	-1.724361	2.158491	1.515853
H	-2.884427	1.486438	0.363901
H	-2.114715	3.042403	0.028903
H	-1.191432	0.202624	-0.581501

Vibrational frequencies

-712.1578	27.0594	60.2245
75.6083	85.3078	89.3301
111.8430	121.2758	136.6067
155.9810	173.2599	182.8933
188.0093	195.4297	309.2565
316.2131	400.2963	444.4501
622.8696	661.2653	692.1466
698.5280	888.4421	1004.9450
1014.4904	1051.4105	1072.7121
1079.8080	1086.7100	1108.1285
1142.5440	1189.1896	1204.0301
1286.2579	1322.9893	1332.5248

1341.8725	1348.0307	1417.5450
1458.5216	1459.8393	1489.3281
1494.9312	1495.9503	1503.8946
1506.3406	1511.4523	1516.7893
1523.1651	1594.6507	1608.8580
1654.4055	1720.1509	1739.9288
1791.4264	2052.2746	2204.8178
2293.9784	2950.6145	2989.9519
3009.3873	3010.1472	3053.4928
3072.9196	3088.4918	3126.3536
3144.4682	3156.4632	3174.5848
3540.8033	3570.2039	3575.2732

P42

Cartesian coordinates

N	-0.437369	2.252742	0.350083
C	-0.574814	1.439122	1.518076
H	-1.244590	2.878535	0.305949
H	-0.904931	1.994960	2.406343
H	0.365126	0.923306	1.733025
C	2.839771	0.736033	-0.436428
N	1.555823	0.525071	-1.104041
H	3.303956	1.706869	-0.651585
H	3.541743	-0.050560	-0.723752
H	2.694853	0.666297	0.644482
H	1.670331	0.572626	-2.109516
H	0.900734	1.262063	-0.833794
C	-2.535186	-0.028845	-1.169171
N	-2.394227	-0.777407	0.073246
H	-3.476167	0.529100	-1.165566
H	-2.507085	-0.640944	-2.082307
H	-1.722413	0.702338	-1.237562
H	-1.535177	-1.327018	0.034556
H	-1.343155	0.661329	1.314133
H	-3.168684	-1.418199	0.192580
C	1.068432	-2.143591	0.972473
O	0.378311	-1.840117	-0.212284
H	0.965191	-1.358321	1.736381
H	2.140767	-2.308479	0.797358
H	0.652243	-3.065388	1.385840
H	0.781949	-1.026738	-0.593014

Vibrational frequencies

37.0097	47.1270	66.9718
69.7286	89.0295	92.5648
104.4039	112.4520	132.2224
158.7669	167.2748	170.0036

174.9362	179.4019	199.7641
216.1040	250.3436	284.5209
387.6670	465.6003	499.0391
925.8510	947.6665	978.1604
999.2192	1026.3776	1042.2000
1060.2172	1090.0261	1096.0779
1101.6477	1118.0652	1166.7143
1193.8933	1197.0562	1214.7875
1340.2187	1381.8460	1384.9497
1421.0024	1464.1434	1472.9880
1491.2786	1497.5688	1503.9592
1505.5827	1507.0951	1509.7358
1513.3794	1528.2102	1528.4934
1568.0377	1695.0723	1699.8495
2844.5986	2981.7088	2991.3364
3017.7647	3020.9542	3031.5615
3064.6776	3092.5509	3103.7265
3104.2431	3106.3986	3126.1916
3382.8797	3439.5790	3460.7499
3473.0268	3593.9054	3600.1041

R43

Cartesian coordinates

N	1.193847	-1.914192	0.719467
C	1.662959	-1.053080	1.695226
H	1.870868	-2.222126	0.039292
H	2.661900	-1.241685	2.074546
H	0.923001	-0.696446	2.404092
C	-2.516343	-1.525343	-0.684896
O	-1.217145	-0.995920	-0.601574
H	-2.436877	-2.604554	-0.832400
H	-3.076621	-1.108639	-1.532640
H	-3.097232	-1.350915	0.231274
H	0.289538	-1.688875	0.304099
C	1.722362	0.436338	-1.766708
N	1.746503	1.302366	-0.587326
H	2.603244	-0.213829	-1.866878
H	1.653029	1.048561	-2.669880
H	0.832676	-0.195914	-1.725319
H	-0.171284	1.835859	-0.316945
H	1.842864	0.726290	0.251440
H	2.549879	1.918659	-0.616065
C	-1.264809	1.858106	1.412791
N	-1.146614	1.682383	-0.033483
H	-0.567675	1.175189	1.903121
H	-2.273302	1.596807	1.743557

H	-1.041263	2.875121	1.759855
H	-1.733086	2.343932	-0.527108
H	-1.273671	-0.020103	-0.440535

Vibrational frequencies

25.0915	43.3626	53.7359
63.7287	72.0203	84.9812
93.6394	98.6441	110.3430
126.3385	129.7478	154.4225
167.4081	198.8062	202.7017
246.7983	248.7607	300.3968
441.5442	547.5566	578.4132
744.7321	826.1500	920.2921
951.9291	997.5739	1015.6521
1022.2154	1080.7699	1085.0694
1092.5169	1119.9648	1165.9570
1186.1081	1204.4700	1217.0397
1275.9567	1347.1884	1370.8608
1385.5410	1463.1700	1472.2272
1485.7350	1489.8209	1498.7130
1504.5019	1508.9537	1513.8277
1523.8729	1531.6537	1576.0461
1677.3586	1697.4084	1699.4048
2988.9252	2992.7826	3011.6021
3042.7197	3081.5300	3087.6987
3109.9832	3125.6122	3126.7174
3127.3238	3233.5179	3254.4068
3357.7990	3423.1090	3451.3079
3592.2615	3596.3017	3666.5272

TS43

Cartesian coordinates

N	-1.647077	0.901494	0.947689
C	-1.608355	-0.225049	1.729370
H	-2.578756	1.126705	0.621702
H	-2.512831	-0.523031	2.263686
H	-0.689519	-0.350602	2.308565
C	0.572486	2.708545	-0.575807
O	0.249078	1.355393	-0.564213
H	-0.011562	3.267385	0.174893
H	0.375921	3.178015	-1.553316
H	1.636176	2.883518	-0.344391
H	-0.662370	1.176779	0.200366
C	-1.291107	-1.121638	-1.660223
N	-0.724631	-1.791330	-0.469782
H	-2.379821	-1.143725	-1.609476
H	-0.953603	-1.625558	-2.566957

H	-0.932248	-0.089522	-1.646124
H	0.335221	-1.606793	-0.425958
H	-1.142219	-1.339739	0.437770
H	-0.914303	-2.788656	-0.458152
C	2.413023	-0.881885	1.038827
N	1.842243	-0.861629	-0.308095
H	1.625080	-0.640197	1.755599
H	3.222478	-0.156040	1.180326
H	2.797073	-1.876770	1.280936
H	2.560180	-1.028879	-1.002923
H	1.422460	0.074379	-0.484521

Vibrational frequencies

-743.5908	51.8128	58.1952
73.5792	92.1902	100.6463
116.7803	132.5470	138.6461
155.2609	160.8453	187.6920
207.0990	271.2733	294.8380
321.9709	324.9721	348.2528
562.1389	587.5274	655.5932
701.4716	905.0498	995.7229
1015.8826	1027.0469	1049.7990
1075.1875	1092.8289	1116.1156
1143.9266	1184.6754	1193.1613
1265.2082	1301.6089	1324.6429
1339.6727	1351.3900	1400.1658
1462.7121	1472.8915	1479.2703
1494.4000	1496.5625	1504.1746
1506.0074	1511.9113	1523.8068
1527.9382	1547.8853	1610.9074
1682.8402	1687.0257	1707.3214
1733.1692	2219.3653	2563.4643
2938.6673	2980.6122	2987.8067
3021.2088	3040.6152	3047.5403
3086.8918	3124.3239	3127.3322
3132.5009	3147.0131	3155.8619
3566.2697	3584.7911	3585.7355

P43

Cartesian coordinates

N	-1.518353	-1.122236	1.219675
C	-0.329284	-1.717747	1.737224
H	-2.133434	-1.860374	0.873592
H	-0.493527	-2.672615	2.252268
H	0.188729	-1.018261	2.398496
C	-2.247013	1.766934	-0.672772
O	-1.208555	1.472139	0.229102

H	-3.218002	1.856398	-0.168714
H	-2.337973	1.010965	-1.466093
H	-2.023634	2.725494	-1.145615
H	-1.406193	0.613537	0.653965
C	-0.069535	-1.375483	-1.830050
N	1.154999	-1.662212	-1.093837
H	-0.644728	-2.294020	-1.983289
H	0.082087	-0.903585	-2.812146
H	-0.679088	-0.692726	-1.231558
H	1.634139	-0.775593	-0.913651
H	0.347388	-1.915799	0.871559
H	1.768486	-2.259715	-1.633506
C	2.379046	1.338808	0.968959
N	1.743842	1.211789	-0.339322
H	1.987283	0.564015	1.632895
H	2.223681	2.309650	1.459820
H	3.455757	1.171964	0.877441
H	2.112264	1.909169	-0.974684
H	0.742506	1.387933	-0.249370

Vibrational frequencies

44.5540	55.2881	62.2415
65.7746	81.7388	87.3872
99.4090	117.9777	131.5391
146.3931	156.2606	178.1495
180.0010	191.0695	196.8753
219.3931	252.6956	274.1660
401.1784	441.5136	537.3331
819.1237	944.5596	964.7867
1014.6592	1025.8348	1040.3101
1048.9844	1094.7124	1096.9920
1112.8145	1116.6752	1160.1874
1195.4506	1204.3168	1206.2253
1336.6022	1382.8855	1392.7161
1417.3530	1466.1997	1471.2658
1479.5080	1494.6528	1501.4476
1506.0544	1508.3136	1509.2079
1512.3625	1528.4872	1534.2730
1541.0981	1690.3592	1706.7964
2787.0910	2987.4447	2990.2477
3001.0809	3034.0885	3045.2042
3070.9141	3082.1005	3110.5114
3117.8156	3118.4107	3119.7167
3402.8199	3462.6444	3489.1048
3524.2402	3595.6564	3598.5197

R44

Cartesian coordinates

C	3.353950	-0.345153	0.560996
O	2.893999	-0.031261	-0.729783
H	2.691396	0.044837	1.348110
H	4.335263	0.117114	0.688864
H	3.464802	-1.426985	0.716532
H	2.053833	-0.497639	-0.853142
N	0.205227	-1.214444	-0.712934
C	0.012030	-1.734885	0.561689
H	-0.073794	-1.821817	-1.469278
H	0.267885	-1.073633	1.382854
H	0.173271	-2.797705	0.698234
C	-3.446146	-0.442615	-0.434236
N	-2.816704	0.059419	0.785061
H	-2.686403	-0.510130	-1.216844
H	-4.206343	0.265321	-0.773931
H	-3.918077	-1.429510	-0.333682
H	-1.446552	1.464836	-0.032688
H	-3.496532	0.130476	1.532277
C	0.489417	2.037526	0.385523
N	-0.557935	1.572267	-0.523483
H	0.491436	1.395234	1.270829
H	0.362947	3.072973	0.727470
H	1.465646	1.929163	-0.092316
H	-0.114051	-0.237669	-0.831589
H	-0.681989	2.218597	-1.291988
H	-2.104363	-0.603311	1.084202

Vibrational frequencies

38.6364	60.9844	63.7450
76.1243	89.5709	95.8630
103.7768	119.1905	125.6629
148.6760	154.9764	170.3151
172.0303	203.5534	214.6010
224.6152	263.7264	309.6791
393.9072	526.3490	573.6159
716.6420	744.4883	912.6741
922.5079	959.5482	1010.4869
1033.9067	1084.0718	1088.7096
1091.8340	1111.8965	1140.7752
1194.0770	1195.2642	1196.1045
1253.4713	1365.0284	1370.0754
1379.3850	1463.1164	1469.1247
1471.8377	1488.0458	1499.6321
1503.6524	1508.2159	1513.8758
1525.2133	1529.6580	1534.2143
1666.5874	1691.4275	1698.3826

2985.8206	3003.0897	3011.8176
3034.4153	3086.4450	3087.9216
3108.7591	3124.1595	3127.3932
3139.4113	3201.8444	3251.7435
3454.3028	3489.4422	3602.4369
3610.0780	3638.8213	3697.2238

TS44

Cartesian coordinates

C	-3.243706	-0.384910	-0.385138
O	-2.554730	-0.002589	0.773869
H	-2.783172	0.016969	-1.303437
H	-4.264946	0.003897	-0.329102
H	-3.301213	-1.476047	-0.498053
H	-1.714439	-0.522920	0.794578
N	-0.127910	-1.286389	0.594224
C	0.170525	-1.696944	-0.686565
H	0.157819	-1.992840	1.265685
H	-0.386236	-1.191916	-1.483124
H	0.376165	-2.750949	-0.893903
C	3.260078	-0.363746	0.438751
N	2.386628	0.158827	-0.619517
H	2.612166	-0.776755	1.213090
H	3.867658	0.437334	0.863398
H	3.913626	-1.155646	0.068612
H	1.578777	0.947402	-0.124635
H	2.907578	0.508216	-1.416317
C	-0.493071	2.021086	-0.462337
N	0.469377	1.439182	0.483578
H	-0.520267	1.388307	-1.352720
H	-0.180578	3.025335	-0.756956
H	-1.497596	2.037393	-0.037265
H	0.119274	0.489342	0.775510
H	0.572150	2.022529	1.305946
H	1.721452	-0.623195	-0.918513

Vibrational frequencies

-878.1463	40.4048	63.2273
84.1581	87.1613	107.4834
115.7641	133.1103	140.8831
145.2034	152.6372	175.7476
178.0156	206.8164	261.0893
292.0405	333.2859	339.0978
555.3453	654.2338	673.7261
733.7984	855.7113	946.0205
1003.2507	1013.7283	1064.0831
1069.6647	1087.2729	1106.1895

1117.6985	1126.0479	1154.7035
1190.9504	1278.9094	1304.8770
1326.0974	1353.3769	1354.4765
1385.6564	1456.5532	1462.6316
1481.2318	1487.1591	1494.0092
1503.2819	1506.4218	1507.5307
1519.8577	1529.6918	1562.4373
1619.2422	1688.6123	1755.6163
1794.8318	2640.4410	2921.6204
2957.1885	3019.3176	3024.3574
3055.0697	3065.1133	3089.3183
3101.0211	3130.2816	3144.9826
3150.3876	3158.5849	3300.5298
3536.4510	3577.7323	3584.6331

P44

Cartesian coordinates

C	2.803671	-0.645294	-0.381091
O	1.614640	-0.531006	-1.125211
H	2.642743	-0.485276	0.695028
H	3.498977	0.119245	-0.734912
H	3.280931	-1.624877	-0.513567
H	0.997696	-1.215067	-0.800057
N	-0.182186	-2.196813	0.205194
C	-0.494192	-1.587970	1.456760
H	-0.900809	-2.887071	-0.017178
H	0.388511	-1.087749	1.864745
H	-0.910881	-2.279860	2.199943
C	-2.559661	-0.097548	-1.099930
N	-2.383990	0.617793	0.157219
H	-1.633474	-0.632647	-1.333449
H	-2.795748	0.539780	-1.964356
H	-3.355784	-0.842424	-1.003963
H	-1.621933	1.293871	0.048168
H	-3.226945	1.120270	0.405473
C	0.889974	2.202771	1.011383
N	0.266721	2.013291	-0.294723
H	0.654128	1.344099	1.645775
H	0.473397	3.087763	1.499844
H	1.983809	2.312044	0.985737
H	0.684774	1.200588	-0.749424
H	0.443911	2.814413	-0.888182
H	-1.263002	-0.800703	1.265505

Vibrational frequencies

33.7426	48.0823	50.0813
54.5876	86.3446	89.4710

91.0136	96.7901	117.9209
142.0864	146.6929	170.1267
179.7110	184.4386	201.3942
216.8895	251.6449	277.6068
417.1468	443.0172	534.2988
836.2247	942.9542	960.1267
1013.5123	1029.3441	1041.7989
1051.7382	1093.4695	1096.4855
1109.4511	1117.6700	1153.0190
1195.0250	1195.8161	1203.8075
1340.4162	1385.1591	1391.2237
1421.0681	1458.6664	1460.1253
1488.4939	1491.3188	1497.1238
1500.4029	1504.1082	1505.7905
1511.8288	1524.8816	1526.5130
1535.0039	1691.7848	1699.3808
2783.8159	2989.7325	2992.1801
2996.6132	3027.8577	3043.0052
3065.1214	3080.2671	3103.1498
3104.5818	3112.2802	3116.8104
3383.2919	3455.6590	3494.5978
3545.4334	3595.9319	3597.5719

R45

Cartesian coordinates

N	0.796361	-2.179703	0.339570
C	0.951209	-1.581864	1.576994
H	1.643360	-2.490625	-0.109599
H	1.710616	-1.994208	2.233336
H	0.039924	-1.218180	2.040928
C	-2.490448	-1.210542	-0.443549
N	-1.318648	-0.755881	-1.189520
H	-2.644275	-2.281317	-0.600835
H	-3.422428	-0.688205	-0.700578
H	-2.311023	-1.063693	0.624686
H	-1.467569	-0.884720	-2.183344
H	0.127356	-1.734735	-0.300128
C	2.250605	0.468763	-1.255359
N	2.025056	1.107912	0.038379
H	3.025980	-0.311018	-1.249420
H	2.535881	1.221563	-1.995240
H	1.316235	0.011341	-1.587657
H	2.877618	1.539318	0.374578
H	1.760523	0.395470	0.721478
C	-1.294010	1.886287	1.213180
N	-0.832408	2.038490	-0.163077

H	-0.876106	0.961334	1.619495
H	-2.383797	1.795448	1.240857
H	-1.002664	2.703848	1.887897
H	0.190967	2.013523	-0.171247
H	-1.136699	2.924922	-0.545694
H	-1.180562	0.248354	-1.024573

Vibrational frequencies

46.7050	52.0560	62.6658
78.7471	88.1714	98.5301
110.0928	116.3477	124.0917
146.5563	169.1008	188.9393
195.3154	206.3726	217.0956
223.4816	249.6633	269.4737
419.3937	492.6429	544.6020
577.9161	737.9149	852.7294
939.9026	961.0643	980.3137
1005.8211	1022.7931	1039.4752
1069.2118	1091.2209	1091.6741
1096.9096	1202.0687	1202.3156
1218.7856	1276.7896	1354.5068
1376.1153	1386.3500	1401.5992
1462.3617	1468.7348	1472.5129
1491.8247	1504.7569	1509.5534
1513.8276	1526.1275	1532.3584
1535.1396	1679.4875	1692.4783
1708.8547	1710.9388	2993.8286
2998.9824	3004.3974	3076.3878
3084.7859	3085.1573	3117.7403
3120.1869	3129.5730	3130.7305
3235.5711	3313.7020	3362.3185
3403.2380	3432.1778	3584.6978
3591.5207	3599.3084	3658.3955

TS45

Cartesian coordinates

N	0.189718	-1.969289	0.136405
C	0.497130	-1.552184	1.411756
H	0.716044	-2.811929	-0.080605
H	0.931073	-2.252332	2.135877
H	-0.242678	-0.880563	1.870296
C	-2.954533	-0.518543	-0.165430
N	-1.784709	-0.387787	-1.032413
H	-3.432475	-1.504784	-0.219923
H	-3.707818	0.240435	-0.401586
H	-2.640448	-0.372226	0.871312
H	-2.037255	-0.601621	-1.990835

H	-1.062042	-1.091514	-0.722088
C	2.653743	-0.221534	-1.021545
N	2.123676	0.488308	0.147891
H	3.523771	-0.834332	-0.769783
H	2.934084	0.482649	-1.810215
H	1.859023	-0.882524	-1.371486
H	2.847961	1.013180	0.627006
H	1.713898	-0.234612	0.818057
C	-0.605391	2.185096	0.932649
N	-0.094791	1.709411	-0.361364
H	-0.572725	1.350097	1.633694
H	-1.635177	2.539404	0.852993
H	0.022168	2.990533	1.319302
H	1.010356	1.189474	-0.171330
H	-0.055667	2.464326	-1.038441
H	-0.755044	0.954834	-0.730458

Vibrational frequencies

-795.9351	27.8660	58.8500
72.1349	92.6155	117.9621
120.9361	141.6324	153.1853
155.3143	161.0794	174.9177
177.4154	185.2939	273.8169
292.4012	315.3763	343.6624
575.8698	611.4307	640.1077
661.4807	767.5461	851.5494
1000.9949	1012.4113	1015.1982
1044.4149	1068.1114	1083.4938
1087.6283	1096.7081	1120.9756
1127.4377	1268.2685	1281.0043
1311.5459	1334.5384	1343.6844
1378.3386	1399.0270	1447.2669
1451.6166	1458.8218	1468.4839
1485.7580	1499.8317	1504.9257
1512.4135	1519.8118	1525.0815
1529.7729	1632.9566	1711.0298
1735.5384	1762.1081	1769.5210
2625.3488	2677.7474	2881.8128
2974.7153	3014.5946	3034.7305
3048.2446	3056.2969	3070.8195
3105.8252	3109.0939	3133.5382
3137.9521	3151.3789	3513.1266
3562.9964	3567.2384	3569.3493

P45

Cartesian coordinates

N	0.587587	-2.316217	0.320424
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C	0.766651	-1.543997	1.510789
H	1.475906	-2.780324	0.116959
H	1.317404	-2.072815	2.301496
H	-0.200333	-1.211223	1.898521
C	-2.786222	-0.825028	-0.363909
N	-1.552927	-0.693702	-1.134282
H	-3.273315	-1.806847	-0.443711
H	-3.505516	-0.063539	-0.678506
H	-2.568614	-0.646771	0.692378
H	-1.731259	-0.874545	-2.114831
H	-0.873356	-1.386467	-0.816890
C	2.334568	0.138447	-1.241643
N	2.265826	0.896187	0.000723
H	3.139679	-0.601860	-1.190471
H	2.492591	0.744621	-2.146041
H	1.394120	-0.405264	-1.371445
H	3.109162	1.439158	0.137552
H	1.363064	-0.639967	1.252356
C	-0.994272	2.062554	1.161045
N	-0.514908	2.052383	-0.216920
H	-0.525402	1.237145	1.703351
H	-2.084296	1.960793	1.270868
H	-0.690906	2.987965	1.658519
H	1.469833	1.537760	-0.050641
H	-0.907857	2.830505	-0.732253
H	-0.824300	1.189264	-0.674525

Vibrational frequencies

39.4715	41.5226	53.2889
64.2449	74.4292	84.5982
86.3374	103.3895	118.7540
124.9341	149.9220	160.4428
171.4195	181.3121	197.6866
210.5009	214.8697	246.2616
401.7240	433.4281	482.7406
546.5917	934.3434	941.6869
966.9560	997.8578	1025.9267
1031.8377	1039.3503	1050.5136
1091.8290	1095.1038	1096.7460
1100.6648	1193.8605	1200.9667
1207.5649	1340.3954	1377.3465
1385.7151	1393.4964	1425.5739
1462.4523	1464.2934	1473.9786
1486.4801	1499.8942	1501.9057
1503.6894	1511.9377	1525.8674
1528.7365	1531.9797	1688.7379
1700.3308	1708.1644	2830.2935

2985.5249	2988.6657	3000.5625
3014.7833	3065.1000	3077.3560
3079.9467	3095.4358	3109.1077
3115.8962	3117.3032	3382.8023
3409.0080	3447.2896	3469.4046
3591.8223	3591.8901	3595.9232

R46

Cartesian coordinates

C	-3.244488	-0.380708	-0.707744
O	-3.314787	0.427312	0.446482
H	-2.260143	-0.320021	-1.192172
H	-3.995688	-0.017085	-1.411368
H	-3.466124	-1.434624	-0.490281
H	-2.637417	0.104105	1.052943
N	-0.735964	-0.571542	1.549111
C	-0.567878	-1.907777	1.220495
H	-0.407835	-0.298898	2.463283
H	-0.928682	-2.192251	0.236874
H	-0.669724	-2.630995	2.021273
C	2.669027	1.398284	1.157866
O	2.554354	1.015027	-0.196978
H	1.843802	1.004238	1.766694
H	2.638932	2.488111	1.201583
H	3.616070	1.061236	1.593457
H	0.855526	1.213376	-0.668667
H	2.535382	0.038762	-0.226718
C	-0.789648	2.313862	-0.797170
O	-0.110835	1.077749	-0.659215
H	-0.749571	2.678243	-1.829702
H	-0.369675	3.082575	-0.137338
H	-1.829412	2.141556	-0.514683
H	-0.491430	0.095167	0.807251
C	1.438524	-1.836443	-1.591857
O	2.020072	-1.650620	-0.308247
H	0.611247	-1.137887	-1.761094
H	1.084434	-2.864605	-1.721568
H	2.217798	-1.644490	-2.330124
H	1.330607	-1.844776	0.350705

Vibrational frequencies

28.1406	40.1136	54.7298
68.6675	74.0479	86.3312
97.9076	104.8787	106.4017
113.3704	120.7197	129.3608
138.2968	149.5308	156.1770
161.6287	166.8051	184.1143

188.4003	207.4980	232.4322
274.4819	284.4481	349.3755
572.8588	642.2633	673.9289
795.9572	816.9787	840.3351
924.3680	1041.6098	1080.9234
1094.5212	1099.0345	1101.5318
1126.6319	1129.8090	1153.7893
1172.3957	1189.6334	1190.8557
1193.0787	1196.7416	1265.3486
1362.8957	1438.1566	1446.1877
1461.6140	1484.9510	1486.7115
1489.3121	1491.4823	1495.9638
1501.2080	1502.3844	1504.2144
1507.7804	1516.8499	1523.5548
1527.0566	1528.3030	1543.9078
1688.0801	2990.6225	3002.3511
3011.3229	3020.8879	3044.8148
3068.3045	3074.3010	3090.3599
3118.6078	3127.3663	3133.3608
3137.4741	3138.9694	3244.6917
3336.0185	3522.9253	3584.7580
3610.4543	3654.1351	3775.9050

TS46

Cartesian coordinates

C	-3.228700	-0.885156	-0.768135
O	-3.339587	-0.147812	0.425829
H	-2.366037	-0.566132	-1.370319
H	-4.136911	-0.718554	-1.351771
H	-3.138595	-1.965260	-0.583519
H	-2.501654	-0.272495	0.902684
N	-0.630223	-0.468797	1.339247
C	-0.154532	-1.732188	1.078112
H	-0.447139	-0.194341	2.299057
H	-0.567210	-2.188520	0.173156
H	-0.033365	-2.433243	1.908660
C	2.287710	1.857804	0.844899
O	2.017483	1.146516	-0.361407
H	1.626101	1.519600	1.648449
H	2.138193	2.924625	0.673005
H	3.326007	1.682029	1.125986
H	0.969609	1.230269	-0.570729
H	2.170343	-0.014998	-0.183242
C	-1.267033	2.211040	-0.634941
O	-0.391064	1.096795	-0.633801
H	-1.287119	2.647938	-1.635691

H	-0.943855	2.982081	0.076713
H	-2.272348	1.877408	-0.364342
H	-0.573238	0.476586	0.215645
C	2.335037	-1.942749	-1.189039
O	2.238470	-1.204361	0.025466
H	1.550357	-1.649206	-1.893291
H	2.242830	-3.007743	-0.969528
H	3.312462	-1.753127	-1.633027
H	1.305823	-1.476933	0.523302

Vibrational frequencies

-940.3534	22.6221	37.4219
70.3161	79.5426	91.4909
99.3621	112.8336	118.2105
126.2328	139.2180	147.1408
147.3185	151.5929	159.9872
163.7287	185.9329	191.3687
198.3859	240.1739	329.9889
411.9941	440.8983	537.4111
607.0536	713.8603	764.9748
974.5042	1041.3996	1064.1685
1088.6276	1104.3515	1107.9952
1118.9834	1139.2051	1157.5727
1171.0308	1175.9101	1188.7563
1194.6859	1202.8728	1211.8931
1223.1573	1300.3310	1342.2298
1365.9235	1442.7547	1465.2641
1472.4502	1479.4247	1488.4421
1492.4587	1498.1615	1503.0360
1504.4520	1509.2557	1510.4322
1513.0975	1521.8009	1527.3016
1531.2462	1579.7644	1623.4895
1695.5570	1760.7333	1788.0905
1899.7386	2174.2992	2988.4253
3011.9217	3037.7071	3038.9969
3047.9487	3049.3818	3093.1970
3113.2670	3124.6335	3128.5394
3131.1174	3132.9799	3153.4264
3158.6724	3555.5765	3629.0863

P46

Cartesian coordinates

C	-3.750769	-0.424915	-0.248755
O	-3.156930	-0.276494	1.021516
H	-3.128800	0.001402	-1.047885
H	-4.701788	0.110636	-0.235932
H	-3.960932	-1.476726	-0.489125

H	-2.285424	-0.693122	0.976918
N	-0.546641	-1.373664	0.285772
C	-0.672815	-2.442161	-0.656469
H	0.425549	-1.388239	0.619617
H	-1.648942	-2.434874	-1.143908
H	-0.529832	-3.411187	-0.153692
C	2.284183	2.055445	0.300993
O	1.926400	1.323911	-0.854797
H	1.807194	1.654762	1.205158
H	2.022126	3.115007	0.204398
H	3.366534	1.981420	0.421887
H	0.956328	1.391657	-0.945686
H	2.231960	-0.363385	-0.429500
C	-1.346426	2.314912	0.233805
O	-0.791473	1.330043	-0.629090
H	-1.542397	3.206492	-0.363302
H	-0.650313	2.579878	1.039555
H	-2.277666	1.954145	0.676313
H	-0.894082	0.460613	-0.208574
C	3.584050	-1.405090	0.525568
O	2.286082	-1.237356	0.003318
H	4.347671	-1.375347	-0.261210
H	3.630398	-2.383740	1.006600
H	3.830036	-0.643414	1.277361
H	0.126899	-2.380300	-1.407819

Vibrational frequencies

20.7684	33.2185	51.9264
60.0253	66.4429	80.8790
84.5861	90.4633	104.0846
110.8607	122.5676	128.2759
146.6342	151.6295	154.0189
161.3316	167.8009	189.8212
198.4010	202.5824	231.3632
266.7153	275.4789	278.7707
542.3135	674.1092	735.7117
825.5790	907.8778	984.1515
1061.1708	1080.1050	1097.0511
1099.9244	1114.2748	1116.9381
1134.8327	1139.7187	1148.9627
1168.0637	1190.3220	1193.0185
1194.7674	1197.8474	1387.9507
1417.9086	1434.8069	1462.6625
1476.6408	1480.2332	1482.6679
1487.5987	1495.4966	1497.3945
1499.6370	1504.6378	1508.6804
1511.5493	1512.3164	1518.4716

1525.6577	1533.6370	1534.9858
1552.3979	2986.8685	2991.3673
3004.1054	3010.1752	3024.2824
3040.2571	3045.7480	3060.4427
3073.8810	3104.9713	3123.8539
3124.4909	3125.8713	3135.2921
3147.5573	3404.7894	3531.3125
3593.1559	3651.2129	3743.5677

R47

Cartesian coordinates

C	-3.155090	0.663130	-1.044417
O	-3.493505	0.305879	0.275344
H	-2.074856	0.829195	-1.159780
H	-3.671475	1.596398	-1.278418
H	-3.471149	-0.093605	-1.775796
H	-2.974183	-0.479675	0.489176
N	-1.254225	-1.605739	0.558195
C	-0.942824	-2.193824	-0.658127
H	-1.186816	-2.207793	1.364982
H	-0.972959	-1.530029	-1.515995
H	-1.249762	-3.223250	-0.804461
C	3.198378	1.733720	-0.302134
N	2.049367	1.142518	-0.987221
H	3.279266	1.294416	0.694440
H	3.041838	2.807418	-0.175635
H	4.153562	1.581888	-0.819364
H	0.640889	1.121203	0.052282
H	1.950217	1.527140	-1.918587
H	2.172484	0.132238	-1.075950
C	-0.769503	2.154201	1.002275
O	-0.108326	0.950618	0.674366
H	-0.785654	2.847458	0.152135
H	-0.291617	2.658066	1.851627
H	-1.802865	1.913123	1.259783
H	-0.842598	-0.676019	0.704771
C	2.179135	-1.651224	0.948359
O	2.054136	-1.779889	-0.455837
H	1.904661	-2.577975	1.466880
H	1.567720	-0.828799	1.340413
H	3.229272	-1.444412	1.164375
H	1.139008	-2.053314	-0.640421

Vibrational frequencies

26.3561	44.3424	55.4081
61.5032	76.6215	88.0791
92.4350	104.6287	105.5510

112.1514	127.1625	139.8584
145.3349	156.6806	160.3280
178.7870	193.5522	203.8248
211.6467	227.0462	233.0662
236.3185	299.9046	331.4872
522.7639	572.3944	646.3952
689.8345	780.8648	893.2615
929.0175	1010.8193	1043.1149
1063.8564	1089.6323	1090.4529
1102.9466	1111.1246	1136.2752
1139.2523	1180.3200	1195.0261
1200.5039	1202.1582	1211.7810
1265.0202	1366.2346	1377.9161
1440.5493	1453.8355	1474.6610
1484.3897	1490.9466	1498.2855
1500.3977	1502.9784	1506.8008
1511.8215	1515.7462	1518.7019
1523.9171	1529.9790	1531.2004
1558.7040	1687.3771	1700.3269
2994.2860	3003.6640	3012.3821
3023.8544	3045.1203	3063.9879
3076.2920	3098.4530	3119.4936
3121.3437	3121.6373	3130.4297
3139.7398	3251.1448	3272.4872
3356.1835	3451.8266	3600.6082
3606.9010	3650.9313	3760.0024

TS47

Cartesian coordinates

C	-3.409083	-1.028832	-0.704138
O	-3.268740	-0.723613	0.663876
H	-2.761917	-0.401948	-1.332761
H	-4.448563	-0.841835	-0.983631
H	-3.185888	-2.083521	-0.919455
H	-2.327171	-0.837897	0.875877
N	-0.400486	-0.922498	0.894360
C	0.102610	-1.913364	0.078157
H	-0.091763	-1.060961	1.853513
H	-0.440145	-2.019608	-0.866823
H	0.349072	-2.880951	0.533225
C	1.963724	1.809342	0.802649
N	1.795184	1.445746	-0.615108
H	1.382729	1.097594	1.389515
H	1.594611	2.816717	0.999096
H	3.014153	1.739969	1.085599
H	0.776510	1.511850	-0.828213

H	2.316777	2.059865	-1.230927
H	2.111023	0.308836	-0.753507
C	-1.844577	2.183290	0.052890
O	-0.906786	1.299293	-0.530579
H	-2.150846	2.910629	-0.702073
H	-1.416664	2.730096	0.905483
H	-2.723454	1.629734	0.396494
H	-0.809786	0.497602	0.059039
C	3.378193	-1.354761	0.120473
O	2.375998	-0.971762	-0.787870
H	3.885200	-2.264430	-0.217762
H	2.963837	-1.544504	1.122167
H	4.135018	-0.565349	0.213136
H	1.315408	-1.470026	-0.416361

Vibrational frequencies

-1044.7784	26.8158	42.5934
60.5432	84.7133	92.8357
96.9873	106.2083	111.2026
124.6156	134.2036	141.1797
150.6587	155.3992	172.7721
187.3840	192.4277	201.5948
209.1148	250.2602	294.4296
343.8368	419.2639	496.9109
557.2616	651.7091	719.4770
765.7063	966.7720	998.3793
1014.3522	1045.9790	1068.6040
1080.8242	1081.8360	1101.3700
1106.5408	1144.8164	1167.4248
1176.8742	1189.4434	1192.5890
1197.7902	1203.4367	1274.9274
1310.3275	1354.2794	1359.7727
1389.7557	1472.9034	1479.5352
1485.1824	1490.3976	1496.1368
1501.2530	1505.7096	1508.5214
1510.1368	1513.5860	1518.2921
1522.8702	1534.4817	1535.1420
1541.6924	1572.4342	1651.4768
1688.8957	1786.5152	2983.5424
2988.0900	2989.5235	3008.4054
3041.9224	3045.2170	3054.4102
3073.4255	3079.2903	3085.3703
3099.8566	3110.4447	3128.4535
3157.3523	3162.2779	3168.8433
3524.7574	3584.5627	3632.2979

Cartesian coordinates

C	-3.605299	-0.936729	-0.470304
O	-3.283329	-0.633361	0.870859
H	-3.028276	-0.325935	-1.176353
H	-4.665876	-0.722361	-0.612109
H	-3.441985	-1.997976	-0.704893
H	-2.338467	-0.798726	0.975807
N	-0.396646	-1.234624	0.678092
C	-0.037522	-2.045175	-0.441879
H	0.133633	-1.545177	1.494031
H	-0.700160	-1.844887	-1.285139
H	-0.039948	-3.117596	-0.202971
C	1.795701	1.899505	0.805464
N	1.898104	1.563501	-0.614995
H	1.189866	1.137885	1.302563
H	1.333125	2.875200	1.000536
H	2.786017	1.888871	1.266760
H	0.955674	1.554003	-1.004046
H	2.428331	2.271968	-1.108224
H	2.609679	-0.092896	-0.820947
C	-1.810692	2.211157	0.010363
O	-1.028882	1.243617	-0.667816
H	-2.113879	2.962381	-0.720350
H	-1.239993	2.712450	0.803972
H	-2.703058	1.755716	0.450293
H	-0.906050	0.487208	-0.074484
C	3.415765	-1.221528	0.529276
O	2.939231	-1.019396	-0.774141
H	3.877699	-2.210144	0.580569
H	2.613065	-1.183868	1.285594
H	4.173733	-0.480543	0.817657
H	1.002781	-1.797973	-0.738676

Vibrational frequencies

23.3781	28.8896	45.2936
59.0286	69.6189	87.9951
91.4037	100.0844	108.6666
123.6589	128.6856	135.1075
152.8838	154.1320	159.3217
167.9103	172.6308	183.8636
205.8330	219.8947	228.1326
236.7653	242.8657	283.1550
395.7941	480.3896	614.4037
745.2838	941.0535	977.5964
991.2519	1036.5873	1042.8043
1086.0232	1090.7522	1096.6478
1107.5569	1117.1624	1136.3624

1149.7620	1151.9260	1191.8945
1197.0014	1200.9044	1218.8551
1338.1048	1382.1025	1410.9053
1443.8840	1452.6473	1466.9286
1473.9869	1483.2991	1493.7123
1497.5544	1501.1999	1504.5204
1508.1012	1511.7827	1511.8482
1512.6863	1530.1169	1533.2252
1538.9166	1562.1291	1682.8943
2880.8222	2955.5688	2999.2349
3009.9289	3018.9757	3024.6686
3025.8320	3060.9298	3092.0527
3096.6235	3110.1573	3128.3695
3131.3309	3132.5847	3139.2408
3401.4471	3485.5098	3489.5926
3599.8072	3689.9922	3769.7270

R48

Cartesian coordinates

C	2.756494	-1.124408	-0.573406
O	3.090821	0.124379	0.002178
H	1.697072	-1.376648	-0.432550
H	3.362823	-1.884583	-0.077260
H	2.983610	-1.155149	-1.646795
H	2.574359	0.797823	-0.459106
N	0.795901	1.745989	-1.018507
C	0.266491	1.018513	-2.073425
H	0.777556	2.749349	-1.120205
H	0.281378	-0.059456	-1.945143
H	0.421928	1.416460	-3.070012
C	-1.423886	-2.931879	-0.059173
O	-0.828692	-1.654676	-0.078497
H	-2.253051	-2.990795	0.657466
H	-0.660734	-3.651086	0.243181
H	-1.797701	-3.224812	-1.047880
H	0.070314	-0.442005	1.258021
H	-1.483056	-1.002079	-0.387008
C	0.055114	0.771012	2.919990
N	0.501796	0.424725	1.575962
H	0.275084	0.007643	3.678408
H	-1.026139	0.935058	2.916837
H	0.526033	1.704414	3.238370
H	1.507845	0.275993	1.548030
H	0.555006	1.420882	-0.069085
C	-2.628304	1.371756	0.060717
O	-2.416479	0.412298	-0.961546

H	-3.027577	2.306737	-0.347877
H	-1.706417	1.581940	0.614403
H	-3.365486	0.956900	0.749779
H	-1.717374	0.752443	-1.549055

Vibrational frequencies

19.1420	41.5997	53.3462
68.4927	75.4972	85.8200
91.1537	100.9580	106.6425
114.3123	119.7339	130.1498
139.1994	147.2258	162.8048
178.5996	190.7545	191.7206
201.8883	213.4837	223.9269
245.0465	264.1662	352.1202
554.1718	594.1939	670.5750
701.3479	807.3034	864.4354
920.1189	1007.4636	1028.1654
1073.5787	1088.4783	1095.4022
1102.7988	1112.2321	1125.2116
1140.9455	1152.5426	1184.4631
1194.4444	1196.8874	1207.9396
1265.5132	1353.8004	1381.8954
1441.4343	1442.4009	1463.6347
1469.7852	1487.7444	1490.4651
1491.7689	1496.0644	1502.6466
1509.0527	1511.0724	1513.7867
1520.5071	1524.1839	1529.2837
1536.7134	1701.9641	1720.8320
3003.4460	3007.6239	3009.9097
3023.5392	3061.9411	3066.0082
3083.2834	3092.4686	3119.1743
3125.3268	3127.3061	3131.7349
3133.8111	3237.6259	3249.9701
3476.7184	3550.4969	3562.6093
3617.1468	3649.2753	3759.9631

TS48

Cartesian coordinates

C	-3.757875	0.479568	-0.990170
O	-2.878565	0.730565	0.084865
H	-3.255586	-0.014731	-1.831559
H	-4.145035	1.438904	-1.337669
H	-4.608901	-0.139322	-0.681507
H	-2.517232	-0.121808	0.401895
N	-1.298780	-1.516648	0.705463
C	-0.807142	-2.069763	-0.485230
H	-1.318306	-2.224803	1.436104

H	-1.118533	-1.485807	-1.359090
H	-0.996816	-3.139148	-0.635595
C	2.942707	1.373348	-1.168024
O	1.703175	0.716569	-1.155342
H	3.184794	1.831781	-0.195349
H	2.947361	2.166178	-1.924244
H	3.748808	0.670841	-1.409830
H	0.619505	1.073902	-0.226917
H	1.824818	-0.348371	-0.846539
C	0.257521	1.926632	1.698489
N	-0.171503	1.137703	0.534169
H	0.485020	2.945403	1.386411
H	1.154247	1.473377	2.119790
H	-0.529069	1.945583	2.452461
H	-1.055167	1.476576	0.137607
H	-0.409325	0.161886	0.804759
C	2.041190	-1.418421	1.025650
O	1.875856	-1.536808	-0.339272
H	2.690412	-2.203419	1.438609
H	1.071167	-1.488102	1.571626
H	2.483355	-0.445338	1.311047
H	0.374329	-1.951759	-0.495736

Vibrational frequencies

-442.8343	26.9948	43.7837
61.9855	68.0311	75.5438
89.5746	98.3960	101.3474
116.2305	127.3407	133.3946
139.4650	148.9197	182.2808
193.2380	203.2946	224.9737
235.7527	267.3679	299.6570
322.6524	387.4278	469.5035
599.1061	646.2822	843.1986
919.3160	1007.2568	1047.7121
1062.9268	1074.3448	1080.5097
1107.2692	1116.2212	1146.8580
1153.0715	1177.6449	1187.3330
1189.4543	1191.2472	1192.2733
1215.6129	1319.4630	1347.3199
1354.8830	1410.4074	1440.7580
1455.9510	1466.2247	1479.0074
1481.7593	1488.8273	1492.8637
1496.3057	1500.1838	1501.6580
1504.7527	1514.0223	1515.1740
1519.2048	1528.6127	1534.1964
1638.4013	1678.3405	1690.1745
1773.6602	1946.2165	2251.2376

2837.1456	2932.5989	2968.7052
3007.0710	3016.4502	3017.3560
3045.8353	3065.1342	3081.2522
3082.3866	3089.4550	3124.4532
3153.3099	3171.9748	3176.2320
3410.8208	3507.1864	3530.2917

P48

Cartesian coordinates

C	-0.972012	2.332448	0.824373
O	-0.578120	2.329516	-0.532325
H	-0.899316	1.331915	1.273212
H	-2.011847	2.664450	0.873648
H	-0.367597	3.026595	1.421366
H	0.385551	2.170892	-0.540005
N	2.136620	1.700911	-0.163911
C	2.453871	0.879971	0.964613
H	2.995554	1.883874	-0.686106
H	1.582976	0.765509	1.610717
H	3.309362	1.268187	1.535043
C	-1.026987	-2.109885	1.755720
O	-0.248896	-1.207800	1.002381
H	-1.349033	-2.975046	1.161428
H	-1.918492	-1.624536	2.173336
H	-0.419644	-2.474755	2.586108
H	-0.797411	-0.895359	0.235992
H	1.247362	-1.794005	0.175633
C	-3.192972	-0.173706	-0.717270
N	-1.776189	-0.273249	-1.067267
H	-3.284601	0.336822	0.244128
H	-3.620037	-1.173012	-0.602796
H	-3.794571	0.377138	-1.450444
H	-1.370960	0.663262	-1.150383
H	-1.660399	-0.741207	-1.957966
C	1.576675	-1.363172	-1.668058
O	1.984377	-1.926094	-0.446284
H	2.396588	-1.471436	-2.381399
H	1.338058	-0.291744	-1.574160
H	0.695514	-1.871040	-2.085381
H	2.729579	-0.129046	0.609832

Vibrational frequencies

23.1463	35.0745	52.2972
56.3859	70.9083	73.4110
86.8984	92.0963	95.9419
113.1471	122.4320	125.4665
139.5632	143.8874	147.5753

155.9475	167.7571	174.4108
179.4969	196.7208	221.5778
244.8266	266.5396	302.8269
372.2937	519.1400	805.2323
823.7071	967.8176	992.2992
1027.0285	1037.0375	1065.4441
1092.4938	1096.0734	1105.4882
1107.5992	1111.8155	1144.0626
1149.3147	1168.3049	1188.4310
1192.2536	1199.4997	1214.4063
1339.5677	1380.2829	1413.4628
1467.0928	1478.7859	1482.1532
1484.5484	1489.5435	1495.5525
1497.7887	1500.7284	1503.3771
1506.2334	1508.0013	1508.9569
1512.8798	1524.4822	1532.6791
1540.5306	1589.3583	1701.3516
2943.9625	2971.6276	2995.7001
2996.5826	3019.3027	3021.9657
3025.2571	3053.2355	3056.5944
3092.6087	3107.7552	3109.5968
3117.3601	3124.5123	3138.8124
3215.2281	3415.3093	3484.6061
3558.7738	3598.6954	3630.8342

R49

Cartesian coordinates

C	2.674116	-0.633072	-1.169327
O	3.226046	0.126614	-0.116387
H	1.630649	-0.919509	-0.980791
H	3.269105	-1.543775	-1.267220
H	2.711874	-0.098854	-2.128902
H	2.646338	0.890114	0.011594
N	0.942410	1.979565	0.189127
C	0.412477	2.078264	-1.093461
H	1.036264	2.852498	0.686456
H	0.251036	1.135190	-1.604347
H	0.714309	2.936962	-1.682043
C	-1.514230	-2.477830	-1.046605
O	-0.897357	-1.228192	-0.832965
H	-2.267147	-2.703382	-0.280326
H	-0.741662	-3.247647	-1.005945
H	-1.992696	-2.528459	-2.031947
H	-0.253835	-0.823678	0.760396
H	-1.583060	-0.513608	-0.863795
C	1.058277	-1.033775	2.215657

O	-0.028018	-0.366847	1.592969
H	0.846692	-2.100353	2.355216
H	1.196187	-0.585764	3.201469
H	1.984482	-0.914115	1.643074
H	0.552573	1.233827	0.771979
C	-3.016186	0.908199	0.821420
N	-2.582659	0.910046	-0.580191
H	-3.436909	1.864335	1.155053
H	-2.162978	0.655622	1.453913
H	-3.773663	0.133686	0.962428
H	-3.358493	1.113540	-1.198993
H	-1.879417	1.632776	-0.734857

Vibrational frequencies

24.3754	40.1497	49.4796
60.3662	66.7187	82.1514
89.7050	96.9775	114.7059
117.3335	134.0324	140.6788
147.5908	156.7745	163.5943
169.7024	175.4841	198.5028
206.5126	219.0443	233.5527
262.3458	283.5301	316.8141
502.8959	566.8576	681.8618
754.8830	826.4422	904.9251
917.1440	1006.1058	1027.5866
1044.7762	1078.0393	1088.5534
1098.3284	1109.9509	1129.4216
1160.4194	1178.4032	1190.2722
1193.1754	1205.8993	1208.8981
1254.2401	1356.0897	1360.3604
1456.1379	1468.5959	1477.5850
1486.8776	1493.5931	1494.5082
1500.1886	1504.5047	1505.8021
1515.9074	1520.3951	1522.3898
1529.8368	1533.5933	1540.8165
1570.3142	1677.8417	1696.7105
2995.7867	3005.6571	3018.6242
3021.7039	3050.4302	3065.4850
3092.3137	3099.0828	3115.8399
3122.3435	3125.7786	3137.2299
3137.5942	3251.7220	3263.1347
3391.9293	3457.6009	3576.8107
3595.9621	3647.7418	3735.5743

TS49

Cartesian coordinates

C	-2.649159	0.729921	-1.139458
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O	-3.243058	0.001646	-0.091592
H	-1.599932	0.978503	-0.930958
H	-3.203942	1.663616	-1.259828
H	-2.689046	0.188995	-2.096829
H	-2.623047	-0.707152	0.138983
N	-0.935680	-1.703353	0.408862
C	-0.555565	-2.140046	-0.838541
H	-0.989729	-2.451916	1.088727
H	-0.719960	-1.423605	-1.646134
H	-0.734254	-3.181887	-1.105711
C	1.905455	2.527189	-0.699779
O	1.289427	1.272311	-0.873740
H	2.417813	2.603743	0.268275
H	1.172187	3.339040	-0.765999
H	2.642127	2.671701	-1.494054
H	0.709613	1.062939	-0.062673
H	1.971425	-0.212081	-0.859538
C	-0.827927	1.235143	1.927409
O	0.032822	0.448457	1.144403
H	-0.653882	2.303530	1.739917
H	-0.667775	1.062415	3.001191
H	-1.880210	1.025001	1.695677
H	-0.490406	-0.587097	0.817261
C	2.533640	-1.361797	0.791276
N	2.137251	-1.232241	-0.628855
H	2.552557	-2.415119	1.069417
H	1.788422	-0.820747	1.377761
H	3.518601	-0.919471	0.940761
H	2.820068	-1.632962	-1.264608
H	1.176184	-1.720063	-0.789698

Vibrational frequencies

-827.1265	28.6207	46.2208
79.9402	90.1356	92.4878
101.4439	110.3986	122.8011
140.7840	146.2852	158.7489
168.2328	177.1566	192.4595
199.2245	205.8812	207.9304
226.6456	239.5877	303.2366
320.8706	377.6036	396.1249
588.0351	622.3983	679.5105
724.9546	916.2768	1002.5905
1038.1228	1040.9068	1055.2162
1089.1275	1106.6310	1110.9928
1130.3133	1141.4489	1188.0635
1193.6893	1195.8488	1203.7189
1211.8977	1294.0120	1321.5534

1326.5315	1343.1785	1460.7832
1474.5740	1484.8494	1490.6503
1492.0069	1502.5039	1504.8981
1507.3793	1510.2278	1515.8566
1518.4807	1523.3763	1527.3489
1530.6093	1543.7787	1602.9181
1618.5441	1658.7576	1714.6788
1753.9777	2326.4707	2716.1174
2894.9501	2983.0015	2985.8305
3015.7634	3033.2675	3041.5521
3058.7462	3062.3721	3065.4786
3068.3937	3107.1041	3109.6159
3158.5130	3158.8611	3165.7907
3567.1753	3584.2894	3677.7050

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Cartesian coordinates

C	-2.660757	0.171261	-1.126514
O	-3.002591	-0.611267	-0.002528
H	-1.655001	0.602508	-1.045407
H	-3.383789	0.986802	-1.192625
H	-2.715438	-0.401880	-2.062833
H	-2.287422	-1.246768	0.130405
N	-0.518973	-2.174754	0.175430
C	0.171658	-2.153771	-1.068755
H	-0.312303	-3.046668	0.663835
H	-0.269355	-1.414118	-1.740939
H	0.240962	-3.134134	-1.555557
C	0.457450	2.783452	-1.043246
O	0.735370	1.406898	-0.936118
H	0.934286	3.366384	-0.244500
H	-0.622358	2.984319	-1.024178
H	0.849400	3.133621	-1.999931
H	0.410068	1.097318	-0.070655
H	2.410966	0.197861	-0.920088
C	-1.195587	0.909442	2.235579
O	-0.178390	0.357344	1.413508
H	-0.978972	1.971706	2.359083
H	-1.195656	0.441261	3.226449
H	-2.179634	0.784462	1.776071
H	-0.449145	-0.528637	1.114524
C	3.147690	-0.381353	0.892741
N	2.898885	-0.605729	-0.529144
H	3.609263	-1.269470	1.333482
H	2.192736	-0.212792	1.395853
H	3.796512	0.479406	1.109322

H	3.768400	-0.722723	-1.034202
H	1.219264	-1.803051	-0.879832

Vibrational frequencies

34.6881	47.3270	49.3080
58.7127	70.7589	76.7775
91.2301	95.2783	105.9048
119.9502	126.4298	138.4237
149.9918	158.1260	161.6309
168.5425	175.7009	181.7822
200.1538	203.3151	213.4079
241.2330	255.1378	287.2037
404.8774	495.6057	616.0240
746.8556	862.6752	928.8997
1010.6422	1027.6548	1060.4238
1087.0230	1090.3534	1096.9839
1114.2463	1123.8018	1136.9048
1142.6134	1166.3544	1188.4550
1190.0060	1194.0383	1196.5080
1339.1231	1371.5927	1417.8901
1440.4060	1454.4009	1474.8673
1480.7915	1486.7011	1492.4211
1495.4402	1500.0309	1501.0833
1507.7931	1511.7846	1514.7020
1522.5134	1531.9863	1533.0150
1535.6758	1543.7209	1690.0312
2728.7872	2995.7941	2997.4232
2998.3750	3027.9032	3036.4191
3051.5401	3062.3641	3080.9311
3102.5367	3119.3508	3120.8127
3124.9508	3127.8410	3139.3053
3498.1885	3499.2442	3574.7876
3607.7920	3627.8436	3753.7789

R50

Cartesian coordinates

C	-3.283429	0.773582	-0.943784
O	-3.521929	0.432417	0.402155
H	-2.213747	0.925580	-1.143593
H	-3.807352	1.710027	-1.147477
H	-3.662662	0.012919	-1.640634
H	-2.995298	-0.358904	0.579870
N	-1.359745	-1.556826	0.516788
C	-1.224037	-2.236314	-0.687861
H	-1.241514	-2.119929	1.345924
H	-1.250929	-1.620760	-1.580034
H	-1.638187	-3.236310	-0.743999

C	3.345701	1.650270	-0.187778
N	2.249014	1.113435	-0.990551
H	3.309352	1.195415	0.804693
H	3.222248	2.728424	-0.059333
H	4.342013	1.466158	-0.609670
H	2.262845	1.501001	-1.925870
H	0.733596	1.122038	-0.114101
H	2.331222	0.092496	-1.062206
C	-0.640414	2.155211	0.893866
O	-0.073209	0.949177	0.431965
H	-0.680262	2.911954	0.100236
H	-0.082064	2.571407	1.742317
H	-1.663886	1.941188	1.208262
H	-0.856711	-0.664185	0.564751
C	2.101178	-1.658340	1.020739
N	2.071951	-1.827065	-0.433187
H	1.723643	-2.523157	1.583576
H	1.497737	-0.786682	1.285632
H	3.127325	-1.466944	1.346053
H	2.659021	-2.605758	-0.707815
H	1.122185	-2.061990	-0.721980

Vibrational frequencies

19.1297	36.5384	55.3407
57.6265	75.6062	78.5916
88.1648	90.0066	100.7451
112.6914	124.6021	142.8833
145.8510	156.9065	162.9702
172.6302	182.7453	199.5439
208.0244	210.3519	213.8001
238.1065	281.6985	332.6151
432.1806	553.5989	563.4224
657.2769	718.4831	917.6817
922.9415	947.7859	1004.1746
1020.1750	1044.1282	1064.1079
1083.0037	1092.5718	1102.6256
1112.4139	1142.1794	1183.2866
1191.2291	1200.7968	1203.2494
1212.8279	1255.8949	1359.7869
1367.3125	1383.1970	1461.5711
1463.5803	1469.3038	1477.6517
1490.7782	1499.3953	1504.1880
1507.8828	1512.0769	1512.7113
1515.0761	1524.9168	1532.4910
1535.5095	1567.8353	1677.7038
1687.7449	1701.2847	2993.2495
3000.5281	3003.0928	3014.5091

3045.7998	3058.6441	3085.3828
3091.9051	3116.1245	3126.5913
3127.4081	3128.1112	3140.0446
3251.5808	3263.8167	3364.4141
3380.8861	3457.9162	3591.2824
3596.4884	3645.9360	3736.9687

TS50

Cartesian coordinates

C	-3.517019	-0.932143	-0.607486
O	-3.269753	-0.645672	0.747119
H	-2.906187	-0.310157	-1.277167
H	-4.571526	-0.727206	-0.811104
H	-3.323838	-1.987246	-0.850461
H	-2.308901	-0.765332	0.877595
N	-0.422799	-0.884262	0.768083
C	-0.127305	-2.015608	0.039513
H	-0.152725	-1.003545	1.740152
H	-0.625283	-2.087297	-0.930348
H	0.009029	-2.974696	0.547984
C	1.931269	1.783472	0.904787
N	1.843590	1.500707	-0.537294
H	1.317991	1.038246	1.413713
H	1.547722	2.777202	1.144156
H	2.964333	1.702333	1.247905
H	2.367689	2.175784	-1.083474
H	0.828576	1.549149	-0.794264
H	2.193307	0.293201	-0.741863
C	-1.715419	2.169737	-0.023577
O	-0.831305	1.273955	-0.662992
H	-2.084228	2.890213	-0.758821
H	-1.221841	2.731652	0.785093
H	-2.565753	1.628214	0.402991
H	-0.723419	0.448159	-0.069474
C	3.388202	-1.418149	0.241138
N	2.456745	-0.990495	-0.809724
H	3.593378	-2.490179	0.193247
H	2.929911	-1.203478	1.207573
H	4.331364	-0.872322	0.167553
H	2.788027	-1.273832	-1.726516
H	1.519705	-1.470630	-0.631183

Vibrational frequencies

-922.1549	17.1093	43.0381
67.6723	85.4577	95.4550
107.2970	113.9230	120.6655
126.6730	142.1712	148.7708

161.6372	178.7497	181.8184
184.6852	192.0408	197.9000
207.9572	243.9964	283.7727
312.5943	363.4742	368.1490
560.5113	607.4343	670.7876
735.1427	797.1993	867.8521
998.6397	1022.5000	1037.3052
1070.0825	1073.6440	1089.8223
1101.4227	1110.4337	1119.6526
1146.0687	1167.6998	1185.8822
1203.3868	1205.7217	1287.3997
1317.6613	1328.5446	1352.1843
1373.7211	1412.6698	1458.9725
1469.5336	1488.2351	1493.6477
1495.9571	1502.9458	1505.2471
1509.0957	1512.2680	1513.0866
1518.7447	1527.6825	1528.4684
1540.3922	1617.5480	1648.6753
1664.7585	1751.7958	1766.9512
2599.2564	2685.4723	2966.9489
2985.1677	3028.2370	3035.0762
3038.1246	3057.6037	3063.3363
3067.1806	3098.7977	3110.6216
3123.2701	3130.0410	3142.0006
3149.6307	3155.8973	3523.1777
3532.5647	3561.9721	3576.2229

P50

Cartesian coordinates

C	-3.628788	-0.975199	-0.655823
O	-3.431958	-0.690429	0.712689
H	-3.005155	-0.342054	-1.299464
H	-4.677645	-0.778810	-0.885761
H	-3.424563	-2.029414	-0.892321
H	-2.488794	-0.800780	0.888434
N	-0.533589	-1.162233	0.851692
C	-0.047357	-2.143407	-0.057766
H	-0.070986	-1.286164	1.753577
H	-0.676248	-2.184230	-0.949626
H	0.046173	-3.141056	0.392028
C	1.755788	1.856062	0.886555
N	1.854365	1.787684	-0.568337
H	1.284882	0.938213	1.250070
H	1.166550	2.702659	1.265628
H	2.753888	1.911181	1.329576
H	2.289128	2.626358	-0.932669

H	0.910216	1.735489	-0.947563
H	2.612096	-0.069937	-0.900059
C	-1.876644	2.170507	0.033013
O	-1.066301	1.246201	-0.669428
H	-2.174520	2.950500	-0.669656
H	-1.332340	2.644137	0.861859
H	-2.774074	1.686022	0.430561
H	-0.936032	0.474076	-0.096321
C	3.873745	-1.175950	0.273095
N	2.878231	-1.053679	-0.785055
H	4.131027	-2.227273	0.430646
H	3.448095	-0.801749	1.208498
H	4.807335	-0.623813	0.091881
H	3.257008	-1.378144	-1.666504
H	0.986509	-1.845875	-0.371448

Vibrational frequencies

23.4624	28.5313	39.4161
53.6357	71.9542	74.8744
76.3028	88.2857	90.4543
107.7478	109.7756	124.8480
135.9228	150.6503	153.1999
162.4628	175.8542	181.2725
205.4061	206.7612	215.0025
220.1210	237.2523	277.6356
442.9503	451.1912	530.9190
621.0272	741.0504	950.8300
964.3906	993.8509	1017.2440
1046.4773	1052.1600	1088.2147
1093.4461	1096.6366	1099.4668
1119.4067	1138.5771	1146.8524
1194.0936	1199.2921	1201.5314
1204.2506	1341.1939	1378.8431
1391.1398	1420.2639	1447.4309
1456.9574	1463.6971	1466.4838
1477.9298	1489.4382	1499.2688
1501.6561	1504.8435	1507.7324
1509.6378	1511.0545	1526.2546
1529.7983	1532.0417	1533.2839
1687.0130	1709.5819	2724.0430
2990.5638	2995.7224	3000.7591
3003.1829	3020.7761	3053.7547
3073.8524	3080.1904	3083.5102
3110.8980	3116.1022	3117.0202
3121.6142	3134.3605	3373.5544
3490.2671	3491.5199	3592.6446
3603.8792	3662.5805	3747.2593

R51**Cartesian coordinates**

C	3.793932	-0.603676	-0.870153
O	3.526608	-0.474657	0.504197
H	2.875007	-0.632674	-1.474328
H	4.327845	-1.544047	-1.022113
H	4.423217	0.211234	-1.253781
H	2.939568	0.289186	0.603311
N	1.299452	1.402375	0.429710
C	1.185982	2.292540	-0.631277
H	1.097954	1.793678	1.338621
H	1.300890	1.864540	-1.620896
H	1.520607	3.310667	-0.470958
C	-3.695148	-1.362443	-0.266076
O	-2.581902	-0.970591	-1.030251
H	-3.542430	-1.205979	0.812045
H	-3.863168	-2.428764	-0.430993
H	-4.608535	-0.828818	-0.561931
H	-0.741241	-1.325378	-0.375962
H	-2.458467	-0.002980	-0.912680
C	0.558926	-2.066175	1.057558
N	0.242729	-1.248413	-0.114516
H	0.335998	-3.133587	0.932327
H	-0.014522	-1.703937	1.915842
H	1.620470	-1.951422	1.286947
H	0.778153	-1.576915	-0.909965
H	0.845709	0.483602	0.271980
C	-2.003933	1.499791	1.147192
N	-2.059920	1.665271	-0.305418
H	-1.592368	2.366187	1.680649
H	-1.387630	0.627781	1.377565
H	-3.007696	1.306639	1.532714
H	-2.685682	2.423459	-0.550643
H	-1.135709	1.924651	-0.651210

Vibrational frequencies

25.4745	29.0776	40.0535
54.5132	64.8220	71.7326
80.3981	89.9119	106.4038
115.4103	120.3769	131.8470
138.0597	140.0095	149.5041
173.2094	180.9881	186.3995
209.3983	210.2224	219.3126
262.8846	282.8199	290.3273
448.7215	501.0832	585.6167
675.3902	708.7205	896.8156

955.3156	978.0748	995.0338
1011.8865	1042.0560	1085.0918
1086.9592	1099.6751	1111.0133
1114.5110	1135.9137	1165.8978
1183.9495	1193.1115	1206.3384
1217.8317	1257.1891	1366.8674
1371.3636	1380.7827	1463.5176
1464.8389	1467.1239	1491.1512
1495.1423	1498.8151	1500.8047
1502.0049	1509.1543	1514.4592
1516.8128	1519.7919	1525.8708
1535.8942	1554.4822	1678.0329
1701.2415	1711.8437	2985.8391
2987.0494	3013.4933	3017.0750
3035.1244	3037.4119	3085.2974
3097.1211	3115.7395	3117.8207
3130.0553	3132.2375	3136.2869
3160.6584	3254.5036	3419.6627
3462.5421	3475.4547	3591.8743
3595.0127	3633.3691	3703.3588

TS51

Cartesian coordinates

C	-3.764489	-0.027916	-0.748531
O	-3.180900	0.320630	0.478067
H	-3.043400	-0.009059	-1.582430
H	-4.552618	0.695806	-0.972934
H	-4.217747	-1.028715	-0.731035
H	-2.458399	-0.326885	0.646172
N	-0.929411	-1.310503	0.666734
C	-0.738050	-2.199441	-0.367605
H	-0.828858	-1.782812	1.560517
H	-1.090562	-1.860824	-1.346493
H	-0.861064	-3.274098	-0.200364
C	2.908897	1.764327	-0.209458
O	1.981138	0.991348	-0.914084
H	2.836114	1.633056	0.884256
H	2.777011	2.835103	-0.417762
H	3.936273	1.507242	-0.500994
H	0.804199	1.231474	-0.579636
H	2.070450	-0.400165	-0.746117
C	-0.603750	2.268462	0.883780
N	-0.365704	1.289863	-0.185507
H	-0.397537	3.279546	0.527725
H	0.069461	2.050998	1.714814
H	-1.636598	2.198212	1.228867

H	-1.016700	1.452605	-0.946741
H	-0.580893	0.322277	0.188127
C	2.420587	-1.685962	0.912629
N	2.047272	-1.504997	-0.498701
H	2.376202	-2.739353	1.192223
H	1.697131	-1.133745	1.511426
H	3.422819	-1.295885	1.093297
H	2.655957	-2.026949	-1.120985
H	1.032581	-1.861019	-0.616369

Vibrational frequencies

-812.6787	19.2869	37.6875
45.0688	69.9386	83.3970
92.2466	93.9723	103.6994
119.5257	124.4405	133.7599
144.8640	165.7325	168.0617
172.9263	182.2644	188.9881
212.1166	250.0671	295.3820
344.3252	354.2739	446.9913
596.3371	625.6571	662.5305
704.4390	862.4602	912.8736
1002.0119	1012.8556	1058.1350
1071.6266	1082.1404	1085.0477
1104.1889	1116.6322	1123.5338
1152.7994	1184.9370	1189.4799
1196.2644	1283.0435	1307.3310
1341.0889	1359.4320	1371.3111
1409.1078	1444.5372	1460.4836
1469.2297	1488.6908	1495.4718
1498.2268	1499.5354	1502.1303
1503.4198	1508.6795	1514.2889
1519.7313	1527.5101	1548.7928
1615.6319	1617.7694	1646.7953
1719.7216	1731.7750	1800.7222
1872.5742	2443.9551	2790.3016
2948.3058	2963.7677	3014.8161
3023.7486	3025.6077	3041.6086
3062.6085	3071.9506	3099.1749
3108.4180	3144.2427	3152.1730
3154.6052	3172.4863	3381.7090
3534.0419	3570.2673	3572.2463

P51

Cartesian coordinates

C	3.772932	-0.705437	-0.584815
O	3.172483	-0.556392	0.676358
H	3.033757	-0.769371	-1.398563

H	4.343475	-1.636526	-0.579298
H	4.465394	0.113798	-0.823072
H	2.626179	0.244992	0.639779
N	1.445025	1.717073	0.274998
C	0.899490	2.269919	-0.922498
H	1.277990	2.377357	1.036612
H	1.182679	1.671551	-1.791159
H	1.196797	3.316499	-1.079189
C	-3.176351	-1.687656	-0.270640
O	-2.418509	-0.845318	-1.102078
H	-2.988874	-1.504092	0.797835
H	-2.983243	-2.750844	-0.470373
H	-4.234889	-1.498964	-0.463957
H	-1.469312	-1.008798	-0.900760
H	-2.422824	1.098565	-0.612811
C	0.239114	-2.044272	0.952001
N	0.214539	-1.299349	-0.312506
H	-0.203596	-3.031605	0.802620
H	-0.377089	-1.517432	1.685189
H	1.249404	-2.152538	1.357756
H	0.767078	-1.795175	-1.003363
H	0.690176	-0.412342	-0.167544
C	-1.812108	1.423730	1.292142
N	-2.157201	1.899908	-0.040447
H	-1.602874	2.270200	1.952903
H	-0.898116	0.823955	1.231896
H	-2.581561	0.802919	1.773093
H	-2.945484	2.533547	-0.001346
H	-0.211865	2.276856	-0.831949

Vibrational frequencies

22.1861	30.9767	48.6986
54.2546	72.1895	76.3415
87.3562	90.9146	100.7536
110.0145	114.3119	120.4603
129.7148	144.0993	150.5415
162.3785	181.9140	184.6528
194.0249	204.2453	219.5891
226.1126	246.4681	291.3755
391.9849	432.5860	480.4194
779.2919	924.8705	949.8605
982.8804	999.0599	1013.2736
1028.9620	1045.5260	1084.9224
1096.2224	1108.4528	1115.6228
1116.5975	1141.8722	1165.3019
1190.0025	1195.9420	1199.3510
1220.0309	1345.4831	1371.7044

1379.9070	1421.4262	1458.1659
1466.1220	1476.1953	1479.9809
1495.9709	1497.2996	1498.1364
1498.6063	1507.0211	1507.9143
1510.2349	1515.6227	1526.5604
1528.2861	1540.1279	1561.5058
1680.0130	1690.6101	2802.4040
2977.2797	2983.8457	2998.7496
3018.6011	3028.9577	3033.6052
3043.3918	3070.9189	3105.9876
3109.7257	3110.3112	3115.6079
3119.8091	3124.9007	3399.5541
3470.3716	3485.2189	3517.8542
3594.9003	3603.6203	3666.6528

R52

Cartesian coordinates

C	-3.577505	0.025062	-0.252750
O	-2.398487	-0.280986	0.459494
H	-3.376681	0.235736	-1.311468
H	-4.013579	0.917566	0.198784
H	-4.317113	-0.783273	-0.193222
H	-1.967298	-1.026007	0.019123
N	-0.431241	-1.841257	-1.019314
C	-0.459171	-0.937728	-2.071417
H	-0.213620	-2.793418	-1.270624
H	-0.756805	0.073670	-1.812625
H	-0.777136	-1.321010	-3.034698
H	1.381154	0.135822	-2.156393
C	-0.043128	3.124125	0.754657
N	0.110180	1.707312	0.453981
H	0.941344	3.575220	0.901552
H	-0.597494	3.244373	1.689198
H	-0.562783	3.703683	-0.022397
H	-0.794844	1.262513	0.321496
H	0.570957	0.019639	1.493650
H	0.665016	1.568786	-0.387806
C	1.484204	-1.513701	2.537344
N	0.444000	-0.983875	1.661943
H	1.540228	-1.022810	3.518126
H	2.457692	-1.398476	2.053514
H	1.327408	-2.582827	2.703691
H	-0.467512	-1.065128	2.101156
H	0.023067	-1.551568	-0.136714
C	2.869345	-0.060233	-0.934986
O	2.039465	0.728251	-1.763838

H	3.521502	-0.720318	-1.521249
H	2.286533	-0.669555	-0.233885
H	3.499096	0.618855	-0.357818

Vibrational frequencies

41.1381	49.3266	62.6252
74.8483	76.6606	82.2430
91.2879	106.6260	112.7172
119.8218	129.8184	141.2410
152.6050	157.3139	162.1001
169.7145	183.4697	186.3280
190.7498	197.5312	208.4224
214.9801	258.6637	306.2304
515.4548	571.4127	586.5405
649.0788	717.1087	783.1278
927.0069	948.2170	1007.3765
1037.9574	1043.6393	1068.7395
1094.2897	1099.2952	1104.7139
1106.5486	1134.0149	1149.4432
1187.5579	1195.5968	1196.2121
1227.1119	1263.1377	1340.0694
1381.3065	1392.0181	1435.4631
1450.2444	1469.9006	1477.3118
1485.7667	1498.7757	1503.7823
1505.6987	1506.9202	1507.7398
1511.0708	1524.6159	1526.4616
1528.2529	1534.9676	1705.6730
1720.9189	1722.7391	2991.7581
3004.3933	3008.8540	3010.9622
3058.6805	3075.3308	3078.9135
3081.5882	3115.0146	3117.2081
3129.5667	3130.2867	3133.3274
3214.5412	3245.2470	3386.6782
3483.6243	3566.5616	3572.9539
3654.4416	3682.6510	3737.1179

TS52

Cartesian coordinates

C	-3.561127	-0.161081	-0.171332
O	-2.278040	0.279161	0.199660
H	-3.519265	-0.971505	-0.911402
H	-4.104400	0.679487	-0.611560
H	-4.137124	-0.519922	0.692144
H	-1.761466	-0.513072	0.542887
N	-0.608168	-1.695836	0.791721
C	-0.470501	-2.260697	-0.460184
H	-0.484245	-2.404144	1.508361

H	-0.974576	-1.727365	-1.273526
H	-0.473616	-3.347092	-0.573001
H	1.099084	-1.582364	-1.218132
C	0.309192	2.579971	-1.601100
N	0.152744	1.280727	-0.949247
H	1.340226	2.921497	-1.495131
H	-0.347511	3.310145	-1.124696
H	0.067318	2.537648	-2.666142
H	-0.814079	0.938972	-0.984222
H	0.324755	1.206600	0.335435
H	0.772984	0.557439	-1.339822
C	1.482657	1.069970	2.384995
N	0.298098	0.834051	1.561509
H	1.637938	2.140772	2.532168
H	2.356117	0.664283	1.873231
H	1.404060	0.589989	3.364115
H	-0.547107	1.211421	1.979866
H	0.093068	-0.193857	1.385312
C	2.799136	-1.127374	-0.406769
O	1.856581	-0.973411	-1.442160
H	3.501246	-1.944748	-0.614381
H	2.304861	-1.334853	0.551363
H	3.378550	-0.202654	-0.314411

Vibrational frequencies

-890.4556	37.1330	55.0338
73.7428	73.9110	81.1920
88.3333	94.7835	106.3241
114.5770	131.8021	142.6776
151.1730	157.1625	173.7839
178.3175	187.4668	202.2476
226.7211	231.3766	262.1338
296.9237	343.5554	354.7445
499.6162	646.6977	656.8301
766.1039	850.2455	876.3889
1004.1432	1037.0700	1045.7899
1068.6647	1090.7193	1107.0628
1111.1159	1122.7098	1123.7693
1136.3155	1162.8516	1170.0644
1185.1794	1190.2281	1282.4112
1285.3392	1321.2438	1333.9524
1373.0165	1386.0100	1469.0322
1473.1568	1477.5110	1487.0916
1495.1834	1497.3947	1497.9972
1503.3759	1509.3034	1512.4294
1513.9228	1520.8940	1524.4329
1530.1857	1583.3626	1705.8160

1717.9180	1764.9735	1803.9942
2756.7463	2933.4402	2991.3633
3004.6890	3028.5417	3045.2519
3050.4498	3051.2503	3056.5873
3080.9937	3097.7937	3112.3864
3120.7547	3120.9375	3123.6940
3140.5909	3147.6895	3323.7651
3420.9947	3541.6789	3564.6230

I52

Cartesian coordinates

C	-3.476126	-0.085466	-0.324972
O	-2.142632	-0.514368	-0.440696
H	-3.556730	0.878779	0.194904
H	-4.043667	-0.831281	0.239751
H	-3.949938	0.022809	-1.309049
H	-1.580058	0.240609	-0.879745
N	-0.605259	1.407279	-1.151521
C	-0.686045	2.316581	-0.119429
H	-0.307166	1.863692	-2.007589
H	-1.381573	2.046602	0.683545
H	-0.648720	3.388505	-0.327987
H	0.650516	1.878053	1.027873
C	-0.078075	-2.021039	2.217144
N	-0.039374	-1.014613	1.149207
H	0.936157	-2.260111	2.536261
H	-0.563668	-2.924621	1.849622
H	-0.636497	-1.634398	3.069076
H	-0.989833	-0.786254	0.763163
H	0.477723	-1.328790	0.286598
H	0.433352	-0.126659	1.437483
C	2.228358	-1.313607	-2.078629
N	0.914286	-1.217986	-1.449140
H	2.580480	-2.347970	-2.057893
H	2.942053	-0.711916	-1.511728
H	2.248679	-0.967194	-3.119784
H	0.226517	-1.752710	-1.969027
H	0.563029	-0.249494	-1.450318
C	2.480596	1.278039	0.715143
O	1.332449	1.336217	1.535793
H	3.194915	2.067998	0.973105
H	2.210303	1.378275	-0.342964
H	2.975774	0.311467	0.858555

Vibrational frequencies

33.8402	59.6818	71.5050
77.2056	86.2203	87.1141

94.2788	103.8230	114.1836
125.0087	135.0750	141.5282
153.7957	165.1332	172.1697
179.5838	201.9782	213.0336
243.4326	258.3786	282.2603
297.8427	341.5117	361.1305
552.0904	635.1030	702.7271
865.9547	927.0800	990.1587
1021.1590	1033.7215	1054.7715
1081.4683	1088.5528	1098.6797
1100.2680	1118.8838	1169.8309
1175.1554	1190.7740	1193.3929
1226.1803	1242.6731	1299.6581
1311.9549	1353.4538	1364.3975
1379.2176	1458.9360	1467.8702
1479.3886	1482.1579	1495.3704
1499.8591	1502.0517	1505.4518
1510.2123	1513.4275	1515.5289
1519.0430	1520.6458	1534.6351
1586.9516	1705.6365	1711.8976
1718.7443	1758.8074	2341.4825
2871.3828	2930.4205	2985.1871
3007.7479	3018.2824	3022.3610
3023.8678	3050.3409	3075.0252
3079.5822	3087.7008	3092.4700
3093.2733	3093.8755	3113.8954
3130.4163	3169.8205	3172.8951
3313.6747	3543.5278	3574.9946

TS53

Cartesian coordinates

C	-3.467018	0.408363	0.236696
O	-2.089297	0.691370	0.299492
H	-3.669874	-0.561880	-0.236242
H	-3.952831	1.187609	-0.355460
H	-3.925816	0.404080	1.233325
H	-1.640447	-0.032445	0.820571
N	-0.764204	-1.405056	1.279365
C	-0.771756	-2.281647	0.207306
H	-0.318705	-1.834416	2.086238
H	-1.587907	-2.079040	-0.498997
H	-0.680596	-3.352869	0.422721
C	2.299276	-1.384707	-0.432192
O	1.203711	-1.463390	-1.290875
H	3.087637	-2.095560	-0.711441
H	2.011311	-1.597299	0.614356

H	2.745204	-0.375881	-0.435217
H	0.230972	-1.979703	-0.570822
C	0.349882	1.626239	-2.568318
N	0.184751	0.855268	-1.332622
H	1.410516	1.704069	-2.807508
H	-0.068660	2.628320	-2.462272
H	-0.152574	1.113350	-3.388468
H	-0.800459	0.772652	-1.035262
H	0.638875	1.288607	-0.504338
H	0.628224	-0.187377	-1.391037
C	2.105577	1.445872	2.157154
N	0.872992	1.334817	1.381885
H	2.527271	2.447228	2.041718
H	2.837113	0.733995	1.768517
H	1.980321	1.250724	3.230296
H	0.161806	1.963992	1.738225
H	0.472774	0.398073	1.467896

Vibrational frequencies

-723.2682	26.2539	54.7545
66.0188	68.3739	77.4791
88.0990	96.0799	99.0207
118.1634	122.6290	128.9947
136.3884	157.1782	160.1907
164.4525	177.1272	195.5330
248.4268	258.2118	264.2768
325.6255	404.0912	413.7208
494.9043	651.7145	704.4849
732.3492	977.0594	1009.5943
1015.9700	1051.2270	1058.4264
1069.3815	1087.8157	1098.3866
1102.1030	1107.3422	1119.5939
1164.9950	1185.7351	1190.2102
1194.0005	1210.0337	1249.7626
1275.2965	1338.3614	1350.2021
1363.6359	1375.8905	1460.5519
1465.4156	1484.2572	1487.0712
1489.6678	1494.6224	1499.3079
1504.3027	1507.9572	1510.3760
1512.8931	1517.2788	1524.9993
1540.9734	1565.2175	1686.0206
1696.6149	1719.1924	1753.6450
1853.9547	2929.3324	2975.8044
2987.4028	2995.2562	3008.5115
3032.7208	3052.0129	3065.0232
3070.7232	3087.5684	3096.8956
3116.1177	3124.5376	3147.6257

3156.0904	3185.4994	3307.1365
3440.5285	3530.3483	3585.4787

P53

Cartesian coordinates

C	-0.963602	-2.808993	-0.482192
O	-0.454851	-1.591539	0.010409
H	-0.459576	-3.123406	-1.405009
H	-2.023035	-2.664075	-0.704354
H	-0.876850	-3.619544	0.252632
H	0.506342	-1.694312	0.176663
N	2.301584	-1.634053	0.225129
C	2.898753	-0.747500	-0.721935
H	2.973818	-1.836475	0.966279
H	2.332493	-0.757818	-1.656510
H	3.958506	-0.952561	-0.916592
C	1.393796	1.270574	1.811776
O	1.860536	1.871965	0.631098
H	1.991194	1.634538	2.651577
H	1.481474	0.170114	1.780580
H	0.339290	1.507202	2.003489
H	2.823998	0.283465	-0.315114
C	-0.649094	1.891118	-2.228694
N	-0.347679	1.294176	-0.932548
H	-0.660161	2.979735	-2.137730
H	-1.612664	1.578008	-2.654202
H	0.134785	1.633645	-2.945751
H	-0.346438	0.277403	-0.983711
H	-1.072686	1.501693	-0.245629
H	1.137107	1.762014	-0.030641
C	-3.420685	0.068110	0.461921
N	-2.263078	0.456075	1.260981
H	-3.107082	-0.042158	-0.580074
H	-4.177346	0.856601	0.492890
H	-3.898979	-0.873796	0.768481
H	-1.560389	-0.277384	1.196055
H	-2.520080	0.560466	2.234433

Vibrational frequencies

24.7770	36.0668	36.8188
49.4300	56.2697	65.2168
68.6543	91.9840	100.2963
104.1301	110.5004	120.8996
131.8408	140.2370	146.5755
154.9243	161.6140	166.4232
179.4120	187.9830	189.6457
235.9356	283.0807	307.3328

421.1984	454.3005	536.4950
872.3841	932.0968	945.8011
1006.0426	1016.6310	1040.3666
1050.4666	1054.1163	1093.2490
1099.5412	1110.5990	1112.3649
1118.0767	1150.6754	1162.7108
1186.4466	1192.9409	1194.8975
1230.2815	1337.6614	1365.1294
1380.8482	1417.0342	1462.9966
1466.6250	1478.9614	1482.9972
1487.4165	1491.9088	1498.6683
1499.7792	1502.2693	1505.0995
1507.4461	1513.3813	1523.2249
1525.2577	1530.1629	1569.5188
1672.4740	1714.6862	2866.7839
2944.7629	2986.9965	2999.1771
3000.5502	3033.9594	3036.6273
3056.0348	3072.8966	3081.7630
3100.7195	3109.9264	3110.5138
3114.7673	3118.6554	3348.8524
3456.1365	3479.5752	3496.9826
3502.5704	3542.1740	3611.6629

R54

Cartesian coordinates

C	-3.772767	-0.582963	-0.503992
O	-3.431135	-0.262150	0.821310
H	-3.058336	-0.167043	-1.230308
H	-4.755041	-0.152608	-0.710086
H	-3.833586	-1.667470	-0.670832
H	-2.543111	-0.618922	0.971051
N	-0.642992	-1.131486	0.635759
C	-0.546322	-2.256238	-0.173134
H	-0.112342	-1.170287	1.493861
H	-1.038300	-2.188226	-1.136865
H	-0.501939	-3.223496	0.313458
C	2.305757	1.752373	0.921134
N	2.320236	1.726742	-0.537685
H	1.474172	1.134005	1.273508
H	2.126597	2.769576	1.279950
H	3.224118	1.379755	1.397644
H	3.059242	2.319412	-0.894815
H	0.327676	1.706037	-0.925820
H	2.502135	0.767716	-0.845709
C	-1.367497	2.338151	0.074677
N	-0.639715	1.400111	-0.780957

H	-1.517619	3.329965	-0.371531
H	-0.806929	2.474303	1.003474
H	-2.337471	1.912280	0.342113
H	-1.085358	1.332546	-1.688045
H	-0.562803	-0.224733	0.138014
C	3.026349	-1.795058	0.440829
N	2.526535	-1.321943	-0.847907
H	2.923855	-2.877181	0.599939
H	2.484098	-1.286038	1.241773
H	4.081724	-1.532452	0.548595
H	3.028096	-1.775748	-1.602372
H	1.548633	-1.595756	-0.939032

Vibrational frequencies

22.3298	36.3785	44.3060
64.9083	72.3697	82.3626
87.0898	90.6888	101.2688
107.6640	111.1844	125.5419
133.4067	135.7995	141.8969
155.2707	163.5926	191.8302
204.5763	209.2979	213.5486
216.8745	266.1682	310.4332
403.9180	478.6984	545.9156
600.6889	686.3031	711.5247
930.5459	938.7157	958.9716
966.8726	1003.6124	1024.5505
1048.1728	1085.3585	1089.5250
1094.3102	1097.3976	1109.9798
1138.5391	1196.8084	1199.7441
1204.8315	1209.9265	1258.0581
1367.5330	1371.0540	1373.7071
1393.7828	1456.0622	1465.1502
1467.4819	1473.4510	1491.0017
1496.5088	1499.4281	1503.5091
1507.8521	1516.8948	1520.3628
1525.2206	1528.3795	1532.0165
1677.6370	1695.2460	1703.2533
1709.3992	2983.1025	2994.7199
3005.8312	3006.5742	3031.0917
3071.7501	3086.3402	3091.9464
3111.1936	3114.4434	3121.8832
3130.0796	3134.3998	3155.9082
3256.4752	3380.2921	3415.8135
3467.5400	3591.0763	3591.7539
3596.4179	3633.1387	3699.7309

TS54

Cartesian coordinates

C	-3.523855	-1.243940	-0.442025
O	-3.161687	-0.550442	0.719484
H	-3.043342	-0.834908	-1.348135
H	-4.606100	-1.157698	-0.576600
H	-3.267691	-2.310929	-0.391898
H	-2.204719	-0.741998	0.875973
N	-0.424184	-1.012686	0.847188
C	-0.029844	-1.983634	-0.050941
H	-0.152784	-1.281089	1.788778
H	-0.499319	-1.930405	-1.038188
H	0.183516	-3.002115	0.287001
C	1.702866	1.686451	1.092387
N	1.655582	1.684451	-0.382626
H	1.138575	0.808924	1.420121
H	1.229208	2.588312	1.482254
H	2.730867	1.628427	1.453742
H	2.109772	2.498290	-0.783006
H	0.520009	1.596727	-0.683898
H	2.130723	0.800651	-0.720845
C	-1.832088	2.223014	-0.194312
N	-0.871840	1.252007	-0.734404
H	-1.996652	3.036967	-0.904605
H	-1.420875	2.651504	0.723474
H	-2.779223	1.739476	0.056251
H	-1.203008	0.888700	-1.621633
H	-0.802991	0.426459	-0.079925
C	3.598770	-1.299986	0.180468
N	2.698483	-0.863535	-0.888709
H	3.815806	-2.374746	0.160034
H	3.129324	-1.079361	1.141891
H	4.547093	-0.757313	0.131135
H	3.053454	-1.168319	-1.788545
H	1.780474	-1.335105	-0.742859

Vibrational frequencies

-358.8504	25.0804	45.7851
55.6752	68.4001	91.0767
101.7003	107.5581	117.7434
120.7771	127.1290	141.1901
154.6009	162.0766	175.1012
181.7871	201.3708	201.9220
226.4189	237.1420	255.0078
301.5586	325.2825	379.6184
558.9336	636.4144	645.2450
709.4614	791.5978	885.1437
946.6566	994.6134	1014.3632

1024.8122	1045.4400	1063.5036
1071.1278	1086.9272	1093.9101
1117.2254	1124.0219	1154.9162
1156.7288	1188.5377	1244.2434
1277.4624	1314.1767	1341.0788
1344.0987	1390.4080	1401.2210
1423.4018	1462.2505	1468.5504
1481.1389	1487.2300	1488.7679
1496.8671	1501.7680	1503.2623
1508.5296	1514.5851	1526.6972
1534.2702	1535.9159	1553.6184
1673.5844	1684.5261	1730.3365
1765.2756	1791.6985	2817.4456
2867.1602	2946.6730	3021.5023
3021.6557	3025.8411	3045.5722
3046.9567	3075.7489	3089.5637
3096.0344	3106.0009	3120.4665
3127.0584	3134.5039	3136.1027
3153.7400	3311.3692	3528.7676
3568.9601	3572.8197	3575.1101

I54

Cartesian coordinates

C	-3.437916	-1.313688	-0.213588
O	-2.915704	-0.683507	0.923605
H	-3.195194	-0.771916	-1.144747
H	-4.528000	-1.347181	-0.125704
H	-3.069414	-2.341483	-0.330562
H	-1.940645	-0.839134	0.909041
N	-0.177183	-1.096156	0.615358
C	0.062475	-1.920571	-0.466582
H	0.101731	-1.575473	1.468069
H	-0.439401	-1.641108	-1.398348
H	0.186695	-2.999607	-0.333824
C	1.513225	1.706876	1.158469
N	1.602104	1.696612	-0.317733
H	0.949516	0.809639	1.428411
H	0.985792	2.599561	1.495387
H	2.511171	1.678243	1.596606
H	2.074033	2.518429	-0.681091
H	0.585617	1.636301	-0.702413
H	2.126507	0.806912	-0.624985
C	-2.006245	2.161875	-0.254991
N	-1.003296	1.270565	-0.847273
H	-2.215845	2.997668	-0.927394
H	-1.609523	2.572543	0.677521

H	-2.932666	1.636568	-0.008406
H	-1.332946	0.920622	-1.739724
H	-0.877935	0.440618	-0.238239
C	3.433477	-1.219660	0.372787
N	2.795098	-0.719826	-0.847839
H	3.746913	-2.267413	0.302515
H	2.707431	-1.144381	1.184815
H	4.308323	-0.614516	0.628045
H	3.376339	-0.910033	-1.656703
H	1.899979	-1.244151	-0.961263

Vibrational frequencies

26.6581	46.6288	51.8373
77.0051	79.3524	92.3925
103.3682	109.9974	114.8219
131.8825	135.5346	139.0914
151.8120	160.7811	175.9472
180.6856	191.7878	221.3913
246.4825	252.7581	262.4565
297.0215	314.3989	354.9257
551.3556	596.1123	652.8490
694.0355	772.9650	933.5893
993.8041	1005.3361	1011.8826
1048.1396	1055.9285	1066.5231
1079.6585	1086.5232	1102.8897
1105.9062	1120.8777	1152.0526
1185.9658	1249.4389	1258.2991
1271.2161	1325.5430	1347.1720
1379.3674	1383.5960	1408.0913
1451.3511	1457.5328	1463.5248
1481.7870	1492.1359	1496.2670
1497.3381	1499.1073	1501.5724
1509.7018	1524.1068	1529.2149
1537.1716	1545.8660	1655.8944
1663.8562	1700.0476	1726.3024
1757.4549	2347.1700	2551.2503
2941.3793	3015.6004	3019.5394
3023.9360	3036.8809	3043.2944
3058.2092	3086.7085	3090.1611
3097.6192	3110.3946	3119.5294
3131.4161	3140.5588	3158.6273
3181.9205	3323.1870	3515.1442
3570.4804	3572.8830	3582.2124

TS55

Cartesian coordinates

C	-3.449691	-1.226183	-0.158764
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O	-2.870558	-0.634803	0.971103
H	-3.199941	-0.689430	-1.090548
H	-4.537562	-1.203284	-0.044964
H	-3.140734	-2.271948	-0.292208
H	-1.903738	-0.822245	0.921294
N	-0.172605	-1.191923	0.582117
C	0.054419	-1.953919	-0.544167
H	0.110275	-1.719259	1.405245
H	-0.476638	-1.632285	-1.446236
H	0.173164	-3.040272	-0.468509
C	1.539895	1.678549	1.187983
N	1.729171	1.659116	-0.274164
H	0.923038	0.809888	1.433985
H	1.036319	2.590065	1.517529
H	2.504528	1.599637	1.693437
H	2.260419	2.462157	-0.593502
H	2.242721	0.537581	-0.603475
H	0.773438	1.674096	-0.711666
C	-1.959022	2.198944	-0.287773
N	-0.979368	1.290957	-0.890619
H	-2.171979	3.026955	-0.969123
H	-1.535337	2.622374	0.627172
H	-2.891077	1.697080	-0.011506
H	-1.336638	0.934571	-1.769512
H	-0.855548	0.470747	-0.280982
C	3.326914	-1.242026	0.356114
N	2.640460	-0.690521	-0.818495
H	3.626785	-2.281445	0.202593
H	2.624597	-1.207337	1.189599
H	4.210273	-0.648943	0.603959
H	3.200784	-0.799803	-1.657667
H	1.728624	-1.236069	-0.935978

Vibrational frequencies

-903.2372	29.7747	53.4326
65.3458	86.2309	89.0062
97.3595	106.4399	123.6116
128.6984	137.3316	140.7340
145.1317	159.3034	165.4202
179.2420	182.7927	209.1486
235.1341	251.9288	268.8142
299.2127	333.8075	347.5134
537.8062	562.9736	619.4088
680.8188	744.9778	832.7759
918.7703	1001.0052	1003.8444
1031.5596	1051.9124	1059.0816
1072.4818	1076.5153	1093.0985

1096.2520	1121.6163	1130.8607
1152.1404	1188.2409	1236.0747
1272.7565	1316.4725	1329.5783
1348.9144	1377.3624	1378.8400
1421.5182	1458.1316	1466.5938
1474.0095	1481.8099	1490.7545
1495.5554	1501.2570	1503.2770
1507.8198	1514.9641	1522.2346
1530.7136	1534.9545	1546.1499
1631.4706	1681.9319	1716.2885
1752.3615	1766.2577	2630.2010
2950.8756	2956.4364	3010.8675
3024.5163	3040.9978	3041.6098
3053.8931	3090.5211	3092.9426
3109.7353	3118.6528	3125.3496
3129.5683	3135.8090	3154.1758
3307.6283	3362.5914	3505.9136
3564.7420	3572.1649	3583.1799

P55

Cartesian coordinates

C	-2.870871	-2.214031	0.624116
O	-1.938213	-1.183402	0.843304
H	-2.913089	-2.525199	-0.429247
H	-3.857526	-1.842304	0.908585
H	-2.655506	-3.101102	1.234460
H	-1.064784	-1.502513	0.541851
N	0.428846	-1.985932	-0.418874
C	0.698867	-1.229468	-1.600433
H	1.099236	-2.754853	-0.364434
H	-0.060801	-0.458005	-1.739622
H	0.765813	-1.867924	-2.494218
C	0.499904	1.155575	1.485627
N	0.841023	1.883349	0.263511
H	0.531343	0.083001	1.282525
H	-0.498039	1.377159	1.888608
H	1.239984	1.365870	2.262623
H	0.841696	2.880806	0.441918
H	2.608318	1.004850	-0.357490
H	0.111697	1.707334	-0.429857
C	-2.553592	2.388533	-0.402985
N	-1.905992	1.209607	-0.969864
H	-2.453008	3.234017	-1.089054
H	-2.045742	2.662700	0.525745
H	-3.620904	2.260700	-0.174700
H	-2.339890	0.961544	-1.850736

H	-2.020198	0.411443	-0.343137
C	3.591412	-0.470569	0.657690
N	3.326991	0.300239	-0.549370
H	4.382566	-1.202897	0.471714
H	2.688661	-1.027214	0.930464
H	3.883037	0.125320	1.535634
H	4.164100	0.777448	-0.859477
H	1.688341	-0.734063	-1.500504

Vibrational frequencies

17.2858	32.4450	44.0000
56.3378	59.9989	66.7278
72.2976	84.0972	95.4007
97.0146	102.9647	111.2329
119.6913	128.6641	139.8418
147.3680	160.7793	177.2959
181.5005	188.6589	195.0528
225.2247	255.2877	275.5778
408.6341	455.6980	473.6018
530.7677	837.5594	947.8679
953.4790	967.6103	995.8755
1016.9553	1035.0790	1041.2112
1048.6251	1086.9473	1094.3492
1098.2166	1112.0196	1113.6552
1145.1958	1185.3188	1195.6035
1200.9262	1206.3715	1344.9804
1377.4398	1383.9365	1389.4681
1422.3680	1461.4207	1464.8735
1469.6283	1480.0069	1488.9241
1491.4487	1499.0879	1500.8953
1502.8175	1508.6246	1514.1065
1520.7570	1524.6353	1528.1003
1528.8692	1696.2072	1704.9878
1705.9148	2851.2511	2982.6324
2989.1502	2998.5623	3002.8709
3003.3694	3041.5155	3059.7815
3077.0709	3083.6038	3099.7049
3112.5792	3113.0502	3125.1839
3126.9061	3389.8114	3437.7665
3452.2021	3485.0785	3535.9575
3587.4526	3595.5456	3597.6855

R56

Cartesian coordinates

C	-1.818950	0.387173	0.322450
O	-1.279162	-0.469735	-0.589680
H	-2.013641	-0.069037	1.303211

H	-2.792085	0.701241	-0.098157
H	-1.229949	1.312145	0.425512
N	1.339949	-0.710089	0.339370
C	1.756459	0.575039	-0.200683
H	0.614409	-1.129386	-0.232085
H	0.968616	-0.609841	1.275673
H	2.143916	0.431151	-1.211558
H	2.571643	0.979090	0.405312
H	0.965694	1.339867	-0.256655

Vibrational frequencies

46.7934	84.6236	110.1125
119.0077	142.5006	163.1233
367.8579	826.4208	878.7137
987.2242	1045.4851	1096.7466
1153.3683	1169.1011	1349.4186
1376.0595	1407.5305	1468.4571
1500.6951	1518.2452	1520.3125
1668.4273	2936.6375	2973.2655
2994.9734	3036.4328	3077.4105
3122.1921	3529.2615	3621.7306

TS56

Cartesian coordinates

C	1.730142	-0.412661	0.261986
O	1.063823	0.478154	-0.567142
H	1.928250	-0.009500	1.266677
H	2.698690	-0.632337	-0.204604
H	1.204270	-1.376655	0.362873
N	-1.079762	0.667073	0.365258
C	-1.738421	-0.491328	-0.198190
H	-0.042222	0.826617	-0.141214
H	-0.909251	0.509818	1.357622
H	-1.862203	-0.353376	-1.272289
H	-2.728671	-0.604720	0.257144
H	-1.191441	-1.430650	-0.028649

Vibrational frequencies

-1631.2320	48.7769	159.4171
184.1872	213.4046	260.0733
569.5651	732.2921	1007.4165
1077.6143	1088.9993	1110.8840
1162.0604	1182.1798	1319.6779
1420.2781	1453.2194	1463.8270
1475.5237	1490.2875	1505.5515
1515.8559	1593.0612	2951.1040
2992.0755	3009.0556	3058.6198
3065.8539	3143.6374	3518.1982

P56**Cartesian coordinates**

C	1.909186	0.229858	-0.444222
O	1.268713	-0.230357	0.718864
H	2.275730	-0.589989	-1.078208
H	2.770112	0.828058	-0.138238
H	1.257697	0.868619	-1.060010
N	-1.358631	-0.725183	-0.244381
C	-1.816984	0.589732	0.100232
H	0.476200	-0.706621	0.434001
H	-2.123812	-1.225790	-0.701810
H	-1.016128	1.136485	0.599618
H	-2.694679	0.545494	0.762685
H	-2.137626	1.145347	-0.794349

Vibrational frequencies

49.5529	94.3910	108.5641
117.1442	138.8991	229.1090
332.0633	745.0541	967.8665
1020.5205	1093.4690	1111.9327
1134.1807	1186.6032	1336.7641
1398.9214	1458.9908	1487.7094
1494.6372	1497.4458	1500.3481
1520.6127	2975.0333	2976.5090
3022.1389	3026.2781	3110.8452
3132.1404	3475.5742	3733.9543

R57**Cartesian coordinates**

C	-1.825583	-1.624074	0.022156
O	-0.834968	-0.890760	-0.593829
H	-1.874232	-2.587641	-0.512001
H	-2.812260	-1.151966	-0.065986
H	-1.608330	-1.844400	1.076058
N	-0.807297	1.106906	0.670461
C	-0.742678	2.070003	-0.412734
H	-1.422601	1.393645	1.419614
H	-0.123862	1.656522	-1.210344
H	-0.331402	3.046155	-0.120109
H	-1.741784	2.227209	-0.825201
H	0.108643	0.864253	1.033708
C	2.559261	-0.211322	-0.333272
O	1.610404	-0.555810	0.648756
H	3.460046	0.134656	0.177579
H	2.209076	0.596416	-0.991476
H	2.833922	-1.068246	-0.962196

H 0.804368 -0.850032 0.190812

Vibrational frequencies

36.5627	67.7202	80.7819
103.5305	110.9865	121.0876
139.7372	163.8192	186.4172
190.6278	212.5500	248.5134
450.9015	760.4490	885.3416
1002.7482	1035.8263	1104.1961
1110.9174	1146.4654	1147.1732
1163.0307	1164.6624	1190.1781
1351.2145	1422.7452	1432.8619
1461.7857	1479.3317	1495.7480
1497.6735	1505.4213	1514.2896
1517.5334	1527.5790	1675.1529
2963.2041	2991.7996	3001.1145
3026.0476	3043.9470	3055.1081
3094.2945	3115.5707	3138.1193
3520.9653	3632.3077	3644.5024

TS57

Cartesian coordinates

C	1.547382	-1.745985	-0.059326
O	0.788234	-0.783838	0.611245
H	1.436466	-2.726606	0.424769
H	2.612072	-1.485015	-0.029726
H	1.240509	-1.863539	-1.109267
N	0.588750	1.116334	-0.671397
C	0.827051	2.094103	0.349075
H	1.355112	0.916358	-1.299117
H	0.038338	2.022626	1.097644
H	0.814200	3.105809	-0.077990
H	1.791008	1.933689	0.836898
H	-0.395274	0.550378	-0.744648
C	-2.443488	-0.195975	0.234902
O	-1.283685	-0.469896	-0.493968
H	-3.127921	0.437617	-0.345179
H	-2.241031	0.322732	1.187551
H	-2.983912	-1.120677	0.478947
H	-0.282880	-0.790688	0.193773

Vibrational frequencies

-1450.4047	73.1097	89.8486
109.2911	120.0242	130.2968
135.0018	148.1550	193.5675
210.8879	322.0204	451.9965
497.1671	579.5939	1014.7824
1084.1602	1087.2226	1116.1155

1129.9840	1168.2082	1172.7600
1190.8253	1195.7381	1263.8951
1294.0264	1443.4846	1468.3038
1481.9796	1486.6934	1491.7833
1501.0464	1504.0906	1507.4725
1512.2885	1616.2782	1641.5976
1721.1136	1880.9409	2956.7390
2977.9834	3017.7276	3018.9321
3032.7546	3042.3356	3058.8999
3100.6719	3156.1902	3630.5678

P57

Cartesian coordinates

C	-2.146898	-0.986501	0.393080
O	-1.343657	-0.966350	-0.761993
H	-2.032560	-1.917341	0.962466
H	-3.189874	-0.901914	0.080980
H	-1.922534	-0.147546	1.071231
N	0.191113	1.718869	0.743280
C	-0.211343	2.026448	-0.596031
H	-0.383912	2.241479	1.405252
H	0.659487	1.985616	-1.258648
H	-0.733885	2.979998	-0.721065
H	-0.870032	1.203636	-0.933201
H	0.954822	0.029270	0.771928
C	2.374067	-0.871192	-0.219962
O	1.141897	-0.879304	0.467973
H	3.203556	-0.586719	0.438336
H	2.364643	-0.191403	-1.082400
H	2.559181	-1.882571	-0.584864
H	-0.427565	-1.091885	-0.463336

Vibrational frequencies

48.2209	62.9014	84.5097
94.8647	107.3002	113.0132
119.2727	132.8116	159.3862
206.2776	236.8745	241.3307
292.9092	724.2699	901.2688
1016.4732	1045.6274	1103.4579
1106.7071	1108.9071	1135.5701
1152.4548	1186.3636	1188.0125
1321.0669	1414.2940	1463.2933
1471.3164	1482.1116	1492.5196
1494.7901	1497.1134	1502.5706
1513.5047	1524.7348	1528.0989
2922.9522	2971.0650	3001.2364
3040.3449	3048.2120	3060.5941

3101.3163	3114.2728	3126.6572
3497.0727	3557.9944	3664.2106

R58

Cartesian coordinates

C	-0.107714	1.993805	0.583980
O	0.017995	1.612582	-0.760496
H	0.297026	1.235197	1.274518
H	-1.151978	2.183101	0.871274
H	0.453771	2.918924	0.733562
N	1.537672	-1.247812	0.701312
C	2.316599	-0.644590	-0.340626
H	1.865502	-0.876162	1.596031
H	2.295387	-1.271563	-1.236543
H	3.355149	-0.421749	-0.067357
H	1.825119	0.308106	-0.616713
H	-0.418452	-1.352973	-0.085194
C	-2.382256	-0.889316	0.303916
N	-1.205752	-0.912707	-0.563025
H	-2.741072	-1.882608	0.603593
H	-3.200211	-0.366528	-0.197367
H	-2.144034	-0.329620	1.211298
H	-0.470932	0.767908	-0.852815
H	-1.392446	-1.448459	-1.401953

Vibrational frequencies

45.2713	79.5569	82.8845
95.9571	104.8635	121.0639
148.7523	151.9664	167.0415
188.0055	206.3659	254.5889
309.8244	481.9749	879.8917
970.5055	996.8245	1035.0121
1053.5972	1090.9988	1096.1733
1115.8453	1147.8299	1187.0949
1199.9109	1331.0812	1374.0453
1414.9149	1466.4787	1475.2238
1485.3138	1495.8716	1503.2173
1508.5138	1509.1715	1524.6236
1551.5298	1692.6085	2920.8399
2961.2634	3010.5182	3015.3555
3037.9157	3089.7928	3098.3320
3105.4657	3124.8691	3447.4354
3469.5193	3487.6754	3600.6001

TS58

Cartesian coordinates

C	0.513423	-2.085494	-0.234383
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O	0.485739	-1.044586	0.664531
H	-0.252387	-2.012466	-1.036719
H	0.338483	-3.056319	0.263377
H	1.491577	-2.180232	-0.743649
N	0.896957	0.885343	-0.620464
C	2.082540	1.270650	0.098220
H	1.116156	0.262120	-1.389896
H	1.802669	1.818702	1.001806
H	2.719263	1.929840	-0.510024
H	2.671958	0.400190	0.403351
H	-0.371982	0.999442	-0.097207
C	-2.509283	0.389007	-0.335369
N	-1.347090	0.659916	0.509015
H	-2.944303	1.317476	-0.711069
H	-3.277157	-0.172324	0.202174
H	-2.182166	-0.208085	-1.187797
H	-0.796094	-0.238217	0.786873
H	-1.571069	1.234775	1.311865

Vibrational frequencies

-1203.0250	73.6835	93.4149
121.5903	136.6994	141.7593
155.0246	179.4212	184.7293
208.6342	304.2039	427.2993
514.3437	542.5870	693.8689
1008.0494	1047.0150	1071.1471
1084.5324	1095.7766	1128.2186
1136.5860	1166.0331	1199.9835
1266.4681	1339.7991	1367.7485
1426.3928	1474.6710	1480.5344
1488.2845	1490.2798	1498.9518
1503.0165	1514.8068	1518.7346
1646.3323	1721.0841	1782.7806
2465.8618	2856.8538	2915.6636
2950.2343	2991.4621	3055.2913
3064.9933	3106.7018	3127.6007
3145.7320	3576.0926	3594.6691

P58

Cartesian coordinates

C	0.588271	2.123812	0.249314
O	0.548020	1.144167	-0.710789
H	-0.215382	2.038119	0.994643
H	0.438368	3.079455	-0.283112
H	1.561010	2.183703	0.755106
N	1.017842	-0.850760	0.608033
C	2.180721	-1.303167	-0.134931

H	1.094667	-1.053918	1.596297
H	2.054881	-1.027237	-1.182731
H	2.361273	-2.386642	-0.078427
H	3.075371	-0.791009	0.229481
H	0.149581	-1.241558	0.246342
C	-2.505726	-0.253366	0.469377
N	-1.721228	-0.826564	-0.618541
H	-3.127266	-1.026321	0.929179
H	-3.160572	0.580585	0.177744
H	-1.820678	0.115526	1.237849
H	-1.126849	-0.103423	-1.016442
H	-2.324466	-1.183016	-1.348624

Vibrational frequencies

31.1929	57.5586	72.7696
89.1082	106.6557	123.0951
151.4406	157.2870	177.2686
183.7564	193.2296	206.4504
404.9587	518.3160	874.6257
927.9158	1013.2629	1024.0445
1028.9888	1094.8711	1104.0765
1146.7947	1152.5670	1167.9226
1191.3511	1358.6683	1376.9233
1414.4150	1422.3151	1462.1853
1463.4510	1500.5726	1504.5521
1515.9868	1518.8433	1528.1883
1672.0294	1694.0483	2952.0902
2989.8098	2990.9105	3013.8371
3044.3542	3074.6393	3082.3214
3113.1269	3134.2010	3468.4526
3509.4625	3613.1498	3617.1627

R59

Cartesian coordinates

C	0.850210	0.719107	2.001899
O	1.440436	0.960990	0.773132
H	-0.146876	0.261948	1.912739
H	0.725009	1.690337	2.505458
H	1.473483	0.093314	2.655759
N	1.543854	-1.112267	-0.068416
C	2.027945	-0.886405	-1.414339
H	2.199786	-1.579322	0.539448
H	1.269430	-0.330871	-1.967531
H	2.246168	-1.815678	-1.956189
H	2.933073	-0.277602	-1.375734
H	-1.231921	-0.560027	-0.620977
C	-1.310252	2.271250	-0.814028

O	-0.612145	1.051542	-0.913320
H	-2.185931	2.214625	-1.463226
H	-0.693725	3.115716	-1.143680
H	-1.652796	2.470280	0.210262
H	0.192900	1.092150	-0.343772
C	-2.339148	-1.534406	0.652921
O	-1.336515	-1.487243	-0.333393
H	-2.083748	-0.942426	1.543713
H	-2.460080	-2.574427	0.962091
H	-3.305588	-1.179613	0.272527
H	0.607107	-1.512112	-0.022044

Vibrational frequencies

20.4957	28.1640	65.1341
78.2991	93.2676	93.5890
100.6632	117.5734	134.8683
142.6802	145.3395	165.5391
181.8690	207.8220	211.0195
242.0482	292.6877	325.4090
498.8494	768.6592	851.4173
987.4926	1011.1769	1061.9554
1104.7284	1110.0507	1121.7174
1143.8507	1149.7738	1161.9323
1166.4834	1177.1550	1188.4549
1190.8600	1348.1369	1437.1521
1454.1237	1463.2760	1484.1940
1489.5234	1494.3034	1499.1879
1500.1186	1501.3292	1505.5580
1513.1051	1516.6650	1531.8375
1542.4352	1682.9794	2961.7341
2988.8159	3000.3934	3014.4733
3024.1791	3032.1770	3043.9080
3061.4038	3103.8539	3116.2331
3120.1090	3147.2906	3321.1302
3459.3754	3571.2309	3659.3583

TS59

Cartesian coordinates

C	0.535357	0.887333	2.073051
O	1.038457	1.158846	0.788975
H	0.054597	-0.098077	2.128954
H	-0.209442	1.638057	2.364441
H	1.354924	0.921602	2.795438
N	1.705014	-0.784623	-0.218266
C	2.093840	-0.190324	-1.464584
H	2.404274	-0.894861	0.500870
H	1.203990	0.261763	-1.907679

H	2.475519	-0.966382	-2.140963
H	2.863164	0.566129	-1.310521
H	-0.916937	-0.419317	-0.608617
C	-2.024336	1.532610	-0.925774
O	-0.837158	0.817631	-0.781656
H	-2.728382	1.005523	-1.585868
H	-1.839525	2.519492	-1.371620
H	-2.541107	1.698763	0.034634
H	0.229669	1.147695	0.132526
C	-1.532715	-1.927276	0.710056
O	-0.717328	-1.517280	-0.351274
H	-1.995142	-1.069353	1.221639
H	-0.957284	-2.488310	1.460188
H	-2.341623	-2.582133	0.361474
H	0.703565	-1.235874	-0.151885

Vibrational frequencies

-662.5468	59.4550	65.0097
85.6953	92.3614	96.4579
121.3042	125.5057	141.7123
157.4760	165.6072	187.8167
200.7122	215.9754	221.0264
340.0592	386.2475	436.8336
484.4737	715.6227	1032.7293
1053.3940	1072.7154	1101.6842
1117.9759	1131.0404	1141.2024
1170.8465	1175.3435	1183.7043
1188.5084	1196.7254	1199.4586
1298.7575	1303.1242	1432.4457
1438.4972	1472.7872	1481.1435
1488.6807	1495.8299	1496.7989
1501.7839	1505.7585	1509.2780
1512.2501	1513.8802	1517.2941
1599.8555	1654.6785	1783.3379
2207.2665	2377.7405	2954.7735
2978.5049	3007.8759	3009.8338
3019.7959	3029.2554	3034.4234
3045.0260	3066.0525	3109.4292
3111.1935	3159.9513	3656.9733

P59

Cartesian coordinates

C	-1.860417	2.050531	0.729844
O	-0.630674	1.704776	0.138871
H	-2.211838	1.286927	1.438393
H	-2.646056	2.214862	-0.018894
H	-1.718969	2.981966	1.280849

N	2.069066	0.618775	0.149943
C	2.374785	0.836572	-1.231801
H	1.396673	1.338908	0.435159
H	3.214193	0.215568	-1.551508
H	2.576298	1.889776	-1.466523
H	1.489520	0.546684	-1.823182
H	-0.125458	-1.227424	-0.487502
C	-1.753339	-1.495940	-1.562878
O	-0.654386	-0.719140	-1.137247
H	-1.425949	-2.418410	-2.055287
H	-2.320749	-0.905695	-2.284156
H	-2.418667	-1.759782	-0.731227
H	-0.751304	0.888555	-0.378869
C	0.070734	-1.263643	2.015681
O	0.830874	-1.691444	0.898662
H	-0.299362	-0.240808	1.876805
H	0.656779	-1.308309	2.939923
H	-0.781489	-1.938305	2.116383
H	1.525815	-1.014588	0.752661

Vibrational frequencies

32.1114	53.5992	63.7527
76.5922	82.7442	98.0069
103.0781	104.5657	122.3500
129.9268	136.3060	146.7209
151.2627	160.6912	206.7728
226.8135	263.8709	277.9266
503.8377	749.3275	863.5964
932.2896	989.2792	1060.5218
1089.1752	1106.1598	1107.3030
1118.9688	1147.4245	1156.8495
1168.0483	1187.5086	1187.8330
1193.8750	1379.4229	1408.9869
1471.4681	1482.8722	1485.1465
1488.2709	1491.1869	1496.2084
1499.8244	1501.2892	1502.4459
1504.8304	1511.3576	1528.5827
1534.0032	1545.6095	2970.0436
2990.0275	3009.4504	3017.9395
3040.0423	3044.8036	3071.7757
3084.4039	3114.4658	3119.8105
3124.2398	3126.4611	3437.9079
3451.7656	3515.8065	3612.4787

R60

Cartesian coordinates

C	0.917800	1.447602	1.603713
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O	1.460903	1.360888	0.339399
H	-0.057447	0.942149	1.690694
H	0.751528	2.516825	1.813517
H	1.586789	1.064744	2.388328
N	1.683346	-0.900880	0.155090
C	2.236723	-1.012193	-1.177867
H	2.334364	-1.157993	0.882666
H	1.467223	-0.735176	-1.901099
H	2.586740	-2.022550	-1.428816
H	3.066747	-0.311674	-1.288889
H	-1.138498	-0.902708	-0.568306
C	-1.981059	1.686754	-0.759197
N	-0.953943	0.756015	-1.226556
H	-2.952188	1.412865	-1.178597
H	-1.780797	2.735902	-1.011586
H	-2.061188	1.613738	0.328104
H	-0.044446	1.018580	-0.833038
H	-0.873585	0.805614	-2.235317
C	-1.981417	-1.591262	1.043109
O	-1.119778	-1.746099	-0.056706
H	-3.011709	-1.370616	0.732651
H	-1.654676	-0.792467	1.726619
H	-1.994085	-2.528229	1.604444
H	0.788124	-1.378677	0.258793

Vibrational frequencies

31.5513	52.0166	58.9381
72.9543	86.9993	96.6866
100.9937	118.9127	122.8469
142.0871	155.4512	167.3156
180.5608	204.6378	207.4461
234.4126	276.4706	286.8204
476.2623	508.5887	816.1861
963.9440	983.7377	1011.6845
1055.5190	1075.2831	1092.2757
1109.2482	1115.9072	1146.6583
1158.1527	1162.7744	1171.0024
1188.1152	1219.0090	1357.0469
1390.4731	1431.8368	1445.6408
1459.2048	1465.5140	1488.6794
1497.4624	1499.1708	1504.3032
1504.9609	1513.7169	1516.1337
1524.9635	1570.0022	1687.8110
1709.9763	2949.6555	2976.2026
3007.4740	3008.0628	3012.9104
3017.9706	3031.4050	3088.4662
3095.0446	3108.3112	3121.5979

3135.7877	3335.2402	3404.7683
3457.7797	3590.5854	3645.8770

TS60

Cartesian coordinates

C	-1.151992	-1.939066	1.061169
O	-1.095408	-1.346659	-0.187753
H	-0.383540	-1.565311	1.765224
H	-1.007243	-3.029908	0.985806
H	-2.131893	-1.791353	1.546134
N	-1.426700	0.834442	0.226543
C	-2.463303	1.049959	-0.743822
H	-1.762839	0.608416	1.152366
H	-2.005607	1.187555	-1.724974
H	-3.044963	1.953663	-0.513116
H	-3.141104	0.194110	-0.792523
H	1.240598	0.293782	-0.699898
C	2.280737	-1.511021	-0.180639
N	1.259674	-0.789505	-0.948163
H	3.284036	-1.169700	-0.441830
H	2.209209	-2.586589	-0.353106
H	2.113271	-1.318703	0.879201
H	0.222001	-1.113400	-0.649633
H	1.387909	-0.916230	-1.946090
C	1.528477	2.159549	0.840238
O	0.869491	1.615250	-0.257957
H	2.290054	1.478567	1.261028
H	0.829841	2.393475	1.662282
H	2.044690	3.096771	0.585834
H	-0.331413	1.265031	0.038639

Vibrational frequencies

-946.8175	17.9611	48.6923
79.4620	82.5571	96.0171
108.1647	125.2230	139.0170
159.0498	169.3246	178.9385
199.5703	207.7047	219.0888
346.2701	418.3825	433.3544
559.5356	641.2580	707.5735
1015.6258	1032.4387	1081.8612
1083.9231	1088.7248	1105.0550
1124.7389	1151.6043	1161.2827
1185.3804	1194.4218	1198.9085
1245.6208	1334.2005	1337.1427
1389.5108	1438.1136	1452.4252
1476.2183	1488.4508	1491.5699
1493.8119	1499.4801	1501.8964

1506.5929	1514.1983	1516.4872
1525.2272	1676.2389	1713.1958
1742.2633	1769.6892	1844.6073
2154.4698	2906.9980	2933.3195
2960.4170	2968.6591	2981.0051
3003.0029	3011.8340	3066.4539
3087.9168	3132.7567	3143.4481
3157.4943	3579.0425	3620.4878

P60

Cartesian coordinates

C	-3.135513	-0.217886	0.195183
O	-2.154477	0.037303	-0.779409
H	-2.720126	-0.249943	1.213594
H	-3.660386	-1.165065	0.013117
H	-3.874395	0.585768	0.156115
N	0.216534	1.638325	-0.092023
C	0.027525	2.971183	0.387810
H	-0.701031	1.237878	-0.340873
H	0.971465	3.425283	0.695422
H	-0.674686	2.993251	1.235224
H	-0.428900	3.598951	-0.393252
H	0.639011	-1.514467	-0.848088
C	-0.038552	-1.826382	1.034829
N	-0.207849	-1.887833	-0.417169
H	0.831537	-2.381664	1.407206
H	-0.932261	-2.210958	1.532648
H	0.081878	-0.779518	1.325169
H	-1.523310	-0.721518	-0.780635
H	-0.316982	-2.846775	-0.724008
C	3.155271	-0.308202	0.208391
O	2.193082	-0.214797	-0.813291
H	2.702608	-0.448286	1.200519
H	3.801373	0.578979	0.249332
H	3.787838	-1.173919	0.000138
H	1.594347	0.526230	-0.592959

Vibrational frequencies

27.0617	37.8514	60.5767
68.3114	81.5133	86.2508
97.9210	102.4300	114.9671
130.1941	137.6511	156.5846
166.7092	192.9741	219.2399
224.7887	248.3517	284.7230
504.5752	579.5973	854.2853
943.0000	977.2259	1019.9929
1030.3905	1068.0521	1088.0053

1111.6026	1113.5626	1128.8603
1153.0908	1159.6404	1188.3589
1191.7145	1220.3293	1380.8988
1388.9586	1428.5778	1464.1119
1482.0307	1488.4885	1490.1350
1493.5081	1497.0551	1499.0453
1501.5823	1511.1504	1512.7919
1528.6355	1538.4712	1569.2430
1681.0700	2974.4099	2980.5495
2990.0132	3013.9484	3021.9746
3036.8321	3040.3634	3088.2191
3107.4970	3109.1055	3112.6806
3121.4887	3319.9787	3374.3109
3463.1558	3532.7981	3602.3030

R61

Cartesian coordinates

C	0.879726	-0.191802	2.115123
O	1.617693	-0.239115	0.946045
H	-0.147242	0.174887	1.961845
H	1.382021	0.512978	2.796347
H	0.838052	-1.162178	2.630508
N	0.505391	-1.760982	-0.247565
C	1.208738	-1.694640	-1.509628
H	0.654056	-2.612241	0.273036
H	1.020279	-0.717284	-1.956988
H	0.900254	-2.473415	-2.220308
H	2.282696	-1.783414	-1.334247
H	-1.418476	0.477023	-0.662875
C	0.768168	2.724543	-0.575014
O	0.314797	1.403023	-0.733501
H	0.174111	3.368522	-1.227214
H	1.822865	2.833928	-0.858804
H	0.651372	3.084682	0.456522
H	0.854887	0.816499	-0.157487
C	-2.994894	-0.069332	0.538395
N	-2.061217	-0.309670	-0.556915
H	-2.436219	0.023708	1.473294
H	-3.669172	-0.922705	0.648068
H	-3.607964	0.835473	0.424288
H	-2.561461	-0.408428	-1.431823
H	-0.479619	-1.477354	-0.296416

Vibrational frequencies

28.7351	54.1520	66.1389
72.2057	87.1239	96.1686
99.4408	109.6219	131.2287

142.6967	151.5398	168.7511
180.7834	190.1082	210.9527
242.3527	281.1019	330.8402
460.5730	545.7397	857.7650
932.3486	966.7484	1026.1649
1039.9783	1067.2277	1095.7985
1108.6280	1119.8431	1145.0791
1156.9074	1163.5992	1177.9397
1186.9617	1201.7720	1353.0455
1373.9727	1439.2735	1455.0440
1461.6409	1467.4677	1490.9701
1496.6536	1498.5739	1503.4706
1506.8775	1509.6282	1517.2177
1524.5391	1538.0491	1687.4898
1698.8875	2955.1489	2991.9169
2999.5832	3003.9903	3015.1879
3023.2929	3046.2068	3079.6510
3097.9444	3109.4204	3115.5345
3142.7131	3332.7295	3404.3921
3458.8573	3600.1736	3652.2417

TS61

Cartesian coordinates

C	0.246810	-0.768864	2.009418
O	-0.187583	-1.246334	0.793497
H	1.198029	-0.199245	1.942426
H	0.421199	-1.575409	2.742659
H	-0.486039	-0.083712	2.486228
N	-2.022032	-0.054696	-0.049634
C	-2.286743	-1.048858	-1.055541
H	-2.288979	-0.399824	0.865539
H	-1.845059	-0.744630	-2.008546
H	-3.367909	-1.182222	-1.204923
H	-1.853550	-2.010781	-0.763702
H	0.586543	0.989009	-0.836461
C	2.654804	-0.826414	-0.750238
O	1.324878	-0.430763	-0.940074
H	3.244494	-0.574107	-1.638199
H	2.728202	-1.910600	-0.596894
H	3.123044	-0.337422	0.118412
H	0.691290	-0.872405	-0.200773
C	0.187946	2.548325	0.512831
N	-0.183385	1.683801	-0.616052
H	0.403001	1.913362	1.371051
H	-0.637655	3.215079	0.764259
H	1.073765	3.140196	0.277416

H	-0.402527	2.224427	-1.445888
H	-1.065190	0.996192	-0.339010

Vibrational frequencies

-393.7265	38.6312	72.0492
85.2908	97.2614	104.0072
111.8608	118.1444	136.1918
148.2148	155.5157	173.7335
187.5923	198.5868	233.6989
312.3352	383.5718	416.1723
503.1850	640.9236	934.8820
997.6976	1056.4492	1075.4224
1086.6422	1098.2459	1117.9346
1126.5958	1148.0542	1171.0505
1173.3836	1188.2380	1195.4212
1294.7865	1336.1146	1357.5278
1416.1705	1441.3428	1454.2413
1482.8081	1485.3425	1487.0636
1493.3266	1501.0947	1506.0597
1510.6131	1511.2291	1515.5023
1543.2020	1638.3181	1683.9772
1701.3041	1759.4020	1952.2773
2829.9933	2861.4406	2887.8940
2957.0580	2980.4067	2997.1244
3039.1625	3072.6808	3074.0069
3074.4973	3111.8134	3150.8769
3175.5228	3576.5294	3589.2701

P61

Cartesian coordinates

C	-0.686987	-1.743151	1.710316
O	-1.464259	-1.527723	0.557133
H	0.104561	-2.485920	1.544921
H	-1.343580	-2.118505	2.497791
H	-0.217623	-0.816977	2.074968
N	-1.619424	1.456103	0.303713
C	-2.083977	1.550515	-1.049942
H	-1.877078	0.514819	0.625833
H	-1.945363	2.558493	-1.448572
H	-3.139069	1.259609	-1.153414
H	-1.509857	0.843724	-1.672319
H	0.837023	0.089297	-0.790296
C	1.465386	-1.534549	-1.713564
O	0.436520	-0.706469	-1.223437
H	2.055911	-1.031101	-2.489071
H	1.006265	-2.419478	-2.157812
H	2.146059	-1.864699	-0.917518

H	-0.843340	-1.324378	-0.165880
C	2.210496	1.186996	1.285653
N	1.343234	1.490688	0.148233
H	1.792888	0.341712	1.836720
H	2.335691	2.021312	1.986509
H	3.198593	0.888743	0.927300
H	1.716542	2.264561	-0.388523
H	0.408110	1.765928	0.461396

Vibrational frequencies

32.4712	34.0626	55.4116
63.8550	79.6636	86.2948
90.3467	97.0353	98.0188
120.2651	136.6453	146.6136
152.0547	172.4147	190.8742
208.7439	232.5677	291.4588
462.5206	531.3538	853.1574
942.4236	980.8702	1028.7738
1038.9001	1057.1340	1090.1310
1096.7653	1108.4593	1117.2881
1140.3510	1169.4342	1187.0104
1189.5483	1206.9404	1364.4828
1390.1033	1418.4173	1466.0855
1472.4117	1483.5462	1489.9664
1494.8998	1499.8183	1501.9238
1503.2165	1505.7970	1510.6820
1520.2521	1526.0279	1576.6709
1697.9663	2967.6740	2982.9027
2997.3632	3020.3157	3026.8228
3037.8529	3055.5656	3095.1997
3101.5927	3114.2004	3119.7248
3127.8930	3262.7843	3408.6607
3415.3649	3595.0323	3600.5647

R62

Cartesian coordinates

C	2.163095	-1.346414	-1.146584
O	0.931254	-0.760538	-0.961795
H	2.681082	-1.576559	-0.201392
H	2.834497	-0.752208	-1.785115
H	1.995916	-2.308775	-1.657205
N	1.521418	1.081861	0.232554
C	1.844705	0.716642	1.592439
H	2.263893	1.557343	-0.259560
H	0.950566	0.295685	2.056170
H	2.182423	1.559889	2.211387
H	2.628432	-0.047960	1.608577

C	-1.601424	1.462805	-1.311962
N	-1.312062	1.789300	0.084050
H	-0.906629	0.682568	-1.632656
H	-1.430031	2.340320	-1.941935
H	-2.628465	1.113578	-1.492000
H	-1.455765	0.956159	0.659801
H	-1.927704	2.519006	0.420254
H	0.620744	1.565492	0.148798
C	-2.281130	-1.788785	0.368725
N	-1.198478	-1.092555	1.057868
H	-3.201836	-1.727716	0.955890
H	-2.082334	-2.849542	0.158736
H	-2.468825	-1.292900	-0.586587
H	-0.361641	-1.098373	0.470972
H	-0.971984	-1.567436	1.923214

Vibrational frequencies

56.3271	66.7893	79.7591
82.7930	103.7754	112.8582
118.9574	140.6037	142.6240
172.2905	182.8939	195.4383
203.3328	208.8077	219.5069
222.6758	264.8601	270.2639
444.1185	491.1943	565.6031
887.8458	948.9226	972.5181
1031.8198	1040.8334	1051.6635
1069.9325	1088.3768	1095.1702
1113.4796	1151.5153	1157.3552
1185.1840	1208.9545	1212.0987
1357.7773	1381.1030	1389.0458
1432.2337	1458.0293	1466.0209
1468.0411	1476.1349	1501.6943
1508.2312	1516.7517	1519.9003
1525.2354	1528.1753	1540.9126
1680.9038	1694.8736	1703.6478
2948.8192	2993.1966	2996.7907
2999.6137	3005.8807	3012.8627
3070.2440	3080.3071	3081.0543
3125.0666	3129.1439	3135.9833
3337.5030	3416.8349	3434.4019
3590.8871	3597.6753	3637.9004

TS62

Cartesian coordinates

C	-0.787134	-2.088972	1.039098
O	-0.302705	-0.835211	0.771343
H	-1.838810	-2.240468	0.695466

H	-0.797833	-2.337419	2.118946
H	-0.209198	-2.899693	0.545228
N	-2.038434	0.756933	-0.139370
C	-2.771013	-0.036395	-1.081903
H	-2.010344	0.272298	0.758229
H	-2.723894	0.398511	-2.084153
H	-3.829470	-0.126613	-0.795135
H	-2.368352	-1.058721	-1.118441
C	0.803058	1.851987	1.234362
N	0.436371	1.854534	-0.200058
H	0.572557	0.842690	1.590588
H	0.206007	2.591423	1.768835
H	1.863374	2.081100	1.347305
H	1.002333	1.089353	-0.701044
H	0.573221	2.758597	-0.639932
H	-0.589491	1.541327	-0.283169
C	2.872845	-0.872919	-0.517324
N	1.593816	-0.443111	-1.075868
H	3.711356	-0.423504	-1.058282
H	3.007654	-1.961903	-0.519975
H	2.926228	-0.543442	0.523087
H	0.814269	-0.781625	-0.450091
H	1.463224	-0.820917	-2.006532

Vibrational frequencies

-127.2552	34.5075	65.1987
77.3900	81.8508	91.7350
117.9717	127.4207	143.0072
152.3586	166.2525	173.1872
201.1997	240.4172	253.8004
284.6393	319.2518	356.8176
392.2884	598.5389	669.8863
999.3109	1006.0454	1010.2992
1045.5829	1060.3512	1081.5766
1092.4752	1116.8898	1128.8843
1146.9591	1181.4640	1185.6739
1285.3139	1325.0604	1347.7681
1387.0536	1404.0314	1410.6539
1459.4263	1462.8014	1475.2470
1481.0152	1489.1655	1495.0691
1501.7248	1504.6796	1508.8005
1523.4219	1541.2163	1666.8160
1680.5691	1697.7385	1742.7531
2471.8109	2617.5472	2803.1746
2847.3117	2883.5720	2902.4705
2979.6086	3015.0813	3026.8260
3031.7175	3076.1209	3092.3348

3115.4289	3132.3012	3154.5534
3508.2669	3573.7430	3584.3184

I62

Cartesian coordinates

C	-1.860417	2.050531	0.729844
O	-0.630674	1.704776	0.138871
H	-2.211838	1.286927	1.438393
H	-2.646056	2.214862	-0.018894
H	-1.718969	2.981966	1.280849
N	2.069066	0.618775	0.149943
C	2.374785	0.836572	-1.231801
H	1.396673	1.338908	0.435159
H	3.214193	0.215568	-1.551508
H	2.576298	1.889776	-1.466523
H	1.489520	0.546684	-1.823182
H	-0.125458	-1.227424	-0.487502
C	-1.753339	-1.495940	-1.562878
O	-0.654386	-0.719140	-1.137247
H	-1.425949	-2.418410	-2.055287
H	-2.320749	-0.905695	-2.284156
H	-2.418667	-1.759782	-0.731227
H	-0.751304	0.888555	-0.378869
C	0.070734	-1.263643	2.015681
O	0.830874	-1.691444	0.898662
H	-0.299362	-0.240808	1.876805
H	0.656779	-1.308309	2.939923
H	-0.781489	-1.938305	2.116383
H	1.525815	-1.014588	0.752661

Vibrational frequencies

20.4912	33.5101	62.4552
64.7752	81.2377	99.7646
103.9364	115.7334	131.7891
153.6159	168.9043	172.9428
206.7205	229.6990	270.8618
311.6200	319.8301	369.9867
618.4348	674.1008	745.7240
992.4747	1004.1112	1012.7124
1048.1579	1079.7290	1086.8264
1091.6342	1131.0123	1148.7287
1156.2887	1189.4619	1189.6730
1307.9415	1312.9934	1348.7177
1393.4066	1429.2194	1465.5999
1474.1272	1482.9981	1484.8874
1486.6542	1491.1894	1498.2188
1504.8198	1511.2252	1523.4951

1536.2139	1547.1849	1649.2160
1671.6886	1693.3995	1762.0374
2182.6536	2709.7631	2798.8048
2879.8689	2883.4896	2896.4593
2926.3859	2971.3476	2991.5844
3013.5040	3019.8419	3078.5646
3085.9737	3114.9016	3119.9940
3156.7557	3576.8240	3580.2473

TS63

Cartesian coordinates

C	0.535357	0.887333	2.073051
O	1.038457	1.158846	0.788975
H	0.054597	-0.098077	2.128954
H	-0.209442	1.638057	2.364441
H	1.354924	0.921602	2.795438
N	1.705014	-0.784623	-0.218266
C	2.093840	-0.190324	-1.464584
H	2.404274	-0.894861	0.500870
H	1.203990	0.261763	-1.907679
H	2.475519	-0.966382	-2.140963
H	2.863164	0.566129	-1.310521
H	-0.916937	-0.419317	-0.608617
C	-2.024336	1.532610	-0.925774
O	-0.837158	0.817631	-0.781656
H	-2.728382	1.005523	-1.585868
H	-1.839525	2.519492	-1.371620
H	-2.541107	1.698763	0.034634
H	0.229669	1.147695	0.132526
C	-1.532715	-1.927276	0.710056
O	-0.717328	-1.517280	-0.351274
H	-1.995142	-1.069353	1.221639
H	-0.957284	-2.488310	1.460188
H	-2.341623	-2.582133	0.361474
H	0.703565	-1.235874	-0.151885

Vibrational frequencies

-337.9021	38.4847	63.3959
76.8822	98.6224	108.5761
109.2493	116.2353	132.3896
153.4369	162.2869	165.2546
188.2339	203.7742	270.9724
285.0441	313.1108	397.4275
637.6238	695.1928	733.5196
955.3532	994.6926	1011.1682
1018.8595	1054.0217	1081.3270
1089.5743	1113.2888	1144.7031

1153.2045	1173.3587	1195.8573
1198.8373	1328.2319	1343.5603
1385.2237	1398.1828	1437.6442
1471.6166	1483.2026	1487.6429
1488.3403	1492.2770	1496.9774
1504.8122	1507.3180	1509.7094
1523.0082	1539.1169	1552.5728
1659.2159	1673.6355	1759.5786
1805.6841	2422.6460	2855.8445
2888.0328	2902.8463	2914.4580
2971.2589	3012.0047	3015.9453
3030.0642	3066.8963	3088.3938
3092.3541	3121.3577	3124.4758
3152.2275	3577.6273	3578.6068

P63

Cartesian coordinates

C	0.850210	0.719107	2.001899
O	1.440436	0.960990	0.773132
H	-0.146876	0.261948	1.912739
H	0.725009	1.690337	2.505458
H	1.473483	0.093314	2.655759
N	1.543854	-1.112267	-0.068416
C	2.027945	-0.886405	-1.414339
H	2.199786	-1.579322	0.539448
H	1.269430	-0.330871	-1.967531
H	2.246168	-1.815678	-1.956189
H	2.933073	-0.277602	-1.375734
H	-1.231921	-0.560027	-0.620977
C	-1.310252	2.271250	-0.814028
O	-0.612145	1.051542	-0.913320
H	-2.185931	2.214625	-1.463226
H	-0.693725	3.115716	-1.143680
H	-1.652796	2.470280	0.210262
H	0.192900	1.092150	-0.343772
C	-2.339148	-1.534406	0.652921
O	-1.336515	-1.487243	-0.333393
H	-2.083748	-0.942426	1.543713
H	-2.460080	-2.574427	0.962091
H	-3.305588	-1.179613	0.272527
H	0.607107	-1.512112	-0.022044

Vibrational frequencies

12.9200	22.0188	50.4949
59.3854	72.6064	83.8390
90.7825	101.1908	103.0465
117.5144	139.2854	148.6912

161.0225	179.2165	197.5295
223.3269	241.9662	284.1883
469.5663	508.5122	560.8771
943.0720	961.0367	971.2641
1021.9415	1029.6758	1056.1899
1062.7991	1085.7792	1094.7192
1112.9581	1123.7934	1165.6248
1186.0934	1209.1940	1220.6859
1376.6772	1386.2920	1390.7789
1422.8990	1465.0306	1471.4464
1484.9498	1489.5220	1494.7149
1497.7738	1504.3298	1512.0922
1516.0898	1523.6615	1535.8550
1578.1918	1683.9750	1706.8801
2967.0976	2983.1865	2999.2458
3009.1115	3013.0007	3033.9519
3074.0808	3083.8975	3100.7816
3104.9823	3117.9622	3119.9177
3270.8183	3339.1624	3390.3652
3466.6387	3594.7475	3599.6903

R64

Cartesian coordinates

C	0.402593	-0.414597	-2.427939
O	1.429226	-0.991458	-1.646991
H	-0.503448	-0.226155	-1.838237
H	0.133504	-1.054084	-3.278785
H	0.766821	0.536590	-2.826700
N	1.871305	0.975014	0.443807
C	3.180241	1.049737	1.010613
H	1.874609	0.294010	-0.334168
H	3.219369	1.753969	1.843737
H	3.917069	1.350730	0.250459
H	3.506780	0.059144	1.363197
C	0.571243	-2.096735	1.539042
N	0.006764	-2.420692	0.229202
H	-0.059146	-2.398966	2.384814
H	0.717747	-1.015300	1.600490
H	1.549300	-2.571940	1.651039
H	-0.160392	-3.416161	0.148836
H	0.995529	-1.643655	-1.047100
H	-0.888426	-1.939387	0.128592
C	-0.908056	2.732524	-0.370055
O	-0.728400	1.842391	0.711961
H	-1.967733	2.990234	-0.421604
H	-0.615324	2.281975	-1.327017

H	-0.336966	3.657323	-0.228533
H	0.225379	1.605827	0.745882
C	-3.452658	-0.204665	0.441871
O	-2.100957	-0.405212	0.104086
H	-4.011018	-1.095226	0.146197
H	-3.884447	0.655961	-0.085395
H	-3.591410	-0.053883	1.520046
H	-1.593417	0.385386	0.379549

Vibrational frequencies

22.0462	31.7732	41.8966
47.8083	57.4595	68.1862
77.7249	79.6312	85.1797
93.2846	100.2763	103.8776
108.5163	112.1846	119.5370
144.7923	149.4029	172.7253
177.0069	196.6319	221.9990
274.4731	300.5044	304.9372
508.2208	647.2319	873.1326
919.9295	939.5045	980.9974
1008.6111	1039.8571	1069.1858
1089.1529	1098.0889	1102.1847
1116.8596	1136.7470	1147.6073
1161.2074	1175.1126	1186.5751
1190.1795	1194.3347	1213.0857
1378.9474	1389.2195	1432.5809
1466.7744	1480.9020	1483.9057
1487.2830	1491.8688	1493.8333
1495.9139	1497.4819	1498.2640
1504.4835	1507.1740	1510.7001
1522.3305	1524.8569	1527.1095
1550.4471	1568.2483	1691.2791
2975.5987	2997.8077	2999.6030
3008.4423	3013.3402	3023.3816
3053.7996	3061.6629	3069.5009
3085.6896	3096.9768	3114.0832
3114.4601	3118.1270	3119.0064
3286.1750	3366.1835	3410.0280
3461.3230	3527.5741	3602.4111

TS64

Cartesian coordinates

C	1.507853	-1.547121	-1.693650
O	2.002671	-1.191454	-0.439418
H	0.430482	-1.348544	-1.803525
H	1.668772	-2.625786	-1.844396
H	2.041406	-1.035342	-2.507907

N	1.734737	0.970007	-0.439894
C	2.606300	1.397001	0.622399
H	2.106116	1.094937	-1.369540
H	2.113073	1.218230	1.579315
H	2.842406	2.467682	0.563367
H	3.537622	0.826493	0.599652
C	-0.164075	-0.602330	2.232254
N	-0.051358	-1.559378	1.111103
H	-1.015598	-0.865855	2.860866
H	-0.333486	0.382923	1.788063
H	0.749165	-0.618015	2.828078
H	-0.050707	-2.522942	1.429286
H	0.854557	-1.390220	0.523001
H	-0.865534	-1.395363	0.435728
C	-1.382484	2.559812	-0.429831
O	-0.827395	1.359312	-0.008447
H	-2.096486	2.973819	0.302169
H	-1.927097	2.463193	-1.386008
H	-0.610941	3.333907	-0.587333
H	0.694041	1.168287	-0.327951
C	-3.245084	-0.718159	-0.383911
O	-1.861660	-0.746618	-0.611015
H	-3.631327	-1.739841	-0.295947
H	-3.777381	-0.233964	-1.213444
H	-3.501800	-0.175795	0.538631
H	-1.454918	0.242646	-0.423090

Vibrational frequencies

-94.5746	31.8992	47.7742
72.7379	82.8155	96.4894
97.8207	110.2637	113.2145
123.6853	134.2685	137.6091
143.2103	157.0527	162.4415
201.3132	209.8703	229.5323
232.7017	268.5430	315.9728
369.5259	408.2310	420.7689
591.1568	653.8840	987.9935
1019.4748	1056.1824	1072.0844
1091.2101	1096.2277	1108.5784
1112.1070	1127.8803	1140.1886
1155.9044	1173.4487	1185.9691
1190.7770	1197.8489	1207.5597
1303.4979	1323.9420	1338.2994
1350.0660	1438.0053	1451.2412
1470.1706	1473.1373	1491.0491
1491.5175	1498.3845	1499.2002
1500.8737	1505.5674	1511.0221

1512.9362	1516.0326	1522.8217
1545.7473	1618.7646	1647.6704
1690.4959	1696.1728	1751.7152
1813.3944	2256.7035	2667.9713
2674.3838	2932.7721	2961.6431
2964.7628	2969.1710	2985.8360
3016.1392	3019.4616	3030.6209
3034.7738	3035.6906	3070.2783
3096.4803	3133.3886	3141.0321
3152.5345	3573.2944	3646.1961

P64

Cartesian coordinates

C	1.695653	-1.400217	-1.803078
O	2.364632	-1.073485	-0.640271
H	0.602640	-1.355260	-1.702353
H	1.961899	-2.445302	-2.033590
H	2.012066	-0.793110	-2.664486
N	1.719105	1.148754	-0.376671
C	2.533958	1.558320	0.749325
H	2.116853	1.428699	-1.261714
H	2.057613	1.228932	1.674890
H	2.688343	2.644437	0.818672
H	3.507826	1.068760	0.686041
C	-0.118688	-0.507439	2.316744
N	0.165726	-1.485927	1.265615
H	-0.998576	-0.822132	2.884115
H	-0.355792	0.452150	1.851977
H	0.708364	-0.364291	3.023837
H	0.324126	-2.403126	1.665138
H	1.016019	-1.238358	0.749337
H	-1.040031	-1.298958	0.057929
C	-2.117975	2.533483	-0.608675
O	-1.169726	1.615825	-0.120612
H	-3.111791	2.367859	-0.172567
H	-2.208739	2.494395	-1.702084
H	-1.790951	3.537037	-0.329564
H	0.747340	1.452101	-0.315778
C	-2.974011	-1.495208	-0.253111
O	-1.710602	-0.985634	-0.611459
H	-2.988016	-2.591860	-0.272342
H	-3.706873	-1.135874	-0.978676
H	-3.287363	-1.161821	0.745756
H	-1.436834	0.708647	-0.375655

Vibrational frequencies

24.0313	28.2649	46.3793
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48.1414	63.1141	77.3703
82.3049	90.7446	98.7490
110.8312	119.2397	127.2959
133.6907	142.2412	148.3348
154.4173	178.0850	190.7874
198.3458	216.4695	243.1997
264.0783	271.3310	309.5656
487.1276	540.5557	810.6324
883.2072	971.3864	1007.4882
1034.6661	1042.9965	1087.3222
1102.1183	1108.2865	1109.2245
1121.0833	1141.5010	1155.7141
1164.6786	1175.3534	1175.7306
1186.6825	1189.3253	1230.2249
1352.8968	1371.3341	1434.4127
1445.4655	1459.6157	1472.2328
1485.4910	1491.4669	1496.7331
1499.7305	1500.3349	1501.7717
1510.7208	1515.9641	1516.5684
1524.8244	1533.1766	1541.8014
1602.3233	1685.1923	1695.0700
2955.5324	2991.0823	2996.7316
2997.8589	3010.3110	3010.8893
3048.3174	3051.0585	3054.6156
3089.3168	3093.3151	3107.9733
3115.8320	3128.6005	3132.3840
3135.6403	3403.4970	3459.0499
3518.1026	3594.4049	3639.4326

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