

Supporting Information

Indenyl-Benzyl Radical Recombination Leads to the Formation of Fluoranthene, a Non-Alternant Polycyclic Aromatic Hydrocarbon

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S1. Methods:

S1.1. Experimental: The experiments were performed at the Chemical Dynamics Beamline (9.0.2.) of the Advanced Light Source (ALS) using a high-temperature chemical reactor consisting of a resistively heated silicon carbide (SiC) tube of 20 mm heating length and 1 mm inner diameter.¹⁻⁵ This device was located inside the source chamber of a molecular beam setup, which was equipped with a Wiley–McLaren reflectron time-of-flight mass spectrometer (Re-TOF-MS). The benzyl ($C_7H_7^{\bullet}$) radical was produced in situ by pyrolysis from benzyl bromide (C_7H_7Br ; 98% purity, Sigma Aldrich, Catalog number- B17905) precursor kept in a bubbler at 293 K. The indenyl radical ($C_9H_7^{\bullet}$) was prepared in situ by pyrolysis of the 1-bromoindene (C_9H_7Br , $\geq 98\%$ purity) precursor synthesized in house using the procedure reported in previous work.⁴ The mixed vapor of benzyl bromide (C_7H_7Br) from the bubbler and 1-bromoindene (C_9H_7Br) stored in a Swagelok particulate filter was seeded in helium carrier gas at total pressures of 150 ± 10 torr at the reactor inlet through a 0.2 mm nozzle. The temperature of the SiC tube was determined using a Type-C thermocouple to be 1273 ± 20 K. The products formed in the reactor passed through a 2 mm skimmer located 10 mm downstream of the reactor and entered the main chamber, which houses the Re-TOF-MS. The neutral products within the supersonic molecular beam were then photoionized in the extraction region of the mass spectrometer by utilizing quasi-continuous tunable synchrotron vacuum ultraviolet (VUV) light. VUV single photon ionization represents essentially a fragment-free ionization technique and is accepted as a soft ionization method compared to the harsher conditions of electron impact ionization with the latter leading to excessive fragmentation of the parent ion.⁶ The ions formed via soft photoionization were extracted and ultimately detected by a microchannel plate detector through an ion lens. Under our experimental conditions, modeling suggested that the residence time in the reactor tube was few tens of microseconds.⁷ Photoionization efficiency (PIE) curves, which report ion counts as a function of photon energy with a step interval of 0.05 eV at a well-defined mass-to-charge ratio (m/z), were produced by integrating the signal recorded at the specific m/z for the species of interest. Due to the weak signal in these experiments, extended data accumulation times of up to 15 min per step had to be accounted for, and each step was repeated three times.

S1.2. Computational: The geometry of the reactants, products, intermediates, and transition states were optimized using the ω B97X-D hybrid density functional method⁸ with the 6-311G** basis

set. The same ω B97X-D/6-311G** approach was used to compute vibrational frequencies and zero-point vibrational energy corrections (ZPE) at the optimized structures. Intrinsic reaction coordinate (IRC) calculations were carried out to confirm connections between transition states (saddle points) on the potential energy surface and corresponding local minima in the forward and reverse directions. The relative energies were further refined using a modified G3(MP2,CC) calculation scheme:⁹⁻¹¹

$$\begin{aligned} E[\text{G3(MP2, CC)}] &= E[\text{CCSD(T)/6-311G**}] + E[\text{MP2/G3Large}] - E[\text{MP2/6-311G**}] \\ &+ E(\text{ZPE}) = E[\text{CCSD(T)/6-311G**}] + \Delta\text{EMP2} + E(\text{ZPE}) \end{aligned}$$

Here, CCSD(T) is the coupled cluster method with single and double excitations and with accounting for triple excitations according to perturbation theory, MP2 is the second-order Møller–Plesset perturbation theory method, and $\Delta\text{EMP2} = E[\text{MP2/G3Large}] - E[\text{MP2/6-311G**}]$ is the basis set correction. B3LYP and MP2 calculations were performed using the Gaussian 16 software,¹² and the MOLPRO 2021 package^{13, 14} was employed for CCSD(T) calculations.

Temperature- and pressure-dependent rate constants for isomerization and unimolecular decomposition on the $\text{C}_{16}\text{H}_{13}^{\bullet}$ and $\text{C}_{16}\text{H}_{11}^{\bullet}$ potential energy surfaces were evaluated using the Rice-Ramsperger-Kassel-Marcus Master Equation (RRKM-ME) theoretical method by solving the one-dimensional master equation using the MESS program package.^{15, 16} Densities of states for local minima and numbers of states for transition states and partition functions were assessed within the Rigid-Rotor, Harmonic-Oscillator (RRHO) approximation. Asymmetric Eckart potentials were used to compute tunneling corrections for the rate constants. Collision parameters for RRKM-ME calculations were adopted from our previous studies of the kinetics of the benzyl + benzyl¹⁷ and indenyl + indenyl¹⁸ reactions. In particular, the Lennard-Jones parameters were taken as (ϵ/cm^{-1} , $\sigma/\text{\AA}$) = (390, 4.46) and the $\alpha(T) = \alpha_{300}(T/300 \text{ K})^n$ expression with $n = 0.62$ and $\alpha_{300} = 424 \text{ cm}^{-1}$ was used for the temperature dependence of the range parameter α for the deactivating wing of the energy transfer function.

Since Variable Reaction Coordinate TST (VRC-TST) calculations are extremely demanding computationally for systems of this size, we used phase space theory¹⁹ for barrierless entrance and exit H loss channels of the $\text{C}_9\text{H}_7^{\bullet} + \text{C}_7\text{H}_7^{\bullet}$ reaction, where high-pressure limit (HPL) rate constants in the temperature range of interest were fitted to the values obtained earlier using

VRC-TST calculations for the benzyl + propargyl reaction, the closest though not direct analogue for benzyl + indenyl for which the rate constant estimation is available in the literature;²⁰ both reactions feature recombination of benzyl with another resonantly stabilized π -radical. For the barrierless H loss channels we also employed phase space theory, with fitting the HPL rate constants in the reverse (radical + H recombination) direction to the most accurate VRC-TST rate constants for $c\text{-C}_5\text{H}_5 + \text{H}^{21}$ for **i3** + H $\rightarrow$ **i1** and for $i\text{-C}_3\text{H}_7 + \text{H}^{22}$ for **i11** + H $\rightarrow$ **i1**.

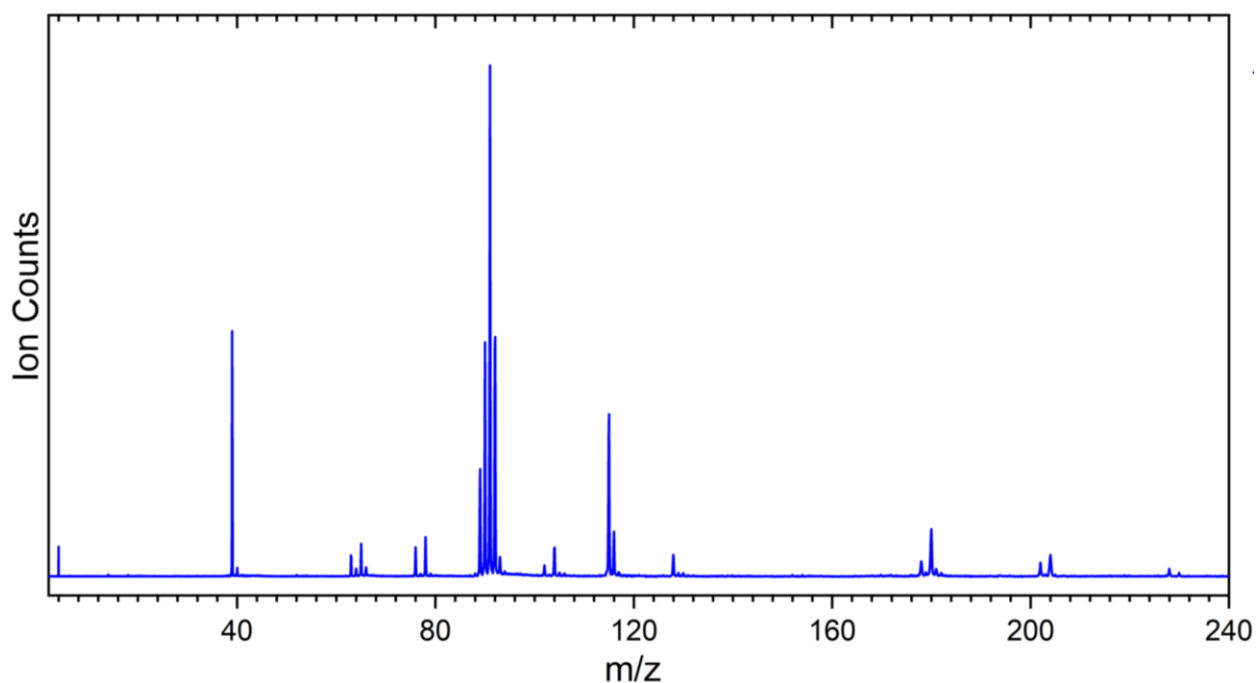


Figure S1: Complete mass spectra recorded at a photon energy of 9.50 eV where the microreactor temperature was 1273 ± 20 K for 1-bromoindene ($\text{C}_9\text{H}_7\text{Br}$) plus benzyl bromide ($\text{C}_7\text{H}_7\text{Br}$)/helium molecular beam.

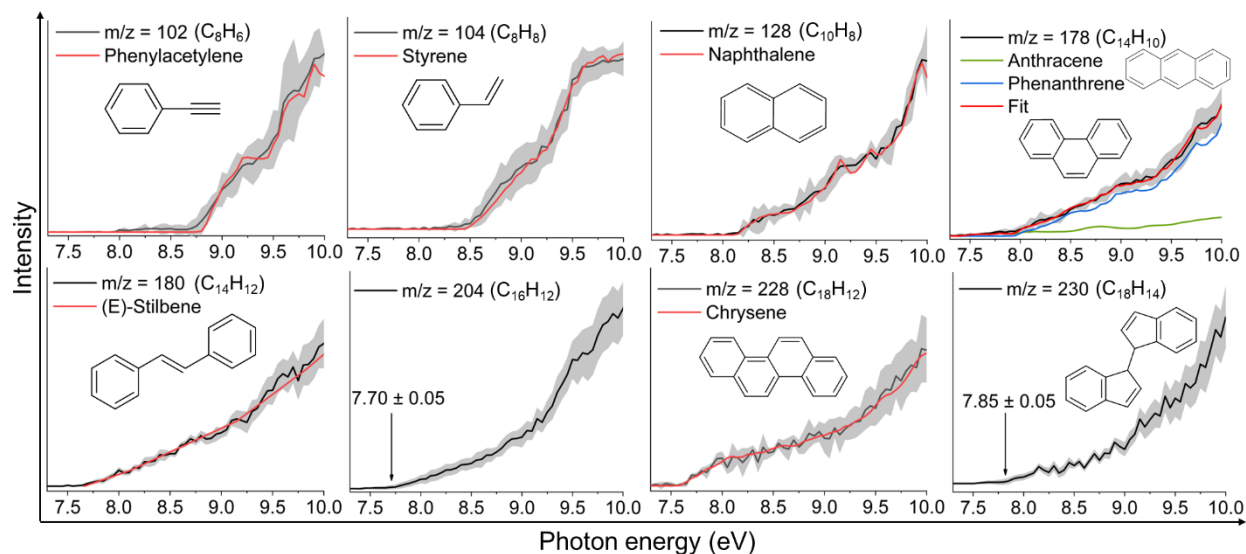


Figure S2: Photoionization efficiency curves for the additional products in the range of $m/z = 102$ to 230. Black: experimental PIE curves; blue/green/red: reference PIE curves. In case of multiple contributions to one PIE curve, the red line resembles the overall fit. The error bars consist of two parts: $\pm 10\%$ based on the accuracy of the photodiode and a $1-\sigma$ error of the PIE curve averaged over the individual scans.

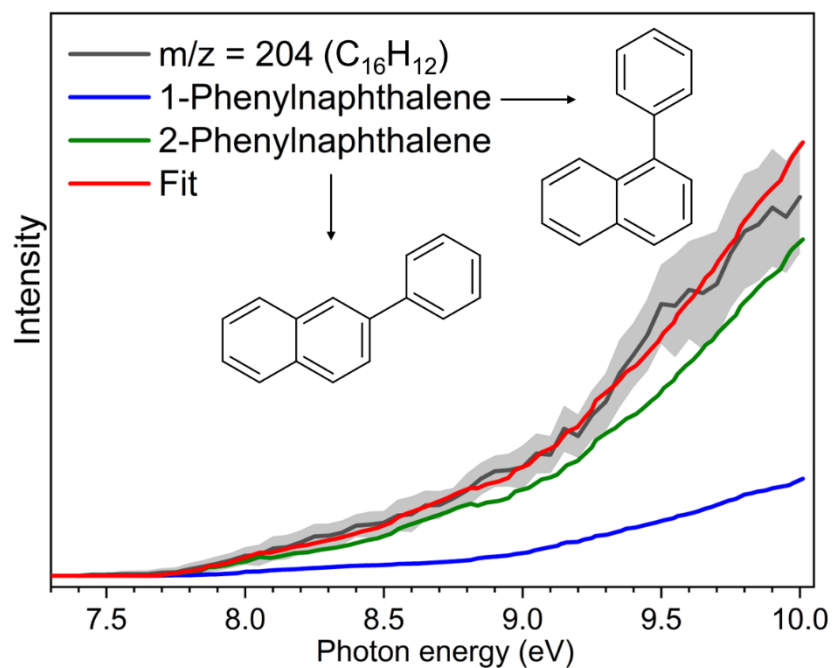
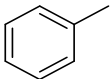
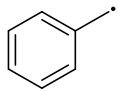
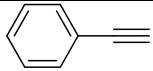
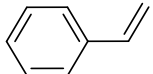
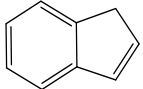
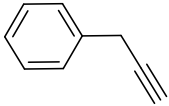
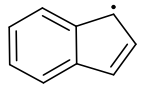
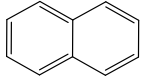
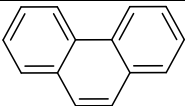
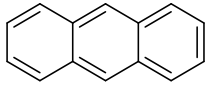
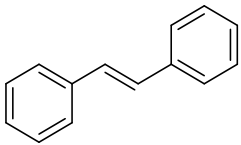
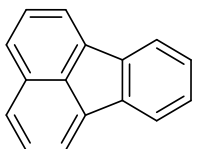
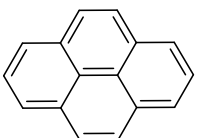
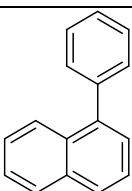
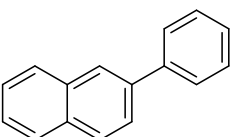
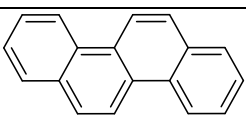
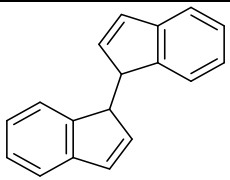


Figure S3: Tentative photoionization efficiency curve fitting for $m/z = 204$ ($C_{16}H_{12}$) with 1-phenylnaphthalene and 2-phenylnaphthalene. Black: experimental PIE curves; blue/green: reference PIE curves; red: overall fit. The error bars consist of two parts: $\pm 10\%$ based on the accuracy of the photodiode and a $1-\sigma$ error of the PIE curve averaged over the individual scans.

Table S1: Assignment of the mass-growth products from the reaction between 1-indenyl ($C_9H_7^{\bullet}$) and benzyl ($C_7H_7^{\bullet}$) radicals.

Mass	Molecular formula	Name	Structure
92	C_7H_8	Toluene	
		Benzyl radical (^{13}C)	
102	C_8H_6	Phenylacetylene	
104	C_8H_8	Styrene	
116	C_9H_8	Indene	
		3-Phenyl-1-propyne	
		Indenyl radical (^{13}C)	
128	$C_{10}H_8$	Naphthalene	
178	$C_{14}H_{10}$	Phenanthrene	
		Anthracene	
180	$C_{14}H_{12}$	(E)-Stilbene	

202	$C_{16}H_{10}$	Fluoranthene	
		Pyrene	
204	$C_{16}H_{12}$	1-Phenylnaphthalene	
		2-Phenylnaphthalene	
228	$C_{18}H_{12}$	Chrysene	
230	$C_{18}H_{14}$	1H,1'H-1,1'-biindene (adduct)	

S2. Mass-growth Products in the Range of 92 – 180 amu:

Toluene (C_7H_8) and a contribution from the ^{13}C -benzyl radical ($^{13}C_9H_7^{\bullet}$) can be identified for $m/z = 92$ (Figure 1b), while indene (C_9H_8), 3-phenyl-1-propyne (C_9H_8), and ^{13}C -indenyl radical ($^{13}C_9H_7^{\bullet}$) correspond to $m/z = 116$ (Figure 2a).²³⁻²⁶ Phenylacetylene (C_8H_6 ; 102 amu), styrene (C_8H_8 ; 104 amu), naphthalene ($C_{10}H_8$; 128 amu), anthracene ($C_{14}H_{10}$; 178 amu), phenanthrene ($C_{14}H_{10}$; 178 amu), and (E)-stilbene ($C_{14}H_{12}$; 180 amu) are also notable (Table S1).^{24, 26-34} One of the major sources of $C_{14}H_{10}$ is the self-reaction of benzyl radicals, followed by dehydrogenation.²⁹

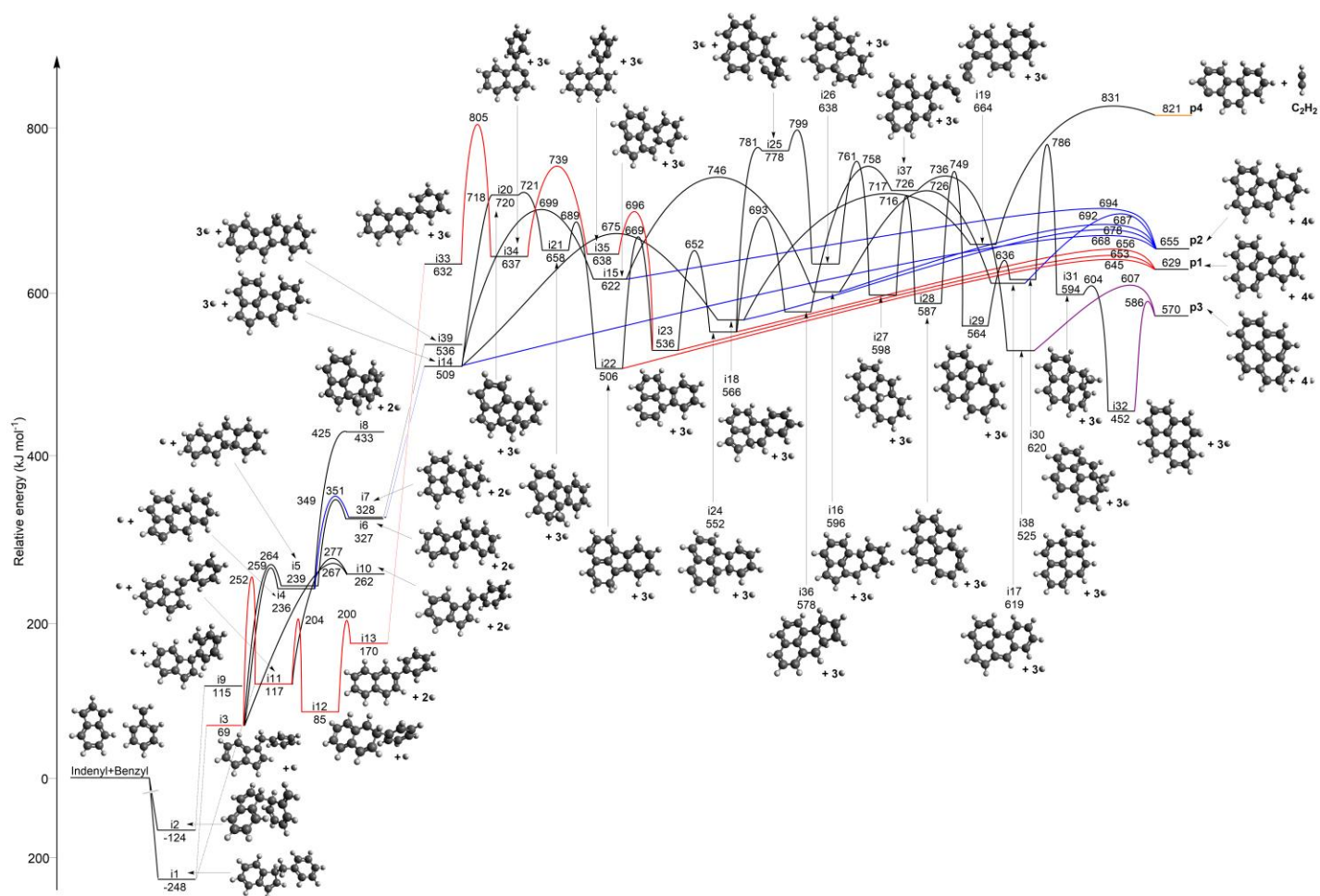
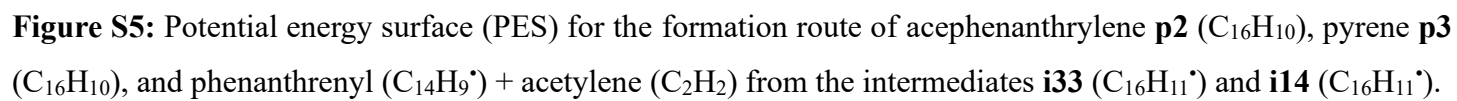


Figure S4: Potential energy surface (PES) for the recombination reaction of indenyl ($C_9H_7^{\bullet}$) and benzyl ($C_7H_7^{\bullet}$) radicals yielding $C_{16}H_{10}$ products.



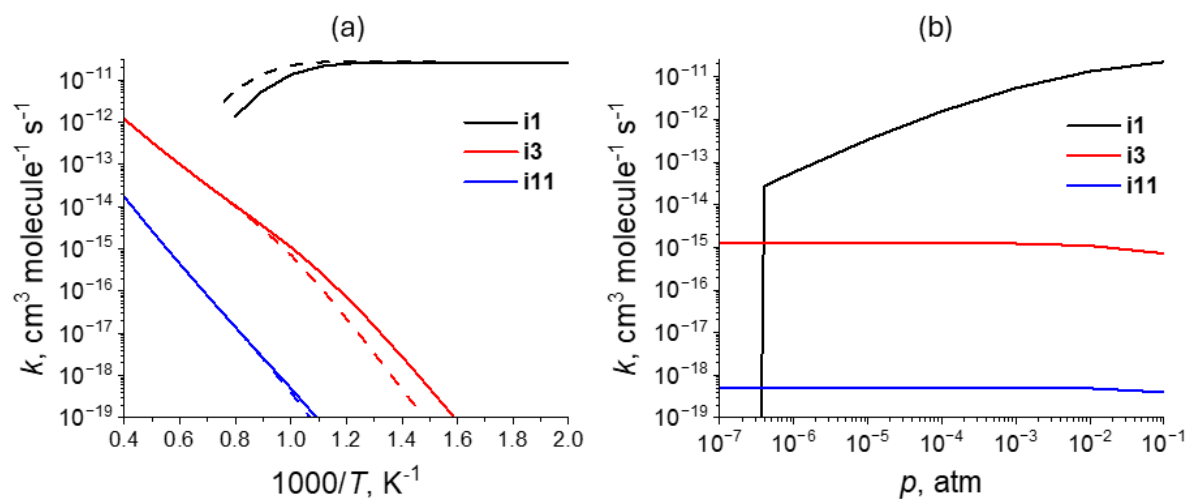


Figure S6. Calculated rate constants for different product channels of the $\text{C}_9\text{H}_7^\bullet + \text{C}_7\text{H}_7^\bullet$ reaction as (a) a function of temperature at 0.01 (solid line) and 0.1 (dashed line) atm and (b) as a function of pressure at $T = 1000 \text{ K}$.

Table S2. Rate constants and product branching ratios^a for the reaction on the C₁₆H₁₃[•] and C₁₆H₁₁[•] potential energy surfaces calculated using the RRKM-ME approach at the pressure of 0.1 atm.

C₁₆H₁₃ ⇌ C₁₆H₁₂ + H								
<i>T</i> , K	i3 → i10 + H		i3 → i13 + H		i10 + H → i3		i10 + H → i13 + H	
	<i>k</i> , s ⁻¹	branching ratio	<i>k</i> , s ⁻¹	branching ratio	<i>k</i> , cm ³ s ⁻¹	branching ratio	<i>k</i> , cm ³ s ⁻¹	branching ratio
1000	4.66E+02	41.38%	4.65E+02	41.27%	2.25E-11	88.39%	2.54E-12	9.95%
1125	7.34E+03	50.03%	7.33E+03	49.99%	2.61E-11	85.17%	4.55E-12	14.82%
1250	5.91E+04	56.49%	4.56E+04	43.55%	2.63E-11	78.13%	7.36E-12	21.85%
1375	2.71E+05	61.04%	1.73E+05	39.03%	2.19E-11	65.94%	1.13E-11	34.02%
1500	8.10E+05	64.26%	4.52E+05	35.83%	1.51E-11	49.76%	1.52E-11	50.19%
1650							2.14E-11	99.99%
1800							2.19E-11	99.98%
2000							2.22E-11	99.96%
2250							2.21E-11	99.91%
2500							2.17E-11	99.83%
C₁₆H₁₁ ⇌ C₁₆H₁₀ + H								
<i>T</i> , K	i33 → p1 + H		p1 + H → p2 + H		p1 + H → p3 + H			
	<i>k</i> , s ⁻¹	branching ratio	<i>k</i> , cm ³ s ⁻¹	branching ratio	<i>k</i> , cm ³ s ⁻¹	branching ratio		
1000	1.82E+04	99.13%	1.40E-16	0.00%	1.65E-17	0.00%		
1125	1.61E+05	99.97%	8.08E-16	0.02%	1.15E-16	0.00%		
1250	7.37E+05	100.00%	2.71E-15	77.63%	4.87E-16	13.97%		
1375	2.11E+06	100.00%	6.87E-15	79.87%	1.59E-15	18.53%		
1500			1.40E-14	75.85%	4.31E-15	23.41%		
1650			2.85E-14	70.35%	1.17E-14	28.89%		
1800			5.20E-14	65.37%	2.71E-14	34.01%		
2000			1.02E-13	59.65%	6.84E-14	40.18%		
2250			2.00E-13	53.72%	1.72E-13	46.01%		
2500			3.48E-13	49.11%	3.58E-13	50.54%		

^a If the sum of branching ratios for a forward or reverse reaction is lower than 100%, the remaining reaction flux leads to thermalization (collisional deactivation) of some other C₁₆H₁₃[•] or C₁₆H₁₁[•] isomers.

Data S1. Coordinates of the reactants, intermediates, transition states and products.

Reactants

Indenyl (C₉H₇)

C	2.139356	0.694412	0.000000
C	2.139335	-0.694380	0.000000
C	0.937290	1.411314	0.000000
C	-0.254828	0.709689	-0.000000
C	-0.254734	-0.709992	-0.000000
C	0.937110	-1.411421	0.000000
C	-1.642000	1.136442	-0.000001
C	-2.451867	0.000377	0.000001
H	-1.981819	2.163530	-0.000002
C	-1.642911	-1.136520	-0.000001
H	0.946753	-2.496196	-0.000000
H	3.081740	1.230171	0.000000
H	3.081561	-1.230380	-0.000000
H	0.946330	2.496103	0.000000
H	-3.532524	0.000896	0.000003
H	-1.982555	-2.163647	-0.000000

Frequencies[1/cm]

200.8697	242.5985	394.7195
418.3795	535.7333	553.1621
566.3149	582.5820	718.8673
751.9667	760.4327	773.6398
816.9399	868.2007	882.8196
902.5067	921.0125	965.5076
1003.8052	1005.2658	1047.4872
1091.0121	1103.7883	1188.2747
1193.0873	1222.7277	1229.0784
1332.7256	1380.6691	1390.8713
1485.2102	1507.3066	1507.8884
1658.5504	1660.9585	3184.1482
3190.3109	3200.8491	3214.1144
3224.6939	3231.4401	3251.1238

Benzyl (C₇H₇)

C	-0.251104	1.213129	-0.000083
C	1.129041	1.206812	0.000031
C	-0.989445	0.000000	0.000000
C	-0.251106	-1.213127	0.000083
C	1.129039	-1.206814	-0.000031
C	1.830845	-0.000000	0.000000
H	-0.791023	2.154298	-0.000026
H	-0.791026	-2.154296	0.000026

H	1.671216	-2.145894	-0.000195
H	1.671220	2.145892	0.000195
H	2.914529	-0.000001	0.000000
C	-2.393083	0.000001	0.000000
H	-2.950021	0.929006	0.000022
H	-2.950021	-0.929005	-0.000022

Frequencies[1/cm]

202.0740	365.8693	393.4902
482.9490	503.0827	538.1424
633.2916	690.9663	708.5794
780.5716	841.8671	843.8226
915.0627	978.4945	991.7167
1001.3986	1007.2864	1050.0037
1126.6390	1179.3221	1191.0655
1289.8052	1333.3473	1356.6714
1487.6995	1495.1484	1511.9325
1610.0578	1625.5518	3160.0714
3181.6471	3184.1418	3196.0543
3202.7863	3215.5710	3263.1014

Intermediates

il

C	4.545488	-0.212809	0.259251
C	3.881532	-1.436259	0.283867
C	3.852904	0.968232	0.007733
C	2.484260	0.901205	-0.218646
C	1.816754	-0.331314	-0.197445
C	2.507748	-1.502577	0.054815
C	1.495300	1.947058	-0.501454
C	0.285896	1.392562	-0.645038
C	0.348651	-0.105651	-0.465932
C	-0.560398	-0.633199	0.664169
H	0.053742	-0.598608	-1.402249
C	-2.023590	-0.386672	0.395421
H	-0.261016	-0.155086	1.601368
H	-0.383185	-1.706790	0.781429
C	-2.684214	0.701718	0.962454
C	-4.022984	0.947979	0.681940
C	-4.722353	0.105811	-0.173308
C	-4.074791	-0.983674	-0.744300
C	-2.737132	-1.225349	-0.460562
H	5.614303	-0.180831	0.439067
H	4.438479	-2.344952	0.482569
H	4.373922	1.919404	-0.010274
H	1.996056	-2.459636	0.074037

H	1.727203	3.001638	-0.581474
H	-0.636612	1.915949	-0.859595
H	-2.140890	1.362988	1.630317
H	-4.521123	1.798063	1.134710
H	-5.767161	0.295018	-0.391653
H	-2.237886	-2.080646	-0.906704
H	-4.614264	-1.648870	-1.409331

Frequencies[1/cm]

33.0606	43.1406	61.4642
108.6524	139.4922	231.7893
245.4426	296.5259	365.9469
412.3807	418.5568	444.3506
484.5980	546.8253	570.2638
575.1634	604.1414	639.7009
641.1382	724.0908	738.0561
747.0034	760.6120	777.6983
809.0544	823.6344	855.6851
872.0252	878.5515	895.8481
933.1192	947.2564	968.5187
985.6404	1000.9061	1009.8747
1016.6797	1021.4447	1026.2640
1055.3591	1063.7955	1083.7802
1098.2414	1114.3802	1144.8488
1177.3339	1184.5128	1190.3473
1196.8322	1212.7034	1226.7328
1241.9576	1264.6889	1301.3898
1325.1883	1347.9888	1348.8711
1360.6565	1370.9229	1403.5402
1494.6379	1500.6488	1507.4627
1513.2696	1545.0091	1640.6526
1662.2760	1673.7336	1684.8850
1692.1937	3033.0670	3055.3827
3104.8861	3172.8227	3178.9879
3179.2303	3186.8293	3191.0064
3198.5602	3200.8830	3211.5996
3213.2316	3213.5012	3238.6076

i2

C	3.035886	1.631420	0.084096
C	1.859766	2.084698	0.674781
C	3.173517	0.298328	-0.290012
C	2.109506	-0.565962	-0.068896
C	0.793860	1.215478	0.900769
C	0.921717	-0.108299	0.519096
C	1.962238	-1.999169	-0.342589

C	0.749411	-2.404857	0.048817
C	-0.049020	-1.262595	0.630760
C	-1.417602	-1.050047	-0.088620
H	-0.270324	-1.466115	1.686070
C	-1.184409	-0.679163	-1.528856
C	-2.301469	-0.062156	0.666691
H	-1.917079	-2.026281	-0.065521
C	-1.538251	0.501122	-2.037069
C	-2.575195	1.231603	0.044707
C	-2.220373	1.498178	-1.219343
C	-2.806492	-0.365835	1.867369
H	-2.637106	-1.332319	2.331232
H	-3.411849	0.345405	2.418605
H	-3.104133	1.970174	0.638979
H	-2.449931	2.462738	-1.658229
H	-0.659951	-1.407415	-2.138343
H	-1.318384	0.739388	-3.071617
H	2.731281	-2.619310	-0.785858
H	0.356749	-3.411270	-0.029583
H	3.853789	2.323848	-0.081535
H	4.093313	-0.056341	-0.742518
H	1.772169	3.125914	0.964120
H	-0.117076	1.575112	1.363989

Frequencies[1/cm]

44.5212	50.6827	85.5087
109.4795	182.7147	207.3145
258.6342	273.1841	371.6313
387.5165	421.2270	436.4210
479.4755	516.8815	521.3015
555.7477	579.3858	595.3515
626.8496	687.8083	719.9499
738.9086	751.1531	767.8268
789.1085	800.1236	806.4246
842.2264	849.9472	878.8398
899.6977	919.2178	942.5031
965.2330	970.3175	983.0958
987.7953	1007.0908	1009.7213
1012.8128	1015.8625	1054.6036
1059.0194	1071.0698	1095.6681
1145.6783	1184.9203	1192.0486
1195.6758	1207.3495	1221.0534
1237.1161	1246.1859	1302.4797
1325.0672	1332.4844	1353.8198
1368.7931	1399.9988	1403.5232
1441.6805	1475.0154	1508.1402
1514.0134	1641.5837	1667.0129

1674.5138	1693.7016	1695.4918
1749.6790	3034.8585	3047.6492
3147.7583	3176.4042	3182.8253
3184.4976	3193.9132	3199.9901
3205.9575	3206.4045	3210.9723
3216.8372	3230.6812	3234.9366

i3

C	4.595682	-0.098456	-0.000089
C	3.974989	-1.342253	-0.000197
C	2.580378	-1.445625	-0.000146
C	1.828830	-0.283740	0.000017
C	2.461259	0.985016	0.000131
C	3.842137	1.079360	0.000073
C	0.389264	-0.054532	0.000080
C	0.179303	1.329075	0.000216
C	1.408290	1.984058	0.000323
C	-0.635401	-1.144822	0.000010
C	-2.058194	-0.645199	-0.000029
C	-2.719593	-0.386746	1.198767
C	-4.014691	0.116024	1.201102
C	-4.666058	0.369003	-0.000098
C	-4.014394	0.116613	-1.201269
C	-2.719304	-0.386155	-1.198864
H	5.678278	-0.041082	-0.000127
H	4.579135	-2.242358	-0.000325
H	2.104855	-2.421192	-0.000241
H	4.335342	2.045577	0.000172
H	-0.791328	1.804723	0.000270
H	1.560934	3.054955	0.000459
H	-0.464427	-1.786751	0.873709
H	-0.464362	-1.786707	-0.873708
H	-2.212124	-0.578491	2.139032
H	-4.516442	0.309263	2.142660
H	-5.677334	0.759451	-0.000128
H	-4.515920	0.310316	-2.142853
H	-2.211597	-0.577439	-2.139095

Frequencies[1/cm]

15.5004	28.3186	61.1995
123.7806	160.0706	206.3906
241.8462	301.3965	340.5080
417.9820	420.2666	444.4282
489.0890	551.3778	559.3277
567.4439	595.9376	637.0691
641.0023	704.0299	723.6114
732.4089	767.2173	769.5178

788.3183	807.8787	844.8420
871.5741	874.2679	884.6867
905.2148	934.5280	948.0252
963.8227	1000.6259	1002.7253
1022.2286	1026.5162	1030.1483
1046.1513	1050.6086	1064.1036
1106.9716	1113.2459	1185.2092
1187.0197	1197.3389	1199.1696
1210.5010	1213.2373	1240.3508
1284.4352	1327.3198	1344.4959
1348.6731	1364.2799	1382.1765
1442.7862	1467.2192	1481.8027
1499.5519	1506.8403	1517.7299
1546.3154	1656.5436	1662.1368
1663.3387	1685.9109	3022.4537
3054.6335	3178.9454	3180.8114
3181.2487	3187.8756	3192.6084
3198.9840	3202.3173	3212.6302
3214.2629	3228.1812	3247.6894

i4

C	-1.993689	2.422519	-0.037057
C	-0.669480	2.207825	-0.093473
C	-0.085198	0.845336	-0.330326
C	-1.122261	-0.211583	-0.229341
C	-2.553381	0.064953	-0.206207
C	-2.973787	1.339746	-0.098379
C	-0.927016	-1.519039	0.020940
C	-2.247448	-2.157101	0.122649
C	-3.217676	-1.224376	-0.035802
C	0.438235	-2.085257	0.269840
C	1.496245	-1.008417	0.158715
C	2.732293	-1.271918	-0.350764
C	3.737640	-0.285102	-0.448438
C	3.480109	1.023754	0.020518
C	2.266540	1.358824	0.529963
C	1.120169	0.398757	0.577107
H	-2.366041	3.435463	0.071826
H	0.011989	3.051781	-0.061708
H	0.316262	0.876183	-1.356404
H	-4.026562	1.582321	0.006929
H	-2.407720	-3.210965	0.313420
H	-4.285998	-1.380267	0.004993
H	0.671887	-2.902262	-0.421866
H	0.462685	-2.525151	1.278240
H	2.955337	-2.280485	-0.688001

H	4.706575	-0.536709	-0.861255
H	4.271148	1.765624	-0.015837
H	2.095230	2.359865	0.911864
H	0.707441	0.371084	1.598136

Frequencies[1/cm]

56.2167	79.9875	152.4610
192.7653	222.1617	261.4165
309.1673	348.0789	362.9061
395.8012	446.3581	482.8462
491.6947	542.9340	553.3830
573.6195	610.5197	623.9796
640.1590	668.8583	698.7581
726.6363	745.2720	755.2444
787.8501	793.3614	804.7380
880.0691	905.5326	937.7465
947.4171	954.8706	975.0598
985.1516	990.6715	1007.2706
1013.8829	1021.2108	1026.4614
1052.2332	1089.9913	1107.8368
1131.8744	1156.4016	1171.5767
1180.5838	1192.1998	1209.5869
1211.8558	1214.4233	1265.8395
1291.1125	1311.7027	1330.0294
1336.8909	1362.6068	1391.4513
1426.0484	1432.6258	1443.8424
1456.2234	1471.0187	1555.3590
1561.5406	1631.1572	1641.4813
1716.3243	1737.0324	2971.4755
2985.8731	2997.2135	3059.7166
3168.5883	3175.3802	3179.0819
3189.2214	3195.6169	3204.4880
3215.7316	3216.1903	3248.8372

i5

C	1.507685	-0.493009	-0.387739
C	1.923960	0.933033	-0.108513
C	0.692551	1.761865	0.200007
C	-0.324102	0.685951	0.460180
C	0.318540	-0.661909	0.607890
C	-1.640785	0.518469	0.199326
C	-1.935395	-0.929207	0.195225
C	-0.790918	-1.633198	0.384702
C	-3.295001	-1.358632	-0.033719
C	-4.240996	-0.433312	-0.298729
C	-3.935403	0.985406	-0.354427
C	-2.691554	1.453180	-0.118224

C	3.228442	1.292795	0.001146
C	4.254757	0.323635	-0.107177
C	3.923085	-1.049323	-0.225317
C	2.633423	-1.470041	-0.322817
H	0.395126	2.394861	-0.645213
H	0.861901	2.425279	1.055184
H	-0.704378	-2.707351	0.477774
H	-3.538370	-2.414875	0.000938
H	-5.264638	-0.742303	-0.480266
H	-4.740372	1.673718	-0.587084
H	-2.477079	2.515911	-0.149387
H	3.490347	2.323465	0.222040
H	5.292585	0.623655	-0.032621
H	4.724049	-1.781515	-0.224232
H	2.399844	-2.526104	-0.409293
H	1.050536	-0.541752	-1.393734
H	0.740727	-0.797209	1.615003

Frequencies[1/cm]

44.9252	80.4311	134.7905
153.4238	212.8148	230.9120
281.3434	349.8646	373.8055
434.9903	458.5956	484.4967
504.6791	531.0480	556.3124
568.7136	583.8800	628.7628
657.6511	684.5856	721.0128
729.3057	754.2899	767.9657
777.1430	797.4282	816.0522
861.5086	884.5386	891.2939
923.6040	947.8814	982.3616
987.8067	990.2159	999.9159
1005.0378	1016.2883	1032.4635
1046.3958	1075.8095	1116.5963
1120.4268	1154.7198	1160.4612
1166.3107	1186.6792	1192.8440
1204.3078	1217.0574	1243.7083
1257.5954	1274.6052	1314.1445
1322.4090	1346.6504	1396.6197
1408.0331	1411.8673	1438.9750
1469.1491	1472.6665	1562.8331
1591.0991	1617.1998	1634.1230
1666.7724	1741.1662	2924.4417
3024.5803	3027.8381	3063.9814
3173.7791	3176.9012	3181.4014
3188.9522	3195.0625	3202.4518
3211.2516	3215.8853	3231.0142

i6

C	1.630291	-0.504096	0.300364
C	1.903726	0.863785	0.174613
C	0.729624	1.711394	0.644825
C	-0.332072	0.654998	0.751333
C	0.276594	-0.703536	0.948911
C	-1.590462	0.509836	0.280350
C	-1.879705	-0.934640	0.154592
C	-0.777205	-1.656404	0.470374
C	-3.188369	-1.342092	-0.301602
C	-4.079768	-0.398021	-0.668190
C	-3.767396	1.019609	-0.609093
C	-2.577093	1.466337	-0.156852
C	3.115299	1.287129	-0.348175
C	4.048976	0.336260	-0.753170
C	3.772120	-1.021352	-0.633604
C	2.559023	-1.450074	-0.100647
H	0.472597	2.500352	-0.066768
H	0.952380	2.192414	1.605568
H	-0.705830	-2.734464	0.521426
H	-3.434974	-2.396763	-0.354978
H	-5.062484	-0.689714	-1.022291
H	-4.524472	1.724385	-0.934643
H	-2.360219	2.527619	-0.103571
H	3.330918	2.345272	-0.454041
H	4.996254	0.656936	-1.171944
H	4.504818	-1.750799	-0.959959
H	2.342860	-2.508857	-0.008059
H	0.426659	-0.901179	2.025081

Frequencies[1/cm]

44.7232	109.1523	141.9290
166.8839	245.0655	254.3292
273.7873	370.7361	418.9616
435.3241	475.6620	496.8232
516.3212	546.0099	559.5951
586.4664	617.7687	679.6148
702.9527	720.2792	745.2804
757.6060	768.9110	777.1327
798.3199	832.9107	848.9428
862.3308	895.2004	905.0239
937.8956	976.2389	987.3990
1000.1988	1012.2829	1013.2067
1016.3242	1041.6903	1059.0703
1105.0864	1121.0229	1155.3382
1178.0708	1186.7561	1188.5564

1190.8522	1202.7604	1214.1000
1241.1005	1249.2937	1287.8682
1314.6145	1330.0321	1354.7700
1395.7213	1410.3900	1471.9148
1480.6018	1507.0167	1524.4829
1596.6373	1621.1338	1656.5701
1671.4138	1687.1998	1744.2552
2979.6435	3030.1486	3093.5794
3181.6649	3181.7165	3188.8695
3189.3305	3199.5895	3202.8203
3211.5332	3212.2578	3231.9258

i7

C	-2.032799	2.368014	-0.159578
C	-0.775013	2.203644	0.279912
C	-0.236191	0.861456	0.697549
C	-1.174352	-0.221756	0.317674
C	-2.541811	-0.003096	-0.128052
C	-2.955511	1.254447	-0.372335
C	-0.880478	-1.526921	0.222285
C	-2.092976	-2.225503	-0.227376
C	-3.089452	-1.326400	-0.419474
C	0.513999	-2.001994	0.462869
C	1.516582	-0.889548	0.172650
C	2.815867	-1.236730	-0.190885
C	3.775445	-0.272688	-0.464678
C	3.437595	1.069989	-0.379376
C	2.146683	1.431744	-0.018994
C	1.177752	0.471541	0.259441
H	-2.388936	3.367682	-0.383689
H	-0.152124	3.078044	0.433449
H	-3.942262	1.462850	-0.773368
H	-2.162224	-3.292810	-0.396265
H	-4.091490	-1.528717	-0.768788
H	0.749661	-2.873088	-0.155517
H	0.636176	-2.326166	1.506067
H	3.076549	-2.288094	-0.266025
H	4.778207	-0.569909	-0.749771
H	4.172953	1.836242	-0.596727
H	1.895042	2.484338	0.038745
H	-0.203588	0.912434	1.802093

Frequencies[1/cm]

47.9954	100.0414	171.3514
208.4469	219.3563	265.5545
303.1603	370.9006	398.6879
439.7770	447.6400	477.2554

518.0898	546.9552	571.7180
592.3573	635.5847	653.2296
671.9533	713.9708	721.1749
743.7861	758.1729	768.5219
805.9826	825.4752	860.6882
888.8594	909.5763	937.4025
952.4291	959.9895	981.3679
998.6994	1011.0437	1014.1966
1023.5510	1059.4993	1084.7656
1100.6373	1145.5340	1150.9484
1185.8475	1193.8696	1200.3629
1210.0524	1219.3651	1230.5695
1248.4231	1274.6592	1305.8228
1316.0383	1343.7672	1362.7432
1397.9599	1433.0294	1461.1640
1478.5214	1500.5667	1532.4206
1554.7494	1641.7649	1650.8432
1684.8645	1727.6266	1741.4598
2936.2101	3010.7442	3081.3123
3175.8737	3180.2509	3189.1216
3192.6965	3201.8525	3207.4996
3214.9209	3216.9146	3249.9053

i8

C	-2.668777	1.811053	-0.116568
C	-1.393848	2.079905	0.409938
C	-0.518938	1.016890	0.601445
C	-1.015130	-0.233515	0.345175
C	-2.190246	-0.528980	-0.321283
C	-3.068176	0.536429	-0.530364
C	-0.086528	-1.349716	0.340929
C	-0.773548	-2.360044	-0.498009
C	-2.010789	-1.906953	-0.816737
C	0.768947	-1.564220	1.563489
C	1.296559	-0.622951	0.529501
C	2.474862	-0.970501	-0.280037
C	3.160680	-0.036483	-0.944007
C	2.767525	1.372996	-0.894405
C	1.773219	1.802894	-0.117338
C	0.995438	0.889537	0.791670
H	-3.343802	2.644046	-0.280595
H	-1.099546	3.107565	0.594747
H	-4.013319	0.408937	-1.046443
H	-0.390027	-3.346575	-0.721595
H	-2.747014	-2.464137	-1.382097
H	1.255533	-2.532459	1.627877

H	0.422013	-1.162916	2.511189
H	2.751254	-2.018566	-0.340974
H	4.017310	-0.314556	-1.547257
H	3.307069	2.077225	-1.518327
H	1.498691	2.853012	-0.104993
H	1.274341	1.130377	1.828064

Frequencies[1/cm]

74.5625	86.4614	168.4268
213.7074	230.8084	315.2553
356.0301	388.4864	416.1491
463.0237	481.0060	496.1224
508.1808	554.0982	576.4670
597.6510	618.4141	635.2150
656.5852	707.6654	739.4903
754.7701	782.3313	788.4647
805.0896	816.0768	847.2950
874.9972	915.2232	916.5792
942.8922	956.3506	966.1424
980.2604	990.6299	997.5634
1008.7374	1013.6131	1051.2715
1064.7562	1084.7543	1091.6653
1116.5198	1141.5289	1188.1617
1194.0253	1208.1157	1230.4928
1245.4290	1269.5310	1297.8618
1306.3387	1339.1761	1361.6403
1371.1410	1405.4508	1418.2625
1461.0039	1492.4505	1504.3011
1518.7210	1580.7797	1666.4573
1683.6282	1707.3343	1742.6205
3003.4101	3117.8929	3174.8143
3178.9733	3181.3410	3193.5426
3196.9015	3206.6309	3209.4088
3210.3819	3215.1169	3238.2389

i9

C	-3.577915	-0.983450	-0.921513
C	-2.546578	-1.895359	-0.714771
C	-3.444291	0.343426	-0.522824
C	-2.261497	0.737437	0.088724
C	-1.360378	-1.501139	-0.097222
C	-1.230412	-0.185724	0.308801
C	-1.820646	2.043540	0.590190
C	-0.582952	1.938063	1.085834
C	-0.074888	0.517451	0.996657
C	1.252974	0.336438	0.289418
H	0.012339	0.140390	2.023174

C	1.622461	1.217974	-0.714709
C	2.112642	-0.761517	0.608686
C	2.818448	1.073482	-1.412721
C	3.332496	-0.876512	-0.114844
C	3.677905	0.019003	-1.101967
C	1.805003	-1.724513	1.582603
H	0.886812	-1.710623	2.153733
H	2.499454	-2.531441	1.782333
H	3.995603	-1.701006	0.125558
H	4.613563	-0.097891	-1.636847
H	0.956446	2.038288	-0.960070
H	3.078139	1.780258	-2.192126
H	-2.421104	2.944005	0.562084
H	0.002023	2.735297	1.525921
H	-4.492541	-1.310015	-1.403653
H	-4.246481	1.053786	-0.691204
H	-2.665523	-2.922287	-1.041307
H	-0.552950	-2.210365	0.050342

Frequencies[1/cm]

48.9822	65.2973	83.0357
155.2090	211.3406	228.6196
272.3911	285.8413	386.5475
408.1705	428.7230	451.5796
470.0771	491.2469	537.6103
555.0388	566.7314	592.3952
617.0602	652.5541	712.2915
731.1500	747.9605	753.5362
768.0231	782.5833	795.6538
849.2319	860.5676	877.8763
886.6764	899.9760	915.5176
971.8223	974.6499	984.7623
987.2414	1001.7581	1011.6380
1027.8149	1060.0036	1073.4573
1095.7125	1137.9512	1143.2698
1181.1391	1182.8472	1190.0974
1192.5724	1227.3786	1246.4911
1278.1731	1301.8128	1315.3572
1322.6910	1341.6321	1350.2833
1398.7805	1471.4917	1504.1649
1507.3295	1513.8250	1517.0541
1597.8571	1634.3954	1641.8539
1674.1335	1691.4111	3050.4485
3170.7880	3182.6671	3183.4554
3190.1806	3191.6144	3200.7877
3201.1380	3212.3951	3212.7866
3214.6170	3236.8383	3270.4551

i10

C	2.572129	0.740799	0.684909
C	3.930359	1.024293	0.649596
C	4.811612	0.155521	0.017304
C	4.328128	-1.009658	-0.567197
C	2.971991	-1.296950	-0.526209
C	2.069552	-0.416276	0.080050
C	0.639641	-0.751538	0.093533
C	-0.395931	0.092795	-0.042159
C	-0.385684	1.535140	-0.333998
C	-1.650326	1.987205	-0.419959
C	-2.448344	-1.492982	0.282535
C	-1.824240	-0.282744	0.033327
C	-2.583149	0.880779	-0.186012
C	-3.968988	0.835858	-0.163510
C	-3.841287	-1.537008	0.302094
C	-4.592447	-0.385523	0.081987
H	4.303580	1.922272	1.128882
H	1.896051	1.402416	1.213247
H	5.872103	0.378346	-0.008290
H	5.010553	-1.698239	-1.052304
H	2.598736	-2.208379	-0.981848
H	0.509362	2.116429	-0.499472
H	-1.949023	3.002247	-0.646835
H	-1.873189	-2.395630	0.460780
H	-4.557770	1.731039	-0.331983
H	-4.345576	-2.477645	0.492027
H	-5.675017	-0.441237	0.103636
H	0.412091	-1.809887	0.204411

Frequencies[1/cm]

44.6662	50.7227	84.0327
143.7314	179.4625	208.6344
271.9273	310.2891	366.6721
420.3569	430.9868	444.9487
512.0919	552.2774	578.3539
591.5078	637.9186	653.4943
665.3013	720.6899	732.6710
750.3809	775.5172	777.6445
822.9683	824.0929	855.1689
874.8024	878.8325	897.5012
917.3887	959.5365	965.6124
976.8777	1007.1392	1007.9226
1023.8041	1026.4728	1050.2373
1056.9602	1064.9114	1102.8946
1117.2811	1143.5095	1186.5426

1188.9164	1212.9956	1214.3978
1228.6650	1270.5312	1306.7665
1334.6403	1347.2964	1357.7211
1371.0192	1424.9744	1492.1592
1504.8629	1509.2921	1542.5578
1612.9124	1650.8950	1666.5497
1680.2283	1688.0411	1735.6127
3155.8654	3181.8433	3183.1358
3188.5784	3190.6209	3199.7415
3200.8443	3210.2922	3212.7052
3217.9922	3224.9676	3255.8744

i11

C	4.432761	-0.832689	0.020914
C	3.520606	-1.764090	-0.468432
C	4.023818	0.451877	0.367772
C	2.684717	0.787000	0.214087
C	1.770295	-0.149626	-0.285594
C	2.177005	-1.426745	-0.625416
C	1.956732	2.028417	0.498048
C	0.665565	1.873182	0.185013
C	0.396655	0.476422	-0.352107
C	-0.640808	-0.251063	0.446812
H	0.082758	0.548941	-1.402111
C	-2.031232	-0.205717	0.208246
H	-0.287230	-0.795286	1.317272
C	-2.915131	-0.921157	1.058004
C	-4.279305	-0.902146	0.852909
C	-4.824945	-0.169084	-0.202411
C	-3.979497	0.546472	-1.048899
C	-2.611019	0.533784	-0.854312
H	5.473825	-1.113469	0.135121
H	3.859283	-2.760367	-0.729328
H	4.737409	1.172663	0.751966
H	1.465359	-2.153072	-1.004086
H	2.410548	2.924842	0.901469
H	-0.120396	2.608523	0.296465
H	-2.497757	-1.492473	1.880718
H	-4.930397	-1.459915	1.516834
H	-5.896759	-0.154784	-0.361367
H	-1.976404	1.104297	-1.522653
H	-4.397543	1.121083	-1.868093

Frequencies[1/cm]

20.8360	53.1385	60.8538
137.9409	165.2332	209.8765
237.5253	300.9053	355.5720

410.9926	417.0163	450.2892
484.5267	546.3221	561.2708
582.2969	588.3350	632.1004
644.9299	676.6580	697.4250
737.5053	756.0621	767.8691
780.1715	804.6088	841.3764
853.6046	878.5263	885.4770
912.1266	919.1527	968.8379
977.5867	990.9828	991.4770
1001.2122	1007.9089	1011.8242
1052.5767	1055.0197	1093.3040
1100.5900	1132.8255	1150.5773
1180.9918	1183.7557	1190.0751
1201.4988	1219.5242	1229.6901
1246.8993	1279.3493	1310.3166
1334.3936	1349.1602	1358.0489
1392.2403	1441.5861	1495.9916
1506.6225	1513.8102	1518.3537
1612.7829	1630.7925	1636.9556
1672.7485	1691.4990	3034.1494
3179.4736	3182.4870	3182.7880
3187.5624	3189.5826	3198.5993
3200.0606	3206.3031	3212.2376
3213.1842	3216.4505	3238.6896

il2

C	-4.208963	-0.372020	0.641802
C	-3.802290	-1.463882	-0.136758
C	-3.353104	0.708163	0.817889
C	-2.090943	0.727571	0.233739
C	-1.663123	-0.382018	-0.562023
C	-2.558974	-1.472690	-0.726852
C	-1.182088	1.850485	0.401359
C	0.037577	1.872013	-0.143448
C	-0.396522	-0.371782	-1.148935
C	0.593382	0.735862	-0.958920
H	-0.079805	-1.221372	-1.745603
C	1.885215	0.204493	-0.335370
C	3.092521	0.251108	-1.024209
C	4.257717	-0.242011	-0.445320
C	4.223182	-0.787114	0.830629
C	3.018673	-0.837405	1.525868
C	1.858665	-0.345321	0.946287
H	-5.188823	-0.369679	1.104522
H	-4.471111	-2.306092	-0.274394
H	-3.667849	1.555187	1.419563

H	-2.243624	-2.318761	-1.328554
H	-1.526743	2.693121	0.993414
H	3.123878	0.676386	-2.022733
H	5.192158	-0.199154	-0.993720
H	5.129891	-1.171956	1.283440
H	0.918408	-0.383641	1.487323
H	2.984995	-1.262141	2.522956
H	0.692362	2.724003	0.008586
H	0.870706	1.131383	-1.949233

Frequencies[1/cm]

25.8889	33.3535	78.4651
164.3413	178.8941	254.8430
277.0532	301.7629	372.4110
407.2668	417.8286	459.0035
508.2670	530.6318	540.7754
561.5083	617.3910	637.7043
645.4689	711.7996	721.8860
726.5238	761.2490	771.8012
785.6527	799.3693	825.5870
861.8833	871.3444	879.1400
914.7115	942.8036	962.0392
964.2868	996.3867	1001.1924
1011.8978	1022.0591	1025.9144
1055.8258	1064.0392	1096.3964
1114.9635	1148.9414	1167.3845
1185.7999	1187.6872	1208.7873
1212.5655	1218.9718	1238.5134
1259.5039	1304.3005	1340.9221
1344.7105	1348.4569	1366.9396
1419.2498	1441.0309	1471.6888
1498.9361	1518.4488	1540.7167
1593.7148	1633.7920	1662.9358
1680.0043	1710.8355	2973.6677
3171.4645	3176.2192	3179.4958
3182.7805	3182.8364	3185.2006
3192.2343	3195.5728	3199.2430
3201.8166	3213.5485	3213.9493

il3

C	-4.552720	-0.066811	-0.036538
C	-4.057056	-1.362779	-0.305798
C	-3.687893	0.969503	0.185387
C	-2.286241	0.762658	0.149795
C	-1.787513	-0.539020	-0.116569
C	-2.709436	-1.592453	-0.345540
C	-1.358428	1.811055	0.371841

C	-0.013304	1.579008	0.330108
C	-0.387221	-0.746688	-0.152442
C	0.498599	0.280363	0.065605
H	-0.015830	-1.740850	-0.381049
C	1.963922	0.050514	0.024234
C	2.810949	0.960583	-0.612824
C	4.181137	0.742675	-0.659845
C	4.729752	-0.388798	-0.068442
C	3.897836	-1.299947	0.570780
C	2.527717	-1.081283	0.617702
H	-5.623211	0.101634	-0.007747
H	-4.752560	-2.175655	-0.481193
H	-4.064514	1.966171	0.391396
H	-2.326596	-2.586496	-0.552589
H	-1.734069	2.806377	0.585917
H	2.388657	1.835605	-1.095176
H	4.821709	1.455900	-1.166328
H	5.799755	-0.558656	-0.104091
H	1.886441	-1.783483	1.139321
H	4.317982	-2.180735	1.043272
H	0.681641	2.388715	0.523543

Frequencies[1/cm]

54.8916	63.8000	92.7118
173.9251	190.2558	263.6119
279.8029	345.1020	404.2909
420.9419	436.1012	493.2941
522.1163	533.0279	561.7832
574.9971	636.6761	646.0921
678.2196	715.7208	723.8703
764.9968	786.7520	794.8003
800.0251	848.9211	872.8071
877.5101	888.1944	929.1909
953.7573	964.3840	987.8221
1001.9301	1004.6076	1017.6793
1022.6264	1025.1049	1048.5319
1057.8254	1078.2263	1116.8036
1166.2285	1172.0459	1188.5449
1194.3949	1215.8289	1225.2296
1265.0814	1299.3283	1311.5712
1325.6429	1359.4989	1391.7690
1412.7241	1434.5990	1475.9227
1498.0770	1514.1172	1548.8799
1567.6020	1645.7921	1657.9919
1678.4588	1685.2151	1717.0938
3181.0159	3182.7051	3183.6213
3184.6507	3186.4345	3188.8954

3197.6704	3199.9741	3203.9220
3205.3609	3213.1797	3215.5777

i14

C	2.163682	2.364076	0.000032
C	0.787388	2.165517	0.000053
C	0.254818	0.865689	-0.000071
C	1.173156	-0.168801	-0.000026
C	2.571358	0.009364	-0.000178
C	3.075877	1.296021	-0.000025
C	0.878637	-1.563396	0.000121
C	2.110431	-2.255877	0.000015
C	3.145206	-1.332039	-0.000110
C	-0.536147	-2.015078	0.000261
C	-1.542518	-0.870890	-0.000058
C	-2.895409	-1.204724	-0.000202
C	-3.884028	-0.233768	-0.000177
C	-3.524149	1.108585	0.000050
C	-2.185125	1.458720	0.000133
C	-1.175531	0.490676	0.000011
H	2.544248	3.379380	0.000114
H	0.137986	3.032667	0.000031
H	4.142611	1.491440	-0.000133
H	2.229697	-3.330771	0.000248
H	4.202027	-1.562002	-0.000266
H	-0.727800	-2.653330	0.873065
H	-0.727812	-2.654182	-0.871871
H	-3.175299	-2.254131	-0.000331
H	-4.928909	-0.522112	-0.000325
H	-4.285441	1.880090	0.000177
H	-1.917166	2.508502	0.000313

Frequencies[1/cm]

54.4053	99.1768	178.4657
194.8344	247.2945	260.8878
301.7676	380.4895	412.0157
437.9376	470.1725	478.5588
546.2017	565.0766	584.1508
595.1897	620.1471	634.6556
684.5910	727.0157	736.6226
745.2680	771.8312	779.4009
819.1958	832.0902	838.0756
880.1102	899.7522	924.3537
927.2749	941.7533	978.1043
988.7907	1012.5129	1045.4140
1062.9871	1079.7546	1085.0940
1097.9323	1155.9173	1185.0274

1191.3637	1201.9164	1210.5995
1212.8554	1257.5345	1286.3612
1308.5846	1323.9710	1328.6393
1366.3387	1397.6169	1430.0631
1446.3378	1481.6491	1501.5013
1510.9704	1520.4703	1554.4107
1635.1591	1657.2896	1679.6419
1688.8238	3014.6103	3040.3558
3174.0594	3187.0043	3192.7774
3200.5051	3206.2944	3213.2163
3218.6789	3224.6286	3243.2101

i15

C	2.252701	2.306331	0.063706
C	0.872488	2.172732	0.154829
C	0.278878	0.895856	0.146995
C	1.152964	-0.175225	0.057082
C	2.538010	-0.062310	-0.069667
C	3.107488	1.201716	-0.059610
C	0.773816	-1.575825	-0.013182
C	2.028727	-2.312258	-0.214921
C	3.054312	-1.433107	-0.232682
C	-0.505813	-1.919978	0.154026
C	-1.531977	-0.859018	0.503556
C	-2.925430	-1.211082	0.066722
C	-3.830672	-0.261411	-0.256744
C	-3.464919	1.113637	-0.304434
C	-2.130068	1.485878	-0.142782
C	-1.140165	0.571681	0.154507
H	2.682120	3.301976	0.082384
H	0.260586	3.063094	0.245134
H	4.178135	1.346806	-0.150027
H	2.106553	-3.386457	-0.309928
H	4.099574	-1.685295	-0.354203
H	-0.840071	-2.953444	0.130797
H	-3.203704	-2.259995	0.084014
H	-4.844813	-0.547978	-0.513431
H	-4.207785	1.860638	-0.555413
H	-1.852617	2.519406	-0.322271
H	-1.560014	-0.884470	1.618552

Frequencies[1/cm]

68.8206	91.7349	171.4863
212.8160	253.5399	261.0655
345.3801	377.8447	397.8954
449.2086	461.4391	486.4063
534.6565	568.3629	569.1573

607.3382	627.9134	642.6169
665.8978	688.4852	724.9893
756.9206	769.6786	786.0665
792.6810	825.3569	840.8866
852.4483	915.0863	919.8383
926.2492	940.8613	969.4712
984.4461	994.5122	1020.7032
1035.4319	1063.8398	1082.5426
1096.7829	1116.8711	1124.4017
1142.2003	1190.9980	1202.3676
1213.0424	1237.1279	1251.3800
1281.9454	1304.0370	1343.4105
1349.8840	1365.6123	1401.0276
1413.8749	1434.1409	1490.4472
1518.2673	1541.1523	1594.1956
1635.4369	1667.3406	1671.1036
1750.7323	2809.2865	3176.2760
3178.9154	3184.2953	3187.7615
3197.3035	3200.2698	3210.8454
3216.9588	3222.7539	3246.0212

il6

C	2.208556	2.319372	-0.051349
C	0.833157	2.156782	0.121957
C	0.281271	0.874706	0.184131
C	1.159561	-0.179823	0.073087
C	2.543495	-0.045520	-0.099598
C	3.080934	1.231372	-0.162999
C	0.812143	-1.580384	0.082120
C	2.053062	-2.303469	-0.068902
C	3.078480	-1.408405	-0.177236
C	-0.523003	-1.932260	0.105314
C	-1.511801	-0.939832	0.166800
C	-1.166313	0.515776	0.466621
C	-2.195982	1.479389	-0.053004
C	-3.452162	1.084985	-0.316740
C	-3.827607	-0.302166	-0.216986
C	-2.877942	-1.264685	-0.014102
H	2.612509	3.324640	-0.098109
H	0.209387	3.038855	0.215073
H	4.144446	1.396646	-0.295648
H	2.146191	-3.380326	-0.100532
H	4.123361	-1.657702	-0.305699
H	-0.832920	-2.968946	0.008095
H	-1.254091	0.581233	1.573085
H	-1.916431	2.522126	-0.146020

H	-4.194486	1.807911	-0.636020
H	-4.859681	-0.585665	-0.386383
H	-3.153368	-2.313800	-0.062518

Frequencies[1/cm]

62.3839	92.2535	193.4821
213.4372	237.7764	270.2185
366.5704	388.3235	402.0544
442.0859	464.8803	491.4706
530.0505	562.8230	577.5542
597.3505	626.5961	637.5736
660.8425	695.5762	739.1930
763.4776	778.7470	786.5521
810.8356	828.6356	834.1166
866.3692	914.5852	920.3192
923.7234	942.9407	972.3060
989.9688	994.4421	1008.1103
1037.3426	1063.2582	1071.5631
1079.8058	1114.2807	1137.3108
1182.7069	1189.5338	1202.1321
1224.5756	1243.9009	1256.0316
1290.6841	1313.3956	1347.3186
1353.7720	1371.2461	1397.5440
1404.0587	1442.7376	1486.8471
1509.2112	1527.6260	1544.2503
1579.3855	1664.5021	1678.6914
1692.5755	2862.7668	3176.3090
3179.0750	3184.0134	3189.4801
3196.4923	3207.4828	3209.8535
3217.4894	3223.5845	3244.1778

il7

C	-2.081285	2.342539	-0.260032
C	-0.769615	2.198802	0.044969
C	-0.222312	0.889925	0.558615
C	-1.179768	-0.192633	0.261510
C	-2.536634	-0.018499	-0.015253
C	-3.024080	1.253085	-0.245645
C	-0.847270	-1.563739	0.173390
C	-2.116214	-2.281250	-0.057211
C	-3.106447	-1.372478	-0.174485
C	0.461316	-1.933354	0.116563
C	1.499707	-0.909065	0.067300
C	2.827902	-1.288366	-0.167987
C	3.836879	-0.347769	-0.283524
C	3.533198	1.002919	-0.162891
C	2.223099	1.398712	0.078352

C	1.196865	0.469787	0.191686
H	-2.441876	3.321670	-0.557745
H	-0.115474	3.062374	0.007847
H	-4.060841	1.434802	-0.503356
H	-2.210531	-3.352868	-0.165783
H	-4.144892	-1.582587	-0.392051
H	0.760407	-2.970098	-0.000454
H	3.059215	-2.343969	-0.269055
H	4.856533	-0.664989	-0.469123
H	4.314412	1.748966	-0.252790
H	2.003880	2.455404	0.183790
H	-0.192884	0.999601	1.666584

Frequencies[1/cm]

71.0264	93.9597	185.8259
202.2184	227.4544	282.8478
362.1831	380.9028	399.3471
439.7214	454.1994	482.0633
538.3345	555.0105	583.0452
619.0302	625.3027	648.8207
667.8574	696.0505	729.3406
744.6283	768.5931	778.5779
804.2574	835.8169	848.5658
865.2801	873.1195	902.7805
910.8784	953.9968	973.2699
986.4007	1006.8876	1010.9550
1028.8032	1074.4781	1086.0992
1094.7651	1143.1170	1152.2733
1191.0253	1200.5209	1206.1178
1217.2624	1226.9879	1251.7005
1260.9039	1295.6699	1314.0690
1326.9633	1348.4956	1393.2493
1437.0290	1464.2728	1498.9817
1514.2377	1541.8836	1594.2051
1606.3933	1635.1609	1656.1658
1676.8385	2823.4037	3180.4345
3181.1811	3188.1632	3190.1921
3200.1902	3204.4186	3210.8913
3215.3305	3224.9148	3247.5379

i18

C	2.106340	2.374947	-0.193159
C	0.739332	2.170730	-0.024641
C	0.234416	0.879983	0.187212
C	1.166510	-0.137058	0.255639
C	2.519543	0.029546	-0.023001
C	3.012360	1.312746	-0.225893

C	0.846422	-1.579275	0.447732
C	2.143872	-2.242930	0.040869
C	3.098803	-1.317470	-0.143751
C	-0.494506	-1.896090	-0.121314
C	-1.493553	-0.897976	-0.103767
C	-2.850963	-1.242236	-0.327567
C	-3.856153	-0.305603	-0.230477
C	-3.548741	1.020327	0.087302
C	-2.224580	1.398797	0.269259
C	-1.185070	0.481534	0.162226
H	2.468280	3.383758	-0.357904
H	0.067943	3.017813	-0.107263
H	4.060431	1.491535	-0.438258
H	2.287377	-3.315478	0.020498
H	4.138644	-1.520100	-0.366657
H	-0.763584	-2.919147	-0.360381
H	-3.090968	-2.275549	-0.555928
H	-4.887137	-0.599835	-0.391008
H	-4.339127	1.755773	0.180721
H	-1.997354	2.434996	0.493994
H	0.771306	-1.753608	1.542167

Frequencies[1/cm]

88.3962	98.5115	197.8202
226.7883	228.4228	281.6469
328.5495	392.8295	410.0379
443.5394	470.4875	500.7222
551.8516	557.1398	584.2985
605.8238	629.0474	639.9734
674.6554	701.8593	723.6132
759.7057	767.1107	774.4959
805.7102	825.1861	854.3401
874.9369	884.8680	919.7849
935.4145	966.7158	975.6386
995.9956	999.4097	1008.4974
1062.4560	1079.1914	1086.2708
1108.7359	1123.8847	1159.8054
1166.0530	1174.9551	1197.7250
1204.5536	1231.4653	1262.6583
1298.9690	1315.0607	1321.7372
1329.6423	1357.5573	1388.2579
1416.5671	1453.9111	1497.6230
1505.5013	1533.8573	1595.8242
1628.2659	1640.1387	1677.7194
1686.6321	2889.9739	3181.6504
3185.7913	3190.5022	3192.6498
3199.3968	3202.1908	3211.2359

3213.1735 3215.3412 3236.5881

i19

C	1.848073	2.432634	0.039533
C	0.517781	2.094735	-0.010383
C	0.107016	0.748216	0.027777
C	1.095437	-0.265403	0.110175
C	2.471579	0.098331	0.106330
C	2.823087	1.434323	0.098915
C	0.674566	-1.633382	0.242586
C	3.665837	-1.983183	-0.627512
C	3.587172	-0.889404	0.089126
C	-0.631135	-1.973810	0.236410
C	-1.659180	-0.987326	0.088453
C	-3.017337	-1.362360	0.055188
C	-4.006739	-0.419739	-0.075435
C	-3.660077	0.935242	-0.176633
C	-2.340535	1.320860	-0.142793
C	-1.302195	0.375503	-0.008939
H	2.144295	3.475112	0.023974
H	-0.217200	2.886430	-0.066646
H	3.872864	1.707216	0.116974
H	3.068229	-2.530167	-1.342827
H	4.453160	-0.608219	0.691278
H	-0.925591	-3.011382	0.355235
H	-3.268694	-2.414998	0.134533
H	-5.048412	-0.718105	-0.101386
H	-4.435864	1.684792	-0.283506
H	-2.110248	2.374723	-0.228661
H	1.427350	-2.396819	0.384248

Frequencies[1/cm]

59.2648	88.0728	101.9309
155.3188	207.0235	239.5596
248.9788	280.6277	376.9649
414.4852	433.3233	448.3912
489.2855	511.3365	532.3713
541.9022	591.7353	596.9707
613.5372	670.3490	718.5760
733.5941	749.2468	775.6615
779.4427	833.4117	836.8911
849.1176	864.4445	891.7685
896.0396	898.3049	926.1967
945.1334	979.3194	1001.3823
1013.1752	1019.2811	1069.2266
1091.2465	1114.0961	1166.7586
1192.0598	1204.5620	1216.4940

1225.2271	1246.1262	1257.3368
1279.9306	1302.5651	1332.6062
1375.9677	1397.1566	1438.0491
1462.6628	1498.0524	1503.9049
1554.2475	1592.3062	1651.5602
1662.4001	1679.9499	1690.2057
1708.6720	3107.3803	3183.2762
3186.5498	3188.0395	3194.5898
3203.9980	3210.5581	3220.5963
3233.0570	3236.6121	3253.9184

i20

C	-2.638317	1.950103	-0.101038
C	-1.300985	2.178708	0.243237
C	-0.455977	1.074590	0.401970
C	-1.059785	-0.162215	0.299198
C	-2.318385	-0.427098	-0.201733
C	-3.155303	0.674648	-0.377614
C	-0.197595	-1.334320	0.282677
C	-1.038459	-2.359681	-0.387799
C	-2.275577	-1.849512	-0.600482
C	0.984638	0.825377	0.323531
C	1.234701	-0.656005	0.273718
C	0.719687	-1.474960	1.457494
C	2.006651	1.696131	0.025687
C	3.234917	1.214743	-0.441632
C	3.421342	-0.170272	-0.695719
C	2.460752	-1.085563	-0.393016
H	-3.287569	2.808326	-0.236393
H	-0.933473	3.196172	0.317382
H	-4.163280	0.576369	-0.764894
H	-0.742088	-3.383701	-0.570781
H	-3.105415	-2.399806	-1.025312
H	0.471293	-0.959197	2.379275
H	1.200478	-2.440090	1.578469
H	1.833493	2.766119	0.078461
H	4.027803	1.911603	-0.684696
H	4.350380	-0.500326	-1.147062
H	2.614551	-2.143507	-0.575312

Frequencies[1/cm]

82.0142	107.3441	169.5580
214.3438	251.2963	305.0377
347.7573	377.9229	424.8221
458.0156	470.5594	506.2861
519.8328	548.7526	582.0652
594.3385	631.4896	645.1831

669.1738	704.9699	724.7865
744.8982	760.2879	783.7615
795.1155	814.0965	824.3213
843.7861	908.8009	924.7327
934.9723	938.1696	955.4930
964.6995	978.6368	990.6475
1013.2736	1028.2695	1061.5996
1065.5138	1076.4259	1100.7535
1119.5485	1138.4759	1175.1883
1189.5757	1234.7679	1261.5658
1301.5442	1313.2366	1316.1087
1351.6719	1361.6961	1402.2020
1412.4834	1446.7830	1482.5293
1496.6175	1516.4075	1552.9398
1576.7257	1610.5522	1662.5981
1685.6948	3124.4286	3183.3914
3184.0202	3187.2352	3197.4968
3202.3000	3208.6590	3215.8040
3216.8604	3221.1742	3240.1085

i21

C	2.490436	-2.170502	-0.004284
C	1.099625	-2.329704	0.138499
C	0.308090	-1.180629	0.232638
C	0.976199	0.019372	0.237264
C	2.312851	0.231802	-0.104260
C	3.112821	-0.930664	-0.155898
C	0.110544	1.186761	0.143641
C	1.067192	2.252792	-0.431724
C	2.408903	1.585659	-0.524543
C	-1.125109	-0.826700	0.104438
C	-1.243209	0.583617	-0.034086
C	0.491084	2.399278	0.960675
C	-2.257447	-1.625709	0.056983
C	-3.501876	-1.028397	-0.126995
C	-3.615453	0.351977	-0.255543
C	-2.486013	1.166991	-0.199759
H	3.102563	-3.063366	-0.072127
H	0.670275	-3.325079	0.125438
H	4.172647	-0.882875	-0.378438
H	0.766214	2.973099	-1.183594
H	3.290779	2.081832	-0.907677
H	1.140828	2.265340	1.818838
H	-0.291942	3.140935	1.078292
H	-2.175986	-2.702116	0.161489
H	-4.392243	-1.645487	-0.168829

H -4.592553 0.798575 -0.400967
H -2.582421 2.243479 -0.294692

Frequencies[1/cm]

100.2717	124.9826	150.7943
207.2241	251.4337	299.8525
352.1835	392.6350	413.8585
450.9476	483.8239	522.7946
524.1589	553.8298	589.2301
598.8047	626.1031	654.1013
671.0166	702.0493	753.9527
765.3741	773.5142	780.5781
822.5272	830.0738	863.0687
886.5603	892.5951	907.1089
941.7131	955.7755	970.2633
985.3307	1010.0646	1017.9530
1042.6045	1050.7419	1060.4667
1069.8731	1083.8224	1094.4150
1135.7606	1160.2808	1185.2193
1189.7933	1210.3890	1262.5539
1277.9056	1313.9805	1320.0226
1347.3044	1360.0979	1377.1875
1387.5473	1471.4724	1483.5734
1493.2107	1508.2799	1526.7850
1621.9365	1647.3598	1658.1720
1691.4505	3128.5540	3182.5934
3184.6130	3185.2946	3189.7179
3200.0658	3200.6576	3209.8732
3212.9889	3225.3565	3227.6966

i22

C	2.107113	2.486778	-0.000004
C	0.703870	2.442616	0.000006
C	0.082322	1.208157	0.000014
C	0.884753	0.047755	0.000018
C	2.281584	0.073885	0.000002
C	2.888857	1.328990	-0.000007
C	0.093079	-1.116018	0.000013
C	2.244007	-2.370499	-0.000013
C	2.944320	-1.227412	-0.000012
C	-1.310494	0.736585	0.000004
C	-1.283157	-0.690521	0.000007
C	0.734632	-2.458401	0.000008
C	-2.516472	1.411073	-0.000005
C	-3.703621	0.675626	-0.000011
C	-3.681379	-0.718038	-0.000009
C	-2.475557	-1.411654	0.000001

H	2.600243	3.452313	-0.000014
H	0.134769	3.365807	0.000005
H	3.970805	1.410563	-0.000020
H	2.775316	-3.316952	-0.000023
H	4.029297	-1.258698	-0.000025
H	0.405249	-3.046848	0.869817
H	0.405219	-3.046861	-0.869779
H	-2.546542	2.495389	-0.000007
H	-4.654772	1.195616	-0.000017
H	-4.615994	-1.267383	-0.000015
H	-2.466717	-2.496484	0.000001

Frequencies[1/cm]

91.2557	121.2968	144.2076
194.2134	202.4714	283.3080
347.0775	354.0205	414.6463
435.9864	465.7470	492.5388
537.7739	549.6831	565.2845
585.9667	608.3479	622.3095
681.1706	719.6871	764.5438
772.3325	774.0278	785.9243
799.3420	832.9525	890.4494
898.8629	930.4609	932.4976
942.8073	964.2868	982.6291
986.0419	1002.5068	1011.7061
1051.4897	1055.8164	1089.6457
1114.2280	1143.8959	1178.1123
1186.7514	1194.4085	1207.8899
1240.0676	1252.4065	1299.9583
1321.7547	1331.0658	1383.5610
1391.0931	1409.5096	1426.5129
1445.3523	1465.2610	1501.5043
1513.5657	1538.9916	1623.3169
1640.3007	1653.7370	1665.6308
1705.0668	2991.4754	3006.2587
3175.5805	3183.2332	3183.9398
3189.4381	3194.0758	3196.9655
3200.4000	3209.3607	3213.4921

i23

C	2.152100	2.429017	-0.071534
C	0.754845	2.395045	-0.024105
C	0.129961	1.160518	0.130109
C	0.912055	0.024331	0.272387
C	2.293217	0.013704	0.102234
C	2.916300	1.267602	-0.037785
C	0.085700	-1.202667	0.475067

C	2.090524	-2.403239	-0.323267
C	2.904252	-1.273201	-0.096394
C	-1.273762	0.714339	0.064153
C	-1.307848	-0.689548	0.168964
C	0.726167	-2.395250	-0.164788
C	-2.447127	1.431936	-0.121531
C	-3.650930	0.739763	-0.214517
C	-3.681760	-0.648088	-0.117079
C	-2.507827	-1.371558	0.087385
H	2.652186	3.384176	-0.187242
H	0.182837	3.309743	-0.131691
H	3.992504	1.325058	-0.162867
H	0.082857	-1.410311	1.564124
H	2.569715	-3.315985	-0.662569
H	3.978220	-1.345965	-0.223966
H	0.136416	-3.279497	-0.377553
H	-2.428218	2.513376	-0.201807
H	-4.574342	1.286637	-0.368084
H	-4.627907	-1.170912	-0.199207
H	-2.539467	-2.452540	0.175068

Frequencies[1/cm]

95.7277	115.7417	157.6797
199.2588	232.5512	284.6640
344.5158	411.4055	437.0264
471.3832	476.7070	496.2430
541.0919	548.9454	560.4024
608.2756	620.9149	636.5856
680.3112	697.6835	752.2181
764.5992	769.5966	785.5939
805.3753	827.9867	854.1227
889.2735	903.3305	914.4962
968.7664	970.8861	974.3450
994.1819	1011.4210	1037.6607
1057.8990	1075.1310	1085.6299
1116.6235	1145.2727	1161.8395
1182.5790	1187.8248	1198.6922
1211.7978	1238.1312	1247.9821
1300.6861	1313.3105	1326.5726
1329.6891	1366.6114	1386.7628
1427.9030	1481.0181	1490.8337
1512.6319	1526.7829	1550.3424
1648.1189	1657.4297	1663.7048
1691.0402	2907.7151	3179.8507
3182.8018	3183.4782	3189.7357
3195.4368	3199.3576	3200.5137

3208.3915 3209.4545 3213.1667

i24

C	2.140573	2.427652	-0.085994
C	0.737925	2.402191	0.081077
C	0.105005	1.177357	0.172021
C	0.896527	0.000441	0.095452
C	2.282579	0.005015	-0.092421
C	2.901147	1.280722	-0.176395
C	0.126694	-1.172486	0.200280
C	2.153881	-2.413128	-0.101722
C	2.906527	-1.265814	-0.191326
C	-1.272701	0.754094	0.268140
C	-1.297253	-0.747256	0.503997
C	0.749493	-2.386957	0.104001
C	-2.445428	1.438996	0.028337
C	-3.621734	0.730595	-0.218676
C	-3.595291	-0.692598	-0.373119
C	-2.481543	-1.417221	-0.117118
H	2.635641	3.390436	-0.152480
H	0.183482	3.332313	0.133193
H	3.974707	1.350510	-0.315219
H	2.647254	-3.375192	-0.187177
H	3.978660	-1.328439	-0.344582
H	-1.411375	-0.886920	1.599029
H	0.200380	-3.319013	0.182433
H	-2.436876	2.520127	-0.067401
H	-4.541841	1.266444	-0.418462
H	-4.486720	-1.188696	-0.741890
H	-2.461705	-2.491187	-0.266648

Frequencies[1/cm]

87.2623	97.2604	168.7508
191.6218	242.4597	269.9026
350.2066	411.8233	423.5152
468.1708	479.6226	494.5823
520.3801	562.9161	569.4505
595.9746	628.7140	640.1754
651.6833	690.7049	742.4144
769.3249	781.0501	799.2738
815.2465	823.1561	855.0242
891.9961	913.9910	927.3227
930.0532	972.9780	984.0387
998.0616	998.3373	1005.4578
1033.5553	1067.2653	1074.2050
1083.3731	1122.9032	1158.9963
1172.3921	1184.4687	1204.2348

1221.4722	1241.3266	1262.4273
1292.9067	1296.6338	1323.6613
1370.2709	1396.2506	1410.3355
1431.6029	1459.2415	1469.5763
1506.7770	1539.3370	1544.6171
1623.3329	1652.4086	1673.1113
1696.0213	2888.4401	3180.4572
3182.0814	3183.1871	3184.0059
3193.0961	3196.9349	3200.8429
3206.6885	3208.5891	3214.1756

i25

C	-0.376124	2.606327	-0.455099
C	0.665273	1.653027	-0.616892
C	0.368849	0.325854	-0.448224
C	-0.958362	-0.027373	-0.139438
C	-2.000679	0.874637	0.024922
C	-1.667185	2.246186	-0.141137
C	-1.083376	-1.429861	-0.047781
C	-3.407905	-1.055506	0.430927
C	-3.270783	0.309455	0.327803
C	1.123375	-0.949152	-0.543917
C	0.253284	-1.971034	-0.324021
C	-2.318738	-1.950841	0.241117
C	2.546364	-1.082015	-0.875582
C	3.579013	-0.477282	-0.274693
C	3.562651	0.384831	0.922685
C	2.635906	0.432881	1.852064
H	-0.138316	3.656460	-0.582563
H	1.669331	1.983854	-0.857145
H	-2.430730	3.008179	-0.024686
H	-4.382784	-1.470958	0.660668
H	-4.130589	0.954711	0.474345
H	0.509050	-3.022371	-0.338167
H	-2.485313	-3.019567	0.323414
H	2.776331	-1.751431	-1.700717
H	4.569050	-0.658611	-0.684824
H	4.447942	1.009158	1.053307
H	1.686653	-0.03031	2.079974

Frequencies[1/cm]

40.2228	77.3673	97.7954
145.6001	166.7731	184.8629
224.9631	272.4891	336.7053
395.8826	418.6055	445.9599
467.1348	500.1778	540.3312
565.4739	583.7175	592.7109

629.4701	669.5091	680.3383
714.2592	755.9788	778.8964
779.7124	794.9815	804.7149
826.5076	846.7459	881.3421
889.9567	919.9106	945.1076
953.9188	955.1760	998.0736
1000.9075	1010.0526	1010.1869
1044.3492	1070.7916	1098.9204
1159.2137	1182.0003	1214.1217
1230.0953	1252.4224	1259.2777
1280.9905	1290.3392	1338.0390
1404.1026	1414.0001	1429.7310
1462.2668	1488.3046	1517.0555
1543.5360	1599.3556	1653.2590
1675.5211	1693.3410	1705.2671
1720.1683	3109.9851	3153.2390
3176.3949	3184.2379	3185.5011
3194.5643	3200.7797	3208.8087
3213.2849	3229.0333	3260.7106

i26

C	-0.236244	2.430157	0.316880
C	-1.187147	1.255169	0.458924
C	-0.476838	-0.032390	0.233491
C	0.930273	-0.067202	0.066924
C	1.757404	1.037609	0.014839
C	1.087898	2.335996	0.128884
C	1.358907	-1.403411	-0.027824
C	3.581057	-0.529720	-0.249656
C	3.126505	0.783762	-0.152667
C	-0.954084	-1.360958	0.222145
C	0.153319	-2.213832	0.082926
C	2.715805	-1.636616	-0.188032
C	-2.351969	-1.728757	0.299965
C	-3.382575	-0.928323	-0.038360
C	-3.322240	0.413123	-0.615027
C	-2.387298	1.358956	-0.465457
H	-0.691035	3.413362	0.397332
H	-1.570384	1.263320	1.495232
H	1.686271	3.238656	0.055452
H	4.643236	-0.706348	-0.377370
H	3.833885	1.604487	-0.207100
H	0.110985	-3.294295	0.038462
H	3.117912	-2.640764	-0.266320
H	-2.577115	-2.747432	0.603635
H	-4.379410	-1.356080	0.020292

H -4.161360 0.660038 -1.261076
H -2.489617 2.283670 -1.026272

Frequencies[1/cm]

72.3891	110.0997	176.7130
229.2383	252.2566	290.8112
356.7546	381.9441	385.2677
420.4615	462.6551	492.6222
509.0113	538.4101	561.6901
595.5426	611.8050	615.6145
653.8343	692.9925	724.0424
754.1137	770.1363	784.5814
797.8795	820.4970	833.9284
838.6088	875.6828	927.9419
933.4206	977.7260	990.7369
997.5572	998.6186	1012.8423
1018.8478	1037.2087	1059.4667
1088.1375	1154.0555	1164.8592
1188.6965	1200.6295	1211.1083
1245.1734	1247.8328	1257.6881
1267.1258	1292.8076	1334.4326
1384.3128	1415.6239	1423.2375
1438.9230	1452.2183	1517.1670
1527.1551	1557.9709	1628.3397
1662.8925	1671.5019	1707.4456
1717.4480	2940.3101	3150.8144
3162.7781	3170.3596	3178.0966
3184.3569	3185.3622	3193.3401
3195.1933	3209.3486	3228.8412

i27

C	-0.223181	2.412376	-0.072439
C	-1.112522	1.283356	-0.009426
C	-0.506721	0.013560	0.516101
C	0.957776	-0.057313	0.276553
C	1.791657	1.038908	0.149256
C	1.130205	2.334443	0.072200
C	1.356267	-1.368973	0.034317
C	3.591087	-0.541520	-0.202644
C	3.148608	0.775291	-0.070123
C	-0.959542	-1.378596	0.107842
C	0.143088	-2.170857	-0.051541
C	2.710280	-1.623527	-0.184004
C	-2.320688	-1.779915	0.016820
C	-3.411381	-0.944308	-0.056950
C	-3.478952	0.462390	-0.177482
C	-2.469439	1.431737	-0.230617

H	-0.673644	3.383607	-0.255299
H	-0.650859	0.049468	1.613389
H	1.732873	3.234530	0.015923
H	4.646021	-0.724566	-0.374406
H	3.852196	1.594084	-0.178141
H	0.114335	-3.231948	-0.266717
H	3.074606	-2.628363	-0.365498
H	-2.508295	-2.848828	-0.034605
H	-4.376411	-1.441894	-0.098597
H	-4.485233	0.850409	-0.305437
H	-2.804843	2.441192	-0.457788

Frequencies[1/cm]

91.3764	126.6453	184.3835
237.1808	274.3310	306.2933
362.2967	379.4390	391.5757
434.2433	487.9396	496.2302
507.9049	548.9217	570.3833
596.0044	623.8890	633.9279
647.1449	722.2157	726.6330
750.8067	773.7710	787.8464
817.9275	843.0953	865.9074
876.6773	894.6720	913.8786
922.1932	939.4045	978.3601
983.6508	990.4619	997.8851
1012.2973	1070.2698	1082.3222
1088.7659	1163.5570	1168.3751
1185.6633	1199.6235	1202.2586
1245.4823	1254.8576	1267.9729
1293.3897	1311.2784	1340.6760
1376.6280	1390.4236	1413.8454
1444.1093	1452.7488	1475.3807
1510.9994	1548.8784	1556.6656
1587.9742	1598.9187	1668.1713
1679.8737	2928.4248	3151.1707
3159.1237	3173.3735	3174.7600
3183.8778	3186.2413	3195.8893
3199.3164	3209.6284	3217.8523

i28

C	-0.372119	2.402546	0.044269
C	-1.163315	1.228832	0.218140
C	-0.482542	0.029004	0.261843
C	0.896213	-0.005325	0.086380
C	1.686595	1.127010	-0.107568
C	0.994052	2.366351	-0.116224
C	1.391099	-1.349337	0.152678

C	3.582430	-0.401201	-0.209595
C	3.081791	0.894507	-0.258764
C	-0.972647	-1.378028	0.506755
C	0.301952	-2.191129	0.377710
C	2.776634	-1.531172	-0.008473
C	-2.083107	-1.733425	-0.452121
C	-3.174829	-0.980469	-0.633132
C	-3.476309	0.325311	-0.055387
C	-2.614065	1.299509	0.299927
H	-0.879642	3.361918	0.020031
H	1.545326	3.290564	-0.253749
H	4.650847	-0.545781	-0.329916
H	3.757171	1.728922	-0.413119
H	-1.360629	-1.457788	1.535669
H	0.333613	-3.267885	0.481565
H	3.222105	-2.518588	0.025248
H	-1.988603	-2.663139	-1.005290
H	-3.943834	-1.372217	-1.294185
H	-4.533961	0.570146	-0.006586
H	-3.033394	2.255931	0.601709

Frequencies[1/cm]

89.2708	112.8866	201.4963
221.1673	245.0733	313.1621
356.4983	382.0359	396.6062
456.7897	484.5955	493.3087
510.7790	541.3730	573.4698
593.4398	619.4764	641.2434
647.6855	691.3517	702.3778
744.6393	751.0450	775.0396
809.1883	831.3875	838.0677
854.7835	884.5567	887.4248
930.2358	984.2154	988.3158
992.0500	1003.2155	1018.8354
1025.7900	1058.7550	1071.8272
1086.4695	1144.8500	1180.0177
1183.5650	1208.5148	1217.2576
1230.0932	1252.9732	1259.4890
1270.6653	1301.7714	1346.8872
1366.1480	1409.1891	1416.9921
1437.3912	1465.1588	1472.5003
1496.6365	1541.7349	1599.4087
1646.1993	1665.1424	1691.7799
1716.2705	2976.2799	3151.7977
3160.3911	3177.1714	3179.0721
3183.5598	3185.6007	3198.5616
3199.1756	3209.8500	3225.5954

i29

C	-0.172119	2.431816	0.080893
C	-1.057226	1.288535	0.058728
C	-0.448936	0.034557	0.068472
C	0.957092	-0.038439	0.030989
C	1.817606	1.049811	0.023586
C	1.189374	2.334485	0.066994
C	1.367310	-1.386852	-0.028669
C	3.621704	-0.558280	-0.086213
C	3.201340	0.755190	-0.030947
C	-0.937879	-1.346705	0.063939
C	0.134221	-2.180762	-0.006540
C	2.714735	-1.649222	-0.090836
C	-2.364917	-1.778328	0.227002
C	-3.459324	-0.822807	-0.143299
C	-3.482843	0.540661	-0.195898
C	-2.457810	1.501074	-0.043256
H	-0.630617	3.415587	0.094126
H	1.796821	3.233472	0.076368
H	4.684476	-0.769149	-0.130440
H	3.929514	1.559464	-0.031735
H	0.088161	-3.262149	-0.019585
H	3.098245	-2.662617	-0.143778
H	-2.525191	-2.046691	1.283820
H	-2.518706	-2.713120	-0.322619
H	-4.416006	-1.310911	-0.311187
H	-4.462714	0.969149	-0.391475
H	-2.777957	2.538565	-0.073167

Frequencies[1/cm]

47.2171	115.4195	140.2525
206.5817	271.6465	291.0441
312.4794	375.3979	414.5024
428.2001	463.9352	498.6715
516.9358	533.5219	576.1288
590.2850	620.2414	635.0475
650.5576	670.1354	716.6055
755.1991	776.1946	787.4473
802.7144	808.9903	851.6033
856.7644	874.0363	912.3471
939.5301	951.9552	983.1005
987.9646	993.9122	1000.2023
1029.2566	1061.2237	1091.8256
1131.5334	1166.1810	1176.8344
1209.0076	1216.1108	1244.2541
1254.6733	1275.9417	1287.3918

1340.5763	1364.9776	1377.3935
1423.9440	1430.7551	1455.7751
1459.6009	1462.6663	1483.8007
1512.4532	1536.1162	1588.8264
1613.4262	1631.7814	1686.7689
1690.3760	2980.8199	3063.2160
3148.6594	3167.5382	3178.4285
3181.7149	3183.0710	3193.3134
3199.1044	3207.8718	3223.3848

i30

C	-0.192258	2.506483	0.128895
C	-1.088234	1.400898	0.102337
C	-0.516252	0.155292	0.207299
C	0.854100	-0.020499	0.128241
C	1.758058	1.038725	0.116208
C	1.178333	2.338709	0.165270
C	1.167925	-1.401631	-0.084786
C	3.468748	-0.671535	-0.168179
C	3.125478	0.667361	-0.011235
C	-1.161453	-1.157544	0.114960
C	-0.046797	-2.108729	-0.151215
C	2.530012	-1.715622	-0.227608
C	-2.336997	-1.511388	0.996237
C	-2.623675	-1.069962	-0.408878
C	-3.151907	0.305155	-0.601234
C	-2.497310	1.434888	-0.273029
H	-0.598804	3.512013	0.081095
H	1.822561	3.211702	0.172713
H	4.519114	-0.922582	-0.271864
H	3.901328	1.425273	-0.007430
H	-0.167194	-3.176888	-0.271127
H	2.863119	-2.733545	-0.394331
H	-2.588330	-0.834045	1.803803
H	-2.449989	-2.566346	1.214406
H	-4.152156	0.375032	-1.016770
H	-2.981599	2.395965	-0.412340
H	-2.974667	-1.830188	-1.097843

Frequencies[1/cm]

95.7539	144.0366	197.2421
262.0229	285.7275	306.7924
332.1691	419.1864	430.0552
460.4631	487.0234	510.2207
542.4395	557.5387	569.9950
586.8748	625.9841	661.0460
668.5790	680.7635	718.2112

749.0688	758.3916	782.2397
805.9422	818.0164	839.8309
843.2499	862.4060	885.7075
935.7417	965.4393	979.1465
988.7617	994.8699	1004.7777
1038.9461	1053.3397	1068.5878
1073.1608	1108.5642	1115.3963
1163.2446	1174.2053	1195.0834
1215.6472	1226.4814	1250.3127
1260.8023	1331.4364	1337.7360
1354.6936	1381.8876	1421.7298
1432.2609	1449.0599	1475.0556
1481.4056	1492.2609	1540.3980
1598.3878	1641.4747	1677.9600
1706.9519	3141.4925	3172.0727
3178.0848	3180.4379	3182.2742
3197.0680	3197.9111	3198.3937
3208.2403	3232.0069	3239.6831

i31

C	-0.415403	2.541348	0.183481
C	-1.270248	1.386721	0.107983
C	-0.631743	0.166750	0.155718
C	0.754736	0.055463	0.086376
C	1.602771	1.162299	0.109901
C	0.951882	2.436551	0.203968
C	1.150341	-1.275403	-0.164050
C	3.389245	-0.422060	-0.275392
C	2.979139	0.877593	-0.057656
C	-1.270125	-1.151929	0.058740
C	-0.084956	-2.135871	-0.181532
C	2.486138	-1.517118	-0.350627
C	-0.834999	-2.181996	1.115467
C	-2.651570	-1.093687	-0.422231
C	-3.295093	0.124170	-0.456920
C	-2.674657	1.354712	-0.148500
H	-0.871539	3.526256	0.192512
H	1.555645	3.337476	0.240449
H	4.446184	-0.619279	-0.417911
H	3.708815	1.680405	-0.044078
H	2.866342	-2.510156	-0.563313
H	-3.246768	2.273983	-0.196509
H	-0.352975	-1.812596	2.013920
H	-0.168645	-2.968820	-0.869018
H	-1.522582	-3.007966	1.260079
H	-3.186090	-2.006714	-0.659561

H -4.341134 0.142155 -0.744923

Frequencies[1/cm]

101.8897	159.1987	168.6843
243.7678	266.6439	334.0647
391.4900	406.9601	446.2006
461.3586	499.1324	503.2830
520.7641	540.0300	565.8496
595.0885	630.3420	658.8176
686.4710	689.3016	711.7598
748.6113	778.2605	781.2619
806.2164	814.7920	837.4179
849.2997	912.9997	931.5068
937.3294	962.2782	971.9978
989.2042	999.6744	1003.4058
1013.4688	1057.6494	1065.9386
1078.4347	1083.6129	1108.8567
1154.8843	1182.8499	1197.9148
1216.7601	1224.1746	1240.7636
1253.3758	1322.7839	1332.6584
1357.3811	1398.6617	1421.5768
1447.3235	1456.2949	1481.3918
1494.9789	1515.7355	1535.6561
1563.5831	1660.7114	1678.0585
1692.1333	3132.1936	3178.9718
3180.5738	3182.4294	3193.2171
3194.8319	3197.7894	3198.4880
3207.4445	3208.6205	3230.7955

i32

C	0.659468	-2.479087	0.000012
C	1.410420	-1.257763	-0.000011
C	0.716989	-0.023611	0.000001
C	-0.721557	-0.021928	0.000011
C	-1.426581	-1.236848	0.000022
C	-0.692442	-2.469318	0.000030
C	-1.441791	1.223756	-0.000016
C	-3.533935	-0.029138	-0.000018
C	-2.839488	-1.226971	0.000013
C	1.449754	1.185818	-0.000015
C	-0.747063	2.430829	-0.000016
C	-2.854366	1.179995	-0.000035
C	0.738778	2.518064	0.000053
C	2.828785	1.141674	0.000003
C	3.515847	-0.078412	-0.000014
C	2.816640	-1.262152	-0.000054
H	1.203321	-3.418002	0.000008

H	-1.249200	-3.400642	0.000044
H	-4.618176	-0.034782	-0.000029
H	-3.372972	-2.171216	0.000027
H	-3.404811	2.114777	-0.000061
H	3.340816	-2.212058	-0.000032
H	1.071069	3.102881	0.870473
H	-1.307485	3.360021	-0.000033
H	1.071154	3.103025	-0.870236
H	3.389654	2.071486	0.000037
H	4.599883	-0.084943	0.000004

Frequencies[1/cm]

67.3261	123.2979	188.4622
214.2461	242.0876	293.0260
357.0672	405.8663	440.5663
452.5469	493.1896	506.2904
513.9353	533.1557	554.6739
573.9780	591.9835	634.0462
689.9544	691.9182	726.9403
738.7687	772.8493	788.4152
810.8393	824.2641	824.9420
851.0711	890.1355	914.7946
951.7262	960.8169	988.3395
998.7890	1006.6870	1013.8698
1059.8363	1108.4435	1119.9209
1127.7502	1171.0016	1199.2572
1203.7237	1212.8670	1218.6712
1232.8311	1264.3491	1268.4013
1333.4764	1353.4673	1373.6571
1399.5971	1435.2836	1450.3308
1456.2108	1470.4531	1483.0520
1496.4602	1545.1859	1564.7466
1620.1870	1645.4337	1678.0503
1697.8169	2992.6860	3008.6249
3176.3199	3180.5542	3182.7576
3185.9086	3187.3772	3193.1990
3200.6241	3208.3095	3209.0121

i33

C	4.553638	-0.106148	0.051382
C	4.047374	-1.408264	0.265754
C	3.701619	0.948026	-0.136476
C	2.298057	0.757039	-0.118741
C	1.792857	-0.560311	0.094601
C	2.698593	-1.634188	0.287072
C	1.374852	1.818583	-0.309051
C	0.025155	1.605679	-0.284676

C	0.401046	-0.684137	0.098515
C	-0.517151	0.302253	-0.063343
C	-1.977109	0.052818	-0.020388
C	-2.860794	1.012453	0.477095
C	-4.226363	0.763985	0.517082
C	-4.730411	-0.448423	0.063300
C	-3.858524	-1.412971	-0.428794
C	-2.494599	-1.164100	-0.471119
H	5.625642	0.053893	0.036509
H	4.736802	-2.231558	0.413390
H	4.090749	1.947473	-0.301613
H	2.302369	-2.629386	0.450488
H	1.760911	2.816690	-0.486308
H	-2.477438	1.952337	0.858746
H	-4.897873	1.517972	0.912060
H	-5.796565	-0.641703	0.094529
H	-1.815455	-1.911223	-0.867379
H	-4.243237	-2.361178	-0.787031
H	-0.655363	2.432908	-0.456664

Frequencies[1/cm]

42.1948	60.0585	92.1505
166.3119	188.1172	263.1089
279.8730	329.6785	409.7869
418.6450	435.2291	504.0197
510.1162	526.3280	554.8253
573.8093	634.7001	642.5261
664.6913	715.1989	719.4845
762.4613	779.8968	790.6472
796.5960	840.5806	870.5721
879.8300	891.2527	943.8098
949.2779	982.7163	994.2972
1002.6175	1019.3676	1022.4892
1025.1266	1047.5751	1058.4698
1086.3735	1117.0829	1155.1420
1176.7836	1188.2427	1189.8658
1213.9724	1240.9609	1272.7813
1299.4004	1323.0576	1353.5534
1362.7472	1392.5491	1412.3727
1460.8146	1492.9729	1508.2564
1540.4322	1552.2264	1618.6275
1653.9953	1676.2197	1682.9930
1707.5641	3182.9094	3183.5855
3184.7543	3189.7632	3194.2818
3198.2699	3202.9289	3206.0300
3206.9285	3216.0156	3217.4570

i34

C	-1.953355	-0.667949	-0.961393
C	-3.277595	-1.084471	-0.949047
C	-4.165047	-0.564095	-0.014198
C	-3.721719	0.378808	0.904746
C	-2.397095	0.796324	0.892456
C	-1.497506	0.274079	-0.036970
C	0.199538	2.068929	-0.189653
C	-0.088716	0.750819	-0.061400
C	1.458264	2.655644	-0.280783
C	2.536218	1.809066	-0.220891
C	0.903155	-1.529661	0.261845
C	1.041297	-0.134853	0.040515
C	2.353889	0.411082	-0.054043
C	3.469386	-0.460003	0.035504
C	2.002936	-2.339531	0.351438
C	3.301997	-1.803115	0.227785
H	1.583367	3.725614	-0.399303
H	-3.618908	-1.812715	-1.676119
H	-1.266062	-1.064427	-1.700787
H	-5.198824	-0.890282	-0.004539
H	-4.408646	0.790510	1.635537
H	-2.047540	1.529145	1.611083
H	3.545849	2.201300	-0.292521
H	-0.088411	-1.950074	0.373947
H	4.465321	-0.036865	-0.045517
H	1.876010	-3.401933	0.526347
H	4.163954	-2.456712	0.296404

Frequencies[1/cm]

43.4605	72.7105	84.4966
168.5619	191.3454	246.1036
286.3115	314.5101	413.9846
419.9783	444.0210	486.5435
506.1387	532.3066	568.1498
579.2337	631.6987	635.3898
666.5427	717.8278	725.6213
757.2185	782.5006	797.4998
803.0507	820.1875	849.2316
876.2261	894.6744	952.0787
974.5264	977.4836	995.1363
1006.5124	1020.3813	1024.0939
1025.5562	1055.0273	1063.4555
1103.7884	1116.7411	1147.2285
1170.6871	1184.3282	1188.8021
1213.2608	1230.0419	1249.9744
1300.4026	1320.2915	1337.6558

1359.5163	1414.0477	1425.2731
1459.3314	1484.8595	1491.2556
1542.4461	1557.4484	1628.8078
1650.6694	1662.2286	1682.2329
1697.0624	3181.5798	3184.0165
3184.6022	3191.2645	3194.4066
3199.9437	3205.4456	3207.1930
3210.2387	3215.9544	3221.6174

i35

C	-3.270842	-1.842360	-0.198519
C	-1.964514	-2.364882	-0.312031
C	-3.455330	-0.498187	-0.033883
C	-2.349724	0.387135	0.037253
C	-1.030879	-0.140187	-0.044640
C	-0.876487	-1.538669	-0.238919
C	-2.536904	1.785271	0.172329
C	-1.463023	2.628373	0.213612
C	0.076914	0.760999	0.036816
C	-0.153509	2.110802	0.146594
C	1.481481	0.271145	0.017094
C	2.403650	0.720978	-0.901048
C	3.721811	0.351722	-0.981973
C	4.176388	-0.563985	-0.030778
C	3.300494	-1.052199	0.934142
C	1.972977	-0.643212	0.961872
H	0.119314	-1.950452	-0.345661
H	-4.124338	-2.508406	-0.253780
H	-1.824051	-3.428734	-0.466253
H	-4.456068	-0.084803	0.038305
H	-3.548093	2.173621	0.234887
H	4.385113	0.746025	-1.743560
H	5.210922	-0.889250	-0.045533
H	1.300711	-1.022331	1.725000
H	3.657138	-1.755882	1.677366
H	-1.609029	3.698161	0.309253
H	0.693356	2.785598	0.202454

Frequencies[1/cm]

42.9306	74.2487	85.3575
166.7860	185.3258	250.3896
289.8153	315.3098	410.6396
429.0728	445.9601	483.0819
509.6636	534.4815	571.1196
586.4404	623.6873	635.9426
668.2018	712.0290	729.4969
757.8926	765.5324	804.5857

812.4486	829.7898	854.3192
878.0634	896.2508	944.0469
969.6117	982.2595	993.1613
1002.4076	1008.9868	1010.5168
1021.1906	1053.4412	1058.2342
1092.8668	1134.4923	1150.8037
1175.0057	1182.2237	1197.9361
1220.4809	1238.9446	1253.0547
1284.8431	1322.7203	1328.4303
1377.6557	1423.7162	1435.3780
1453.1467	1484.2119	1494.6919
1516.2466	1571.8487	1605.6224
1660.1763	1668.9328	1670.9244
1707.2009	3182.4906	3182.6454
3184.6458	3189.1128	3194.3276
3196.8221	3200.7902	3209.1683
3211.9850	3213.0715	3221.2704

i36

C	2.137741	0.374163	-0.006170
C	0.774731	-0.000351	0.059228
C	0.412759	-1.408387	0.013925
C	1.447394	-2.352421	-0.155166
C	2.783488	-1.962135	-0.224185
C	3.135676	-0.632752	-0.137778
C	2.476003	1.746079	0.033643
C	1.498551	2.707220	0.112617
C	0.146035	2.340298	0.146060
H	1.187753	-3.404289	-0.208702
H	3.552976	-2.717139	-0.340399
H	4.177029	-0.333800	-0.185356
H	3.522739	2.028451	-0.006145
H	1.769550	3.756377	0.145587
H	-0.620938	3.104394	0.207168
C	-0.224035	1.008544	0.116268
C	-1.613753	0.568649	0.077181
C	-0.912666	-1.809046	0.171108
C	-2.710851	1.135360	-0.461538
C	-1.960038	-0.814829	0.548837
H	-1.163151	-2.864021	0.141928
C	-3.814138	0.175661	-0.417347
H	-2.766628	2.119740	-0.908530
C	-3.389561	-0.980104	0.118256
H	-1.989791	-0.776692	1.657797
H	-4.815728	0.380506	-0.773209
H	-3.977831	-1.869216	0.300227

Frequencies[1/cm]

83.0833	111.1501	172.5259
205.4912	247.3261	275.9034
317.0771	385.3605	415.1595
444.6164	477.3737	494.4013
525.3442	546.9617	560.0573
613.8247	615.9458	637.0019
682.0258	712.1106	731.2680
764.7095	787.9972	798.4716
807.6197	830.2818	842.0069
863.4858	884.0592	901.0707
929.9873	936.6875	970.8241
989.3114	1003.4759	1004.1695
1033.1383	1065.7317	1089.0741
1096.2709	1117.6570	1135.7321
1154.0862	1172.7639	1193.5398
1212.9855	1236.9702	1243.4952
1261.6388	1293.7991	1318.1792
1375.8050	1376.5774	1402.4222
1411.5771	1449.6322	1468.3367
1496.6115	1538.7187	1596.9967
1607.2256	1634.0993	1672.1229
1688.4893	2914.7638	3183.1019
3184.3492	3190.1208	3193.4967
3195.5811	3208.8985	3210.8286
3212.6729	3224.9955	3242.7780

i37

C	-2.167353	0.591563	0.101089
C	-0.891091	-0.014127	-0.032922
C	-0.806133	-1.437433	-0.091599
C	-1.947970	-2.198740	0.019700
C	-3.208080	-1.594367	0.191009
C	-3.317219	-0.231969	0.224578
C	-2.265823	2.001288	0.097023
C	-1.142017	2.768690	-0.052933
C	0.121781	2.168788	-0.171516
H	-1.872867	-3.279814	-0.034927
H	-4.091806	-2.215226	0.283063
H	-4.286441	0.241480	0.339956
H	-3.242494	2.462274	0.198573
H	-1.219441	3.849571	-0.080552
H	0.982075	2.814037	-0.299134
C	0.280010	0.796724	-0.133780
C	1.610282	0.135492	-0.166562
C	0.493542	-2.039834	-0.331953

C	2.758144	0.829723	0.016936
C	1.612716	-1.306375	-0.382244
H	0.533753	-3.112255	-0.493100
C	4.132785	0.314783	0.075690
H	2.700101	1.906065	0.141642
C	4.553041	-0.819861	0.591963
H	2.562165	-1.782550	-0.592921
H	4.891045	1.001915	-0.306100
H	4.144227	-1.671573	1.116627

Frequencies[1/cm]

39.9289	76.4668	138.8492
170.5750	178.6824	213.1432
248.5022	277.0996	341.1164
398.6644	447.8248	457.2700
479.8359	489.8265	513.8992
531.6531	552.0439	600.2275
641.0113	666.0711	694.6829
707.9722	761.6251	772.4198
792.7972	804.5066	832.0445
833.7538	852.6893	872.6940
896.8265	906.0830	925.6383
938.6902	945.0011	1001.9205
1009.2828	1021.2642	1058.3878
1077.8314	1116.0745	1137.2058
1153.5517	1184.4696	1215.9002
1231.9659	1248.5555	1268.2462
1278.8514	1324.6645	1346.2612
1398.7199	1418.5981	1433.4072
1448.9314	1489.9785	1514.3628
1566.8210	1614.4367	1655.2555
1662.4103	1674.1546	1681.9861
1721.3474	3099.6387	3183.4541
3184.3009	3185.2626	3187.5073
3191.5145	3203.3694	3210.8500
3216.6850	3217.6420	3253.8031

i38

C	1.410393	-1.240802	-0.017378
C	0.728071	0.010978	0.069950
C	1.472279	1.218311	0.026871
C	2.882031	1.152866	-0.018429
C	3.524616	-0.059646	-0.057718
C	2.786623	-1.256887	-0.076760
C	0.613607	-2.460324	-0.131105
C	-0.711771	-2.453804	0.009143
C	-1.460351	-1.210505	0.402592

H	3.450605	2.076863	-0.032463
H	4.607216	-0.099056	-0.096295
H	3.305612	-2.206718	-0.154687
H	1.137298	-3.382826	-0.361299
H	-1.284283	-3.370581	-0.092915
H	-1.544145	-1.270098	1.512147
C	-0.682335	0.055356	0.141059
C	-1.357792	1.273655	0.046034
C	0.765348	2.454200	0.016258
C	-2.778682	1.282790	-0.074064
C	-0.594602	2.479299	0.000736
H	1.332096	3.379157	-0.005252
C	-3.489817	0.077602	-0.230369
H	-3.293470	2.233142	-0.157967
C	-2.877490	-1.130866	-0.082623
H	-1.123379	3.425682	-0.048503
H	-4.541968	0.118004	-0.491492
H	-3.426344	-2.056919	-0.216457

Frequencies[1/cm]

80.6383	132.7509	195.5226
218.3255	246.5273	342.1647
385.7738	400.3480	446.4381
461.5342	493.1917	504.0926
514.2777	527.1766	542.1143
557.8543	590.6299	657.8047
682.8065	686.0222	715.4522
739.3841	776.1365	781.3245
806.6595	821.3094	835.0635
859.3824	866.3302	931.0851
959.8605	973.4207	990.5244
1000.9790	1001.0816	1007.2548
1076.7419	1088.1524	1100.6066
1110.7696	1152.5363	1170.9184
1183.7996	1201.2145	1212.0770
1225.7430	1245.0303	1264.2200
1269.4560	1314.8262	1344.6928
1383.4082	1418.7076	1427.8043
1434.8743	1439.4369	1471.7296
1504.6407	1551.5759	1578.2153
1630.1977	1662.8308	1671.8265
1734.2342	2824.9501	3172.4465
3179.6539	3180.2738	3181.8910
3189.2151	3193.7935	3195.0269
3199.5596	3206.9046	3209.6083

i39

C	-1.719993	-0.518578	0.000382
C	-2.019773	0.856753	-0.000160
C	-0.746650	1.688978	0.000152
C	0.306451	0.629431	0.001063
C	-0.264695	-0.654708	0.000976
C	1.742315	0.502128	0.000321
C	2.011766	-0.900163	-0.000148
C	0.737479	-1.613931	0.000092
C	3.316834	-1.354344	-0.000572
C	4.359495	-0.418999	-0.000639
C	4.096211	0.944284	-0.000172
C	2.780062	1.417980	0.000360
C	-3.334243	1.286234	-0.000680
C	-4.356307	0.337717	-0.000691
C	-4.059925	-1.021705	-0.000125
C	-2.739475	-1.461019	0.000448
H	-0.683515	2.339164	0.880390
H	-0.682369	2.338231	-0.880703
H	0.625635	-2.689471	-0.000582
H	3.536309	-2.416674	-0.000905
H	5.386677	-0.765612	-0.001044
H	4.919387	1.649463	-0.000205
H	2.581491	2.484379	0.000818
H	-3.571322	2.345115	-0.001105
H	-5.390703	0.662169	-0.001116
H	-4.866797	-1.745916	-0.000092
H	-2.512098	-2.521198	0.000906

Frequencies[1/cm]

61.7873	110.5740	155.0521
173.8435	224.7215	289.0964
306.4963	332.1986	396.2918
424.1025	440.1401	521.8227
546.0234	559.1447	564.1858
596.1560	635.6899	639.1207
688.3874	734.6829	753.7786
768.8271	783.1680	784.6569
805.7565	812.7417	841.0624
889.1190	897.5697	919.7815
935.9283	962.7150	976.1385
1001.9464	1010.3330	1037.4574
1051.3258	1058.1974	1085.6467
1116.9935	1152.2099	1153.8011
1183.0230	1185.2232	1194.2760
1196.0600	1215.5610	1247.7739
1287.5044	1315.3359	1326.5453

1353.5619	1388.4844	1425.1211
1449.8705	1496.2833	1505.3842
1508.6412	1518.2686	1563.8615
1653.9564	1655.7508	1658.3801
1690.9683	3041.7942	3075.7088
3182.3342	3184.4973	3190.1058
3191.2980	3201.3547	3201.4329
3213.0633	3214.0486	3236.1461

Transition states

i3 – i4

C	-2.067116	2.367110	0.153773
C	-0.783264	2.204130	-0.201699
C	-0.229719	0.869021	-0.620618
C	-1.185704	-0.218921	-0.310889
C	-2.580298	-0.000887	0.042689
C	-3.006182	1.254154	0.277970
C	-0.899046	-1.524221	-0.191997
C	-2.139770	-2.222307	0.173489
C	-3.147343	-1.323720	0.293553
C	0.500660	-2.019881	-0.332304
C	1.516798	-0.907092	-0.107964
C	2.836670	-1.253553	0.151663
C	3.823978	-0.293582	0.332719
C	3.499334	1.055894	0.224877
C	2.194248	1.429002	-0.025836
C	1.162143	0.470642	-0.116327
H	-2.431002	3.362419	0.384214
H	-0.142246	3.075222	-0.280812
H	-0.130327	0.941147	-1.719609
H	-4.016344	1.458645	0.618005
H	-2.219287	-3.289074	0.341098
H	-4.170992	-1.525654	0.573470
H	0.663276	-2.443803	-1.333396
H	0.698205	-2.833978	0.373033
H	3.099927	-2.305754	0.204248
H	4.844624	-0.596841	0.535122
H	4.267634	1.813210	0.330438
H	1.949413	2.481220	-0.108849
H	0.614782	0.548503	1.624448

Frequencies[1/cm]

-982.2762	49.4926	98.9041
162.2408	205.8119	226.7082
253.8084	296.3298	368.4723
375.5385	417.6615	436.7977

449.0444	479.5127	506.5970
532.0497	548.0230	572.8859
595.0307	636.0398	656.6645
669.4946	711.3625	721.9922
737.3870	755.4922	765.2516
804.7934	826.6772	861.2262
881.4769	910.0847	937.3684
951.5163	958.8453	981.7316
998.8668	1006.8363	1012.3967
1025.0055	1059.1568	1079.7662
1101.1583	1144.4963	1153.2470
1184.7376	1191.5520	1198.9808
1212.6255	1220.2419	1225.4951
1249.4262	1277.3378	1299.5917
1312.9926	1341.0635	1363.1883
1398.9983	1436.7602	1461.6138
1475.2740	1494.4991	1515.2392
1556.2719	1617.9194	1644.8584
1662.9085	1728.1996	1741.4391
2943.4481	3008.7599	3067.5855
3175.7406	3181.7333	3190.7124
3193.8206	3204.8013	3209.5565
3217.0364	3217.3788	3250.2814

i4 – i7

C	-1.912850	2.450159	-0.101104
C	-0.603277	2.190236	-0.335908
C	-0.099942	0.830890	-0.509340
C	-1.111033	-0.207888	-0.362212
C	-2.514344	0.108056	-0.152404
C	-2.899505	1.399526	-0.012608
C	-0.930073	-1.532491	-0.087956
C	-2.240560	-2.121092	0.167856
C	-3.193585	-1.155040	0.108678
C	0.423881	-2.131625	0.167859
C	1.484903	-1.053419	0.196850
C	2.675290	-1.199736	-0.476243
C	3.626641	-0.171133	-0.525582
C	3.399410	1.028045	0.165624
C	2.228020	1.213683	0.854647
C	1.158249	0.249109	0.771631
H	-2.242834	3.477710	0.006587
H	0.099077	3.010416	-0.442774
H	0.585251	0.746744	-1.350875
H	-3.929018	1.657994	0.213662
H	-2.410101	-3.167182	0.390302

H	-4.255602	-1.274873	0.268297
H	0.689106	-2.882852	-0.585080
H	0.393070	-2.659731	1.130602
H	2.883068	-2.137300	-0.983117
H	4.551937	-0.318291	-1.069869
H	4.165270	1.795836	0.177090
H	2.058144	2.125285	1.416728
H	0.465289	0.242552	1.609719

Frequencies[1/cm]

- 811.8701	58.3137	99.0840
135.9679	207.5215	221.8944
261.8481	315.8410	326.2873
367.5617	420.9207	448.9781
497.0618	529.2856	558.3935
568.9143	601.9289	614.2768
633.2083	668.0293	690.9067
732.4114	740.2388	754.7704
761.1457	798.4377	807.4378
851.5114	877.4025	920.9810
932.7117	944.1541	958.4884
972.7745	993.0034	1000.0170
1001.7899	1033.9992	1041.3401
1046.8187	1084.6858	1096.9596
1103.6559	1118.9267	1159.5104
1170.4788	1188.0357	1195.5488
1196.8705	1207.5238	1211.2985
1278.0237	1322.0110	1331.8789
1360.8144	1368.3036	1379.5508
1436.6630	1448.8995	1458.2069
1476.6231	1505.5773	1517.7917
1565.3330	1568.8283	1624.0048
1634.4333	1705.0239	3016.9021
3056.2017	3124.2608	3141.8461
3176.3189	3178.9835	3185.6469
3189.4162	3201.1736	3204.7272
3213.9437	3215.0807	3246.7262

i4 – i8

C	1.985990	2.423448	0.127123
C	0.654428	2.170659	-0.158908
C	0.184534	0.840066	-0.249125
C	1.130358	-0.162837	-0.091752
C	2.489810	0.082902	0.218754
C	2.921256	1.386517	0.326025
C	0.922996	-1.560407	-0.198569
C	2.166101	-2.195086	0.053756

C	3.122470	-1.228885	0.310196
C	-0.441554	-2.077938	-0.527270
C	-1.479118	-1.015331	-0.240506
C	-2.601140	-1.276095	0.481564
C	-3.573497	-0.286363	0.751753
C	-3.401951	1.021327	0.242416
C	-2.300913	1.357912	-0.475151
C	-1.194063	0.385664	-0.750982
H	2.318123	3.452226	0.208071
H	-0.029981	2.999752	-0.293532
H	-0.480053	1.104765	1.695756
H	3.954914	1.627262	0.549886
H	2.337528	-3.262964	0.050460
H	4.164507	-1.408446	0.537040
H	-0.667771	-2.993611	0.026512
H	-0.473158	-2.345070	-1.595848
H	-2.756952	-2.280867	0.863889
H	-4.450600	-0.534134	1.336028
H	-4.168377	1.766586	0.426797
H	-2.195177	2.361234	-0.872862
H	-1.067239	0.319951	-1.848131

Frequencies[1/cm]

-638.278	63.3428	73.7293
179.4709	198.8079	206.9914
278.0854	300.2470	317.3662
352.7612	370.5137	383.9962
454.5252	458.4819	485.1521
521.5700	549.0265	561.9851
580.4317	601.6341	613.5635
630.2492	669.5805	727.8048
734.1961	761.3791	769.8475
793.7780	799.2092	819.3340
843.9380	889.9106	910.4142
931.6155	941.3628	956.4859
985.1524	990.1074	1009.2227
1020.3512	1037.5440	1052.2345
1065.6748	1102.4398	1131.7207
1167.1024	1179.4616	1189.5854
1193.8322	1207.6596	1224.3576
1246.5949	1267.0789	1289.9545
1311.7538	1329.7231	1360.5097
1399.5003	1410.4207	1426.0273
1445.8886	1461.6510	1479.0578
1500.8483	1525.6187	1566.1900
1630.4630	1638.8423	1666.3760

2925.7024	2982.7214	3085.3542
3171.7814	3181.1886	3187.9387
3198.7046	3202.4474	3215.4354
3218.7968	3224.9541	3243.7985

i3 – i5

C	-4.136033	-0.463050	-0.383199
C	-3.823354	0.929221	-0.555839
C	-2.589973	1.415529	-0.259955
C	-1.592849	0.521682	0.244431
C	-1.891276	-0.903595	0.360631
C	-3.209670	-1.358231	0.057246
C	-0.286863	0.723111	0.610782
C	0.307643	-0.617316	0.886524
C	-0.747583	-1.579620	0.750692
C	0.690069	1.798282	0.216599
C	1.879270	0.956377	-0.178882
C	3.184559	1.187809	0.169429
C	4.149010	0.175176	0.040245
C	3.779866	-1.095855	-0.423510
C	2.479804	-1.366959	-0.778294
C	1.456073	-0.368624	-0.615341
H	-5.139608	-0.799655	-0.619958
H	-4.596699	1.593657	-0.924558
H	-2.363022	2.469857	-0.379118
H	-3.461154	-2.406940	0.172982
H	1.070536	-0.746395	1.649118
H	-0.671645	-2.632349	0.982558
H	0.946082	2.494078	1.022053
H	0.297063	2.390888	-0.618316
H	3.467430	2.150616	0.583115
H	5.178311	0.372436	0.315062
H	4.537071	-1.865630	-0.525387
H	2.205466	-2.338486	-1.172537
H	0.638009	-0.405708	-1.334368

Frequencies[1/cm]

-734.4359	52.8852	94.1124
130.0005	168.5794	201.7176
249.3114	324.0849	342.1453
391.1698	447.5439	469.7315
500.9469	539.3845	551.1020
556.1837	558.2223	611.0113
656.2043	695.8336	721.4571
726.0297	735.3768	761.2846
773.3266	791.2158	813.5384
848.7125	861.9369	877.5309

901.3570	946.1291	955.7277
977.4483	982.9124	996.4871
1005.3667	1007.7895	1010.6675
1033.9104	1051.7065	1065.2318
1106.1561	1131.9299	1142.9564
1167.8136	1175.9609	1183.3846
1196.9898	1210.0430	1226.1943
1262.3581	1276.7064	1316.4759
1339.9324	1353.5413	1391.3789
1407.5752	1437.3404	1451.8929
1475.3794	1482.8524	1501.7669
1567.1837	1578.0048	1606.9778
1630.5208	1686.3987	3032.4497
3074.5249	3116.0161	3171.4000
3179.3228	3181.7470	3185.8454
3188.1572	3199.3870	3205.6603
3209.8386	3215.1823	3238.9237

i5 – i6

C	-2.067116	2.367110	0.153773
C	-0.783264	2.204130	-0.201699
C	-0.229719	0.869021	-0.620618
C	-1.185704	-0.218921	-0.310889
C	-2.580298	-0.000887	0.042689
C	-3.006182	1.254154	0.277970
C	-0.899046	-1.524221	-0.191997
C	-2.139770	-2.222307	0.173489
C	-3.147343	-1.323720	0.293553
C	0.500660	-2.019881	-0.332304
C	1.516798	-0.907092	-0.107964
C	2.836670	-1.253553	0.151663
C	3.823978	-0.293582	0.332719
C	3.499334	1.055894	0.224877
C	2.194248	1.429002	-0.025836
C	1.162143	0.470642	-0.116327
H	-2.431002	3.362419	0.384214
H	-0.142246	3.075222	-0.280812
H	-0.130327	0.941147	-1.719609
H	-4.016344	1.458645	0.618005
H	-2.219287	-3.289074	0.341098
H	-4.170992	-1.525654	0.573470
H	0.663276	-2.443803	-1.333396
H	0.698205	-2.833978	0.373033
H	3.099927	-2.305754	0.204248
H	4.844624	-0.596841	0.535122
H	4.267634	1.813210	0.330438

H	1.949413	2.481220	-0.108849
H	0.614782	0.548503	1.624448

Frequencies[1/cm]

-982.2762	49.4926	98.9041
162.2408	205.8119	226.7082
253.8084	296.3298	368.4723
375.5385	417.6615	436.7977
449.0444	479.5127	506.5970
532.0497	548.0230	572.8859
595.0307	636.0398	656.6645
669.4946	711.3625	721.9922
737.3870	755.4922	765.2516
804.7934	826.6772	861.2262
881.4769	910.0847	937.3684
951.5163	958.8453	981.7316
998.8668	1006.8363	1012.3967
1025.0055	1059.1568	1079.7662
1101.1583	1144.4963	1153.2470
1184.7376	1191.5520	1198.9808
1212.6255	1220.2419	1225.4951
1249.4262	1277.3378	1299.5917
1312.9926	1341.0635	1363.1883
1398.9983	1436.7602	1461.6138
1475.2740	1494.4991	1515.2392
1556.2719	1617.9194	1644.8584
1662.9085	1728.1996	1741.4391
2943.4481	3008.7599	3067.5855
3175.7406	3181.7333	3190.7124
3193.8206	3204.8013	3209.5565
3217.0364	3217.3788	3250.2814

i3 – i10

C	2.583525	0.709047	0.727597
C	3.936735	1.005881	0.649729
C	4.796551	0.174606	-0.058840
C	4.297051	-0.965207	-0.677765
C	2.944995	-1.265675	-0.595075
C	2.065951	-0.422477	0.090243
C	0.634228	-0.762725	0.136324
C	-1.631641	1.998530	-0.408282
C	-0.370807	1.534422	-0.297910
C	-0.401261	0.094365	-0.025451
C	-3.962546	0.860089	-0.208602
C	-2.577241	0.897078	-0.204850
C	-1.829487	-0.273201	0.020943
C	-2.463533	-1.480468	0.256503

C	-3.857506	-1.516049	0.250650
C	-4.597210	-0.359857	0.020120
H	1.923009	1.338107	1.312959
H	4.323875	1.883333	1.155163
H	5.853655	0.407089	-0.117113
H	4.963059	-1.624368	-1.222800
H	2.558956	-2.157389	-1.078099
H	0.440505	-1.029823	2.281999
H	0.405084	-1.825413	0.166392
H	-1.916827	3.018187	-0.631491
H	0.532871	2.109836	-0.433723
H	-4.543612	1.759178	-0.382682
H	-1.896357	-2.385833	0.445682
H	-4.370766	-2.453843	0.429924
H	-5.680275	-0.409204	0.021798

Frequencies[1/cm]

-578.6425	46.2203	50.2964
82.1840	130.7556	172.8252
203.7089	239.7276	262.6042
276.3351	322.7109	390.2192
419.0684	430.5901	447.9112
521.6608	552.5294	576.5867
591.3784	638.0621	653.6809
668.9188	719.7285	732.1825
750.1324	775.1026	777.9396
822.7981	825.1922	854.2862
872.4716	878.7142	898.7989
919.9648	956.2876	965.1009
973.5096	1004.8741	1008.3620
1023.8523	1025.5640	1050.7655
1056.7348	1065.5989	1107.5526
1116.8773	1143.1048	1186.8740
1188.8311	1211.6311	1214.5570
1226.4228	1268.4244	1303.3786
1334.2052	1347.0360	1358.6094
1370.5235	1423.8012	1491.8165
1503.6452	1509.0116	1542.2966
1598.3725	1647.6487	1665.6950
1671.8874	1681.7209	1686.0140
3162.4100	3183.1787	3183.7094
3189.7112	3190.3699	3200.0208
3200.6874	3208.3134	3213.4423
3217.2736	3226.4552	3259.3358

i3 – i11

C	2.533097	0.849748	-0.446416
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C	3.883777	1.119903	-0.608493
C	4.841568	0.170069	-0.272771
C	4.433647	-1.068824	0.216706
C	3.088451	-1.344334	0.381506
C	2.105602	-0.387938	0.063084
C	0.711233	-0.739422	0.229688
C	-1.794558	2.030209	0.336052
C	-0.505811	1.613290	0.449803
C	-0.452208	0.162700	0.303062
C	-4.023137	0.769478	-0.093881
C	-2.649780	0.881099	0.098192
C	-1.836175	-0.272317	0.074532
C	-2.387094	-1.526584	-0.155762
C	-3.760327	-1.626352	-0.344519
C	-4.570248	-0.488868	-0.311371
H	1.801847	1.586096	-0.753307
H	4.190581	2.078639	-1.011563
H	5.895649	0.387756	-0.398971
H	5.171311	-1.821412	0.471628
H	2.778672	-2.310839	0.766182
H	0.056179	-0.314648	1.353049
H	0.461332	-1.794747	0.222916
H	-2.137941	3.051645	0.425290
H	0.344601	2.240718	0.670416
H	-4.656217	1.650160	-0.079728
H	-1.767439	-2.416527	-0.193997
H	-4.207924	-2.597037	-0.524896
H	-5.638872	-0.590948	-0.463483

Frequencies[1/cm]

-1705.0387	39.3952	50.5208
90.0402	153.6138	176.2951
214.1241	270.8353	290.4864
349.1833	419.4525	428.2592
445.4599	496.3875	552.6987
575.5137	585.8458	622.2062
635.0818	658.2344	709.6417
718.6249	729.0404	742.0519
771.6880	783.6149	799.2627
817.7396	856.0335	863.0567
881.9183	888.4030	925.2175
939.2409	961.5147	999.4218
1003.4810	1015.2939	1017.5133
1028.5896	1055.0978	1061.1689
1101.0809	1120.1290	1128.3960
1143.9901	1184.6276	1186.4725
1204.4585	1215.5765	1220.5245

1268.0408	1306.1132	1334.4907
1341.4069	1358.0682	1370.2181
1422.3464	1439.8256	1495.6362
1509.1746	1516.8281	1539.3833
1566.9285	1636.3222	1651.4836
1660.1746	1677.6279	2184.5677
3179.8704	3180.1514	3186.6946
3190.0319	3195.1023	3199.0515
3200.3886	3212.1184	3213.9381
3224.4925	3232.4020	3259.3670

i11 – i10

C	2.596442	0.736721	0.651888
C	3.957098	1.002035	0.599987
C	4.819446	0.124243	-0.046609
C	4.314858	-1.034555	-0.626965
C	2.956956	-1.305933	-0.568499
C	2.070999	-0.414314	0.050354
C	0.647144	-0.734714	0.084075
C	-0.395655	0.138804	0.108423
C	-0.399046	1.575065	-0.247478
C	-1.662904	1.983955	-0.455154
C	-2.436119	-1.473302	0.377033
C	-1.823545	-0.261690	0.108139
C	-2.585029	0.869158	-0.230526
C	-3.968148	0.789259	-0.309407
C	-3.824364	-1.551985	0.293486
C	-4.581149	-0.432541	-0.044972
H	4.348164	1.893034	1.077952
H	1.937946	1.402915	1.196358
H	5.882036	0.334667	-0.085766
H	4.983007	-1.730247	-1.121596
H	2.566922	-2.212650	-1.019457
H	0.492362	2.170010	-0.376631
H	-1.965153	2.977696	-0.758106
H	-1.855610	-2.346376	0.656066
H	-4.561493	1.658534	-0.571202
H	-4.321860	-2.492950	0.498778
H	-5.660811	-0.514639	-0.100426
H	0.405031	-1.794724	0.107244
H	-0.372449	0.593496	2.034136

Frequencies[1/cm]

-826.1143	49.6790	53.3594
88.4083	154.7241	181.8032
204.9341	264.0899	312.3119
332.6604	348.2190	409.5308

422.0329	432.8145	449.9573
513.0964	552.2709	578.2311
592.7473	637.0031	641.1619
656.6069	718.4251	732.5173
749.6291	773.3400	775.4873
815.4470	823.9544	856.0942
872.9795	878.8955	887.0666
901.8270	956.5017	966.4614
973.7678	1006.8953	1009.3402
1022.8376	1026.3464	1045.2528
1055.9844	1065.5873	1107.1329
1123.7400	1146.2389	1186.2604
1189.4219	1212.2847	1218.7801
1229.9419	1270.1515	1306.7471
1335.5621	1347.4390	1361.8752
1372.5225	1421.0362	1490.7604
1504.0886	1510.2669	1542.4416
1610.3752	1636.2366	1657.0367
1668.2350	1676.7004	1688.0846
3162.1396	3183.0231	3183.4666
3189.8209	3191.2013	3200.7686
3201.4159	3211.0433	3213.2896
3218.4965	3226.5059	3262.2693

i11 – i12

C	4.493743	-0.255751	0.411606
C	3.989862	-1.451804	-0.093075
C	3.677857	0.864889	0.507789
C	2.342896	0.783464	0.115191
C	1.824777	-0.443488	-0.366086
C	2.657076	-1.546990	-0.488364
C	1.390677	1.862531	-0.033983
C	0.075093	1.488448	-0.242746
C	0.396630	-0.397776	-0.681323
C	-0.478420	0.201543	0.346430
H	-0.023456	-0.856873	-1.568932
C	-1.957926	0.009633	0.205684
H	-0.143916	0.026240	1.371769
C	-2.717630	-0.350419	1.316721
C	-4.090359	-0.538277	1.211153
C	-4.725853	-0.366850	-0.011533
C	-3.978532	-0.005902	-1.126641
C	-2.607299	0.180877	-1.018665
H	5.532691	-0.193996	0.714800
H	4.638085	-2.316328	-0.180264
H	4.080572	1.806112	0.867081

H	2.268799	-2.482432	-0.876978
H	1.718912	2.882267	-0.197776
H	-0.636149	2.150203	-0.726144
H	-2.227391	-0.485682	2.275319
H	-4.663692	-0.818803	2.087576
H	-5.796663	-0.512374	-0.096014
H	-2.037715	0.465406	-1.897839
H	-4.465626	0.131499	-2.085549

Frequencies[1/cm]

- 692.4125	41.6014	68.0065
77.9333	161.7290	182.7113
253.9718	275.6547	373.1432
394.7316	416.8308	420.6575
467.9087	523.5249	539.3028
553.6942	583.7078	631.3264
638.6987	667.8973	693.3636
697.3938	724.4781	767.2668
779.1185	783.3947	822.1180
862.0611	871.1261	879.8714
893.4430	931.8122	946.1748
967.9226	1002.8272	1003.9518
1007.9668	1023.1732	1024.7128
1058.0942	1064.8150	1110.0441
1131.2169	1142.4499	1176.6806
1186.3181	1188.5074	1191.9578
1213.6558	1217.5459	1240.4597
1244.9120	1266.9055	1308.4878
1328.2746	1357.1388	1364.3677
1371.5302	1439.9974	1463.3015
1503.0856	1508.1883	1521.7799
1547.5393	1637.2045	1661.3635
1661.7665	1685.9099	3074.8947
3179.0087	3181.9535	3182.4594
3183.2261	3188.3893	3193.3938
3199.7204	3201.0606	3202.7486
3206.2508	3213.3197	3214.6939

i12 – i13

C	-4.543225	-0.081285	0.180582
C	-4.035795	-1.381555	0.388711
C	-3.688889	0.961702	-0.068234
C	-2.292510	0.753667	-0.125570
C	-1.779895	-0.556158	0.074720
C	-2.687361	-1.613088	0.339875
C	-1.375162	1.818417	-0.356578
C	-0.037914	1.591431	-0.426349

C	-0.384097	-0.765909	0.024884
C	0.495552	0.261382	-0.305801
H	0.007163	-1.757736	0.225313
C	1.965749	0.056477	-0.131586
C	2.609394	-1.051463	-0.684894
C	3.964661	-1.260979	-0.476317
C	4.701972	-0.361477	0.285774
C	4.071887	0.745109	0.838942
C	2.712941	0.951433	0.633589
H	-5.612831	0.089761	0.221049
H	-4.720396	-2.198326	0.586963
H	-4.076119	1.963339	-0.224014
H	-2.294441	-2.611945	0.498432
H	-1.764700	2.823153	-0.483363
H	2.042210	-1.739107	-1.303266
H	4.449714	-2.123361	-0.919487
H	5.762004	-0.522353	0.445281
H	2.224302	1.805232	1.090108
H	4.636761	1.449123	1.439528
H	0.647148	2.407092	-0.627510
H	0.515337	0.008898	-2.099516

Frequencies[1/cm]

-1052.9863	51.4228	65.7093
91.0321	169.1019	196.2475
254.7368	282.9829	330.7878
401.5757	420.4653	426.7456
444.3726	493.5331	521.0855
531.1674	546.6225	560.0386
591.8110	636.9964	644.5014
673.5249	716.8099	723.9004
765.5519	783.5533	786.9651
797.2487	843.0119	871.3930
877.3227	885.0198	912.3518
951.0743	960.4212	986.1828
1001.7180	1006.0209	1016.6583
1022.4874	1025.6053	1041.6672
1056.7113	1073.7999	1118.6147
1164.5589	1171.7030	1188.6913
1191.2941	1217.7520	1223.1728
1261.2288	1296.5375	1308.1799
1322.4482	1361.0309	1381.3200
1404.2032	1429.8630	1473.7482
1497.6504	1502.2432	1546.8055
1554.1348	1625.7342	1657.3571
1669.5767	1683.9281	1696.3759
3182.2786	3183.8262	3185.1195

3187.2677	3188.8121	3192.4179
3197.9045	3200.9740	3205.3084
3208.3043	3214.1247	3216.0930

i14 – p2

C	2.172747	2.354151	0.036952
C	0.800206	2.181318	0.047119
C	0.245245	0.882397	0.020941
C	1.154005	-0.158534	-0.008984
C	2.551319	-0.006367	-0.025585
C	3.072468	1.267661	-0.002295
C	0.824548	-1.546154	-0.041052
C	2.097814	-2.267069	-0.080149
C	3.110404	-1.367694	-0.070529
C	-0.493884	-1.903906	0.010802
C	-1.511577	-0.864253	-0.011736
C	-2.869649	-1.225880	-0.043760
C	-3.861964	-0.272157	-0.059488
C	-3.520942	1.084895	-0.039984
C	-2.197093	1.465902	-0.008313
C	-1.164918	0.513955	0.005951
H	2.572716	3.361730	0.057901
H	0.162361	3.056912	0.076130
H	4.141399	1.450252	-0.012854
H	2.200896	-3.342964	-0.105482
H	4.166136	-1.601976	-0.093015
H	-0.602171	-2.327313	1.979668
H	-0.812820	-2.935554	-0.097257
H	-3.128297	-2.279762	-0.051150
H	-4.903527	-0.570597	-0.085147
H	-4.299600	1.838932	-0.050991
H	-1.949458	2.520756	0.002860

Frequencies[1/cm]

-766.6044	95.5016	102.2932
186.2501	229.2141	249.8127
263.3359	290.0539	345.9232
398.2967	412.1235	424.6005
455.3922	474.7843	526.7735
574.3268	576.6250	596.1699
623.2176	646.9039	679.7095
685.4896	739.1367	775.7880
777.9531	778.9917	797.0605
839.7474	846.0932	870.4985
892.9958	935.0862	939.1409
953.4516	967.3728	983.7434
998.8738	1015.9026	1067.0344

1072.7890	1084.0774	1100.4650
1118.6172	1166.3407	1189.9386
1202.6954	1214.1878	1236.7826
1255.6486	1308.0304	1333.2455
1356.2086	1370.5399	1394.5868
1430.7781	1475.9421	1499.1533
1519.7039	1526.3640	1572.2999
1598.5867	1654.5423	1682.3267
1685.5196	1699.8716	3183.4766
3188.0232	3188.6154	3194.1328
3201.4736	3207.6004	3214.1669
3219.1461	3226.7439	3248.2937

i14 – i15

C	2.188732	2.345883	0.013310
C	0.807820	2.169085	0.036658
C	0.256492	0.873531	0.022639
C	1.167799	-0.175431	-0.017674
C	2.563781	-0.020188	-0.034208
C	3.083164	1.270707	-0.021934
C	0.853923	-1.576110	-0.021743
C	2.108408	-2.279913	-0.037854
C	3.125833	-1.362909	-0.055871
C	-0.478453	-1.939094	0.033528
C	-1.520144	-0.893991	0.098669
C	-2.917929	-1.238468	-0.042093
C	-3.873642	-0.267244	-0.089561
C	-3.522607	1.098062	-0.049907
C	-2.189115	1.461236	-0.002011
C	-1.159144	0.520616	0.036646
H	2.583047	3.356045	0.026771
H	0.168694	3.043336	0.069327
H	4.152169	1.452536	-0.035584
H	2.222893	-3.355096	-0.047475
H	4.182090	-1.593914	-0.083892
H	-1.128781	-1.381047	1.206614
H	-0.818942	-2.969494	0.024245
H	-3.189647	-2.287760	-0.083324
H	-4.916347	-0.550908	-0.179143
H	-4.293098	1.857822	-0.087159
H	-1.931586	2.513847	-0.021943

Frequencies[1/cm]

-1567.9983	84.6289	103.7537
201.8754	236.8559	250.4746
266.2242	360.4987	398.1783
414.4484	440.9217	472.9928

514.0399	555.7001	572.0399
583.9379	615.2407	639.4876
643.8742	669.7045	730.5806
739.5181	759.2564	771.9118
775.6510	823.3636	832.0399
833.9712	861.5520	904.0892
910.2171	926.4461	938.1765
958.4960	985.7929	994.8013
1047.4257	1063.2949	1074.5027
1081.5673	1102.7346	1127.3076
1162.6435	1183.7620	1198.9782
1211.1722	1226.6466	1255.9936
1295.3866	1310.9533	1349.7527
1366.2805	1371.2673	1407.2054
1449.4685	1481.4528	1491.0013
1500.6864	1530.3240	1558.8993
1604.6049	1636.2082	1657.4725
1674.1871	1879.0836	3184.5277
3185.1552	3194.8328	3197.2328
3201.2153	3205.3068	3213.2761
3222.4804	3224.1135	3244.1212

il5 – p2

C	2.191796	2.338011	0.022549
C	0.818165	2.172514	0.045882
C	0.256075	0.876311	0.036930
C	1.158744	-0.170590	0.009163
C	2.553747	-0.025320	-0.027257
C	3.083644	1.247238	-0.018219
C	0.820585	-1.564335	-0.019645
C	2.098547	-2.286409	-0.085926
C	3.108972	-1.388753	-0.084542
C	-0.478361	-1.917900	0.038544
C	-1.503210	-0.877307	0.149433
C	-2.873409	-1.239986	-0.029071
C	-3.850710	-0.286377	-0.123192
C	-3.507912	1.075993	-0.103047
C	-2.183652	1.459872	-0.045585
C	-1.152043	0.517996	0.031613
H	2.597212	3.343573	0.034446
H	0.184213	3.050958	0.076441
H	4.153513	1.422358	-0.043719
H	2.200710	-3.362178	-0.120242
H	4.164303	-1.623510	-0.121819
H	-0.804401	-2.952992	0.037866
H	-3.128638	-2.294034	-0.042211

H	-4.888774	-0.580839	-0.225082
H	-4.284794	1.828607	-0.170066
H	-1.937443	2.514578	-0.084619
H	-1.501773	-0.932285	1.873218

Frequencies[1/cm]

-1164.5939	96.4923	99.1129
196.8104	235.0009	252.1016
271.0487	369.9726	392.4866
407.5430	441.6744	469.6267
498.1455	515.2238	528.6912
574.4660	579.1036	603.3544
619.3737	647.7732	670.5895
679.3125	739.9953	770.4447
774.7988	782.4032	799.9708
837.3438	847.4869	860.7280
890.6092	929.6074	933.1047
939.1503	967.8440	976.8348
998.7615	1008.3869	1062.0723
1069.8017	1082.9978	1095.0765
1121.0286	1167.7189	1183.1065
1200.9922	1216.9497	1236.4386
1253.8147	1301.3819	1327.7585
1350.9148	1367.7568	1391.2007
1429.6775	1466.3388	1492.7832
1514.3144	1523.5813	1578.5881
1594.5579	1668.8779	1679.7515
1683.0764	1719.8472	3186.8219
3188.0585	3191.5568	3195.3710
3201.7588	3207.2554	3214.3187
3218.9485	3225.6000	3247.7637

i15 – i16

C	2.221411	2.332377	-0.008258
C	0.832224	2.172867	0.021972
C	0.279018	0.881461	0.027784
C	1.171623	-0.182046	-0.002061
C	2.564507	-0.041804	-0.027344
C	3.099902	1.252296	-0.032063
C	0.832228	-1.589070	0.000178
C	2.081284	-2.298463	-0.025080
C	3.108309	-1.387991	-0.045074
C	-0.495181	-1.946202	0.027894
C	-1.503524	-0.941465	0.083886
C	-2.928692	-1.252320	-0.034628
C	-3.870262	-0.291257	-0.083836
C	-3.513951	1.105609	-0.060175

C	-2.208938	1.477589	-0.007433
C	-1.137622	0.533005	0.059466
H	2.625593	3.338883	-0.010176
H	0.200191	3.052749	0.040931
H	4.170782	1.421052	-0.052692
H	2.187019	-3.374473	-0.031442
H	4.162456	-1.629870	-0.073168
H	-0.814012	-2.983441	0.021306
H	-3.200924	-2.300321	-0.092332
H	-4.914961	-0.567792	-0.166190
H	-4.292488	1.856176	-0.108650
H	-1.946809	2.528467	-0.036421
H	-1.370869	-0.288949	1.137466

Frequencies[1/cm]

-1856.6602	87.1584	100.5457
199.8222	228.0187	238.2143
263.9410	353.5838	394.8442
409.4298	422.9939	471.4652
492.5983	537.1747	566.5038
578.0793	605.0909	632.9702
647.6248	649.7979	687.9581
735.9307	739.7372	759.8549
773.5275	813.9763	817.7745
822.8923	837.4107	875.9035
880.3304	919.8751	932.4704
970.0921	978.6506	997.5295
1005.5670	1051.4520	1076.1681
1085.1954	1098.1074	1100.4419
1160.1807	1181.1050	1200.1717
1210.7096	1227.1446	1245.8397
1288.7414	1317.2529	1326.9500
1377.8710	1380.3388	1403.1686
1427.3211	1475.7920	1488.2142
1501.5994	1526.8822	1557.4733
1581.0203	1619.0388	1671.5294
1691.6882	2178.0455	3183.4224
3189.3349	3191.7240	3198.7859
3204.2274	3210.1199	3212.7000
3221.7417	3225.9766	3242.5515

il6 – p2

C	2.175080	2.337454	-0.040820
C	0.802126	2.162947	0.016967
C	0.255542	0.864957	0.046419
C	1.159747	-0.176226	0.018637
C	2.554203	-0.024008	-0.037010

C	3.073817	1.252435	-0.067695
C	0.827217	-1.568564	0.026362
C	2.105481	-2.286424	-0.013209
C	3.114529	-1.385190	-0.051704
C	-0.481025	-1.927059	0.019262
C	-1.499021	-0.911261	0.023573
C	-1.161517	0.486919	0.134362
C	-2.207641	1.439358	-0.027790
C	-3.516424	1.044827	-0.113989
C	-3.850311	-0.321005	-0.093201
C	-2.857039	-1.271149	-0.040275
H	2.572962	3.345788	-0.063693
H	0.162466	3.037225	0.045934
H	4.141919	1.435067	-0.110975
H	2.211980	-3.362398	-0.015214
H	4.170173	-1.618142	-0.090052
H	-0.792597	-2.966717	-0.009822
H	-1.173145	0.487794	1.910332
H	-1.960907	2.493791	-0.042072
H	-4.299156	1.788846	-0.206871
H	-4.889188	-0.623990	-0.150324
H	-3.113089	-2.325344	-0.066562

Frequencies[1/cm]

-1110.8633	94.9766	99.9341
200.8333	232.1440	245.1156
281.5842	377.8415	397.1543
410.5013	443.4253	468.8863
475.5978	492.7004	537.4974
575.3758	579.5937	594.5160
628.5346	645.7110	670.9811
679.6384	740.4260	768.2630
775.0937	783.8528	800.0715
837.5050	849.4031	869.2483
887.7742	931.8560	934.7260
939.3393	965.0410	982.3167
998.0999	1011.7388	1060.8792
1070.8059	1082.6583	1098.4376
1119.5357	1162.5586	1185.3068
1203.8229	1218.7608	1240.7368
1252.1234	1303.4792	1334.5332
1356.3945	1364.7749	1396.8027
1428.5372	1466.0177	1482.1345
1516.2104	1530.4240	1572.1107
1587.5910	1670.0568	1676.8915
1685.3207	1702.4317	3183.6560
3186.3754	3188.0999	3195.0699

3201.5060	3209.9994	3214.4925
3221.3940	3225.4946	3247.1688

i16 – i17

C	2.209833	2.327701	-0.053078
C	0.829516	2.191175	-0.011388
C	0.255957	0.873632	0.094025
C	1.177902	-0.192093	0.037487
C	2.553952	-0.052396	-0.009445
C	3.099441	1.244347	-0.041845
C	0.817275	-1.587354	0.026300
C	2.069456	-2.315005	-0.016162
C	3.091112	-1.409934	-0.040816
C	-0.505265	-1.919341	-0.004418
C	-1.519319	-0.911793	0.008552
C	-1.174469	0.494744	0.067903
C	-2.228142	1.458897	-0.012846
C	-3.532362	1.055690	-0.062929
C	-3.877245	-0.314040	-0.049766
C	-2.884034	-1.261921	-0.022426
H	2.617459	3.331289	-0.115683
H	0.197343	3.069272	-0.037007
H	4.168416	1.415165	-0.080162
H	2.167631	-3.391029	-0.037978
H	4.144320	-1.654548	-0.086495
H	-0.823752	-2.957441	-0.041942
H	-0.418594	0.705806	1.232300
H	-1.980603	2.512854	-0.035558
H	-4.316018	1.802182	-0.130198
H	-4.918139	-0.610746	-0.081486
H	-3.139704	-2.316659	-0.040684

Frequencies[1/cm]

-1554.3389	98.2359	111.6702
192.4729	218.0065	237.6965
281.1179	377.0947	397.7999
416.7488	440.4234	466.3903
496.3458	554.1006	560.6410
585.3202	614.6921	636.4267
653.4037	662.7912	706.9658
713.2022	750.0866	767.7259
780.6506	815.1870	825.6538
830.7348	854.3010	868.6914
915.8184	936.0403	950.5385
971.9778	976.8430	997.3182
1007.1205	1043.6072	1058.7579
1075.8476	1083.8266	1107.6401

1163.3600	1171.6417	1192.6719
1207.9093	1233.9289	1255.4067
1293.6408	1329.9580	1334.8704
1370.7445	1377.6438	1409.0316
1448.2493	1471.8099	1480.1229
1512.4356	1535.5789	1548.2211
1573.1070	1637.8690	1648.2911
1662.9621	1673.7491	3179.2183
3184.0472	3185.3597	3192.9030
3209.6459	3213.2592	3219.2444
3222.5884	3223.1944	3247.1804

i17 – p2

C	-2.156854	2.333493	-0.101424
C	-0.794521	2.170496	-0.008057
C	-0.235098	0.861666	0.168650
C	-1.151467	-0.188018	0.043095
C	-2.542472	-0.032551	-0.030613
C	-3.060962	1.242389	-0.089827
C	-0.816863	-1.572444	0.040260
C	-2.096591	-2.294192	-0.021959
C	-3.104493	-1.394255	-0.065993
C	0.490974	-1.926054	0.046432
C	1.512962	-0.899619	0.022439
C	2.868271	-1.269181	-0.054140
C	3.866160	-0.321286	-0.104963
C	3.535121	1.036791	-0.077194
C	2.213931	1.426614	0.004579
C	1.182721	0.481845	0.052626
H	-2.556563	3.336981	-0.195840
H	-0.152436	3.042733	-0.017224
H	-4.127573	1.424899	-0.158108
H	-2.200515	-3.370085	-0.047960
H	-4.159085	-1.625469	-0.131292
H	0.807224	-2.964549	0.033786
H	3.119887	-2.324556	-0.076664
H	4.904240	-0.626629	-0.166087
H	4.317280	1.786168	-0.116831
H	1.973189	2.482644	0.037236
H	-0.190563	0.903711	1.895517

Frequencies[1/cm]

-1135.3171	93.7969	102.7351
195.2653	228.9644	242.9964
278.7909	378.8026	395.1851
413.6767	442.8648	454.8331
488.1854	523.7482	535.4428

572.5397	584.2879	595.3698
630.6011	647.4677	667.8439
686.2093	742.7219	771.6970
776.4358	778.0701	797.0691
836.4462	861.7646	872.0787
893.4273	925.0083	930.9274
939.4901	964.7134	981.9411
997.4483	1015.4564	1058.9625
1072.4347	1079.3552	1097.9975
1116.3924	1167.5230	1188.9724
1204.6189	1218.6531	1242.4523
1253.0885	1299.1240	1330.6709
1351.1337	1362.6401	1389.1674
1432.1774	1474.8511	1489.6537
1510.8257	1526.2862	1580.7269
1605.6811	1655.9081	1670.1364
1688.0618	1698.2846	3183.2972
3187.2042	3189.2224	3194.2007
3203.6855	3207.3726	3216.3346
3220.4031	3226.1917	3247.9578

i14 – i18

C	-2.157747	2.362097	-0.024745
C	-0.773684	2.165925	0.010451
C	-0.243287	0.870853	0.047534
C	-1.169870	-0.160658	0.060368
C	-2.560090	0.003325	-0.013455
C	-3.063757	1.303864	-0.045343
C	-0.866981	-1.572591	0.065592
C	-2.134873	-2.264747	-0.035550
C	-3.136219	-1.330225	-0.065174
C	0.555324	-1.944421	-0.008120
C	1.541801	-0.891923	-0.012907
C	2.906359	-1.234465	-0.064643
C	3.889557	-0.267528	-0.067659
C	3.538365	1.081506	-0.008555
C	2.202742	1.442247	0.040995
C	1.182456	0.488576	0.033467
H	-2.535821	3.378157	-0.052559
H	-0.124735	3.033233	-0.005010
H	-4.129445	1.497303	-0.096256
H	-2.258475	-3.338028	-0.061415
H	-4.193738	-1.549498	-0.119427
H	0.848055	-2.981025	-0.114172
H	-0.228866	-1.848722	1.108565
H	3.178960	-2.284100	-0.103591

H	4.933034	-0.557931	-0.110854
H	4.306249	1.846018	-0.002751
H	1.944221	2.493593	0.083941

Frequencies[1/cm]

-1702.2493	86.7705	104.7870
200.4055	239.9822	246.5214
276.8495	359.5578	389.8397
414.4585	448.6672	472.2143
506.3532	556.3442	572.9591
589.3319	613.3017	640.1112
647.6980	681.6382	706.5772
738.3757	756.8760	763.2794
774.3349	789.4804	825.4718
831.1711	868.8862	883.7228
902.0609	912.1410	938.7704
968.1584	988.4636	1004.4116
1053.5828	1072.9069	1077.6945
1086.7725	1101.9586	1121.7876
1163.7063	1183.3363	1195.8481
1211.5322	1228.5174	1269.2126
1305.2450	1316.2034	1338.7377
1344.3142	1370.0503	1397.7944
1442.0254	1475.7926	1501.0342
1511.0725	1512.7931	1557.1921
1613.8881	1644.4905	1665.1052
1683.1510	2207.8006	3182.0052
3185.4736	3194.4581	3201.0149
3205.6903	3213.5003	3218.9277
3220.1283	3228.2803	3248.6047

i18 – p2

C	-1.181330	0.498398	0.041048
C	-2.222648	1.437403	0.083606
C	-3.543393	1.045716	0.027537
C	-3.871667	-0.311187	-0.077468
C	-2.871610	-1.254820	-0.116479
C	-1.512490	-0.885355	-0.052376
C	-0.497375	-1.905042	-0.074211
C	3.104285	-1.345637	-0.083545
C	2.111264	-2.258103	-0.023729
C	0.816723	-1.551660	0.099556
C	3.043947	1.288594	-0.081729
C	2.532887	0.008340	-0.023119
C	1.143630	-0.150464	0.072787
C	0.225535	0.881335	0.055771
C	0.767204	2.182896	0.001192

C	2.138813	2.366723	-0.055200
H	0.904235	-1.705584	1.967767
H	-1.985924	2.491807	0.164287
H	-4.329323	1.791327	0.064032
H	-4.910495	-0.616630	-0.123817
H	-3.120752	-2.308331	-0.191145
H	-0.803334	-2.942148	-0.164386
H	4.160237	-1.566661	-0.161358
H	2.223839	-3.332896	-0.041114
H	4.108990	1.476129	-0.161711
H	0.121036	3.052770	-0.013708
H	2.528838	3.377405	-0.100699

Frequencies[1/cm]

-966.6115	94.2233	107.8559
198.0605	238.5200	247.4321
284.8774	314.2314	383.4832
408.9633	423.8771	457.8219
472.3958	479.2919	513.5740
571.2160	577.0440	595.7236
621.2749	645.9184	666.3850
684.2430	739.4811	771.7675
775.2317	780.3200	794.5192
836.9542	845.1022	873.2422
883.3349	913.9913	932.3588
940.2049	964.7674	980.8471
999.4906	1014.5167	1066.9132
1071.8282	1083.0900	1096.7222
1121.6681	1166.4305	1188.4820
1203.7390	1215.2513	1241.1834
1255.5917	1306.8819	1336.3781
1353.4668	1368.0521	1396.2032
1425.2282	1470.9707	1493.8329
1515.2824	1528.1379	1576.7771
1604.6380	1649.0109	1680.7139
1684.8006	1695.3618	3183.6830
3187.6360	3191.4052	3193.9457
3200.9436	3207.0692	3213.5069
3218.3905	3227.2355	3250.6909

i18 – i19

C	2.008107	2.420492	0.010722
C	0.656677	2.149308	0.090686
C	0.186641	0.825468	0.196356
C	1.143890	-0.192206	0.292710
C	2.502626	0.075855	0.030149
C	2.942410	1.381907	-0.064617

C	0.760578	-1.575737	0.502536
C	2.586343	-2.234970	-0.521293
C	3.273368	-1.124531	-0.315848
C	-0.564920	-1.923829	0.330504
C	-1.561058	-0.932164	0.061965
C	-2.909660	-1.305708	-0.114887
C	-3.898126	-0.359422	-0.251708
C	-3.567165	0.999945	-0.206237
C	-2.254439	1.389527	-0.036045
C	-1.223357	0.447067	0.094139
H	2.341990	3.448706	-0.069780
H	-0.042832	2.974180	0.039182
H	3.987135	1.597289	-0.260869
H	2.863669	-3.261100	-0.721262
H	4.352065	-1.059899	-0.454889
H	-0.891646	-2.940227	0.522047
H	-3.157669	-2.361941	-0.134018
H	-4.929542	-0.663648	-0.387955
H	-4.342916	1.750373	-0.305902
H	-2.025324	2.447591	-0.007598
H	1.353575	-2.177342	1.186244

Frequencies[1/cm]

-618.5197	76.9939	102.3632
181.2383	216.4573	255.1673
268.8745	328.5588	389.1520
423.6821	449.7416	465.1639
502.6153	524.4372	527.0942
559.9329	591.1615	606.0952
620.4362	679.2055	684.2032
696.3468	754.3352	768.8084
773.5684	790.3353	832.2624
835.1039	862.0706	872.2990
888.7670	904.2591	910.3126
925.1068	967.5048	974.5239
995.8144	1009.9730	1072.1624
1096.8462	1102.2658	1160.3820
1173.5787	1191.5153	1195.3369
1214.1716	1227.0529	1236.7399
1289.4454	1301.0662	1324.5739
1365.1932	1382.4863	1427.3518
1455.1695	1462.5028	1503.3597
1530.6306	1556.9973	1619.5572
1630.7755	1652.9296	1675.7752
1684.3340	3129.8625	3141.4795
3183.0742	3187.7119	3192.0588
3194.4973	3201.8019	3208.7982

3216.1821 3225.2771 3242.6747

i19 – p4

C	-1.665555	2.540045	-0.002650
C	-0.347139	2.146637	-0.032395
C	0.022780	0.785558	0.021905
C	-1.007961	-0.187008	0.109619
C	-2.324502	0.276215	0.147309
C	-2.694935	1.583112	0.086714
C	-0.680731	-1.584092	0.155835
C	-4.437891	-1.603870	-0.699714
C	-4.057102	-1.214198	0.383771
C	0.605057	-1.991514	0.122403
C	1.684396	-1.048611	0.040569
C	3.021082	-1.494635	0.009490
C	4.063206	-0.604001	-0.069388
C	3.795106	0.771363	-0.119960
C	2.498290	1.228180	-0.091276
C	1.408100	0.337414	-0.010837
H	-1.914484	3.594788	-0.050032
H	0.415828	2.910946	-0.102548
H	-3.736941	1.883452	0.105336
H	-4.652580	-1.851183	-1.712561
H	-3.997800	-1.089637	1.441818
H	0.848166	-3.048453	0.155520
H	3.214207	-2.561754	0.049372
H	5.086881	-0.959586	-0.092355
H	4.613490	1.479596	-0.181873
H	2.324279	2.295801	-0.131160
H	-1.494256	-2.297534	0.210119

Frequencies[1/cm]

-377.4344	31.1899	44.2952
95.6451	100.5346	104.8757
205.7200	237.8446	243.6547
251.9995	409.6771	415.2256
442.6357	458.9212	501.9425
507.2716	522.7387	563.7514
571.0142	598.9193	626.6319
683.5150	703.2736	725.2122
728.8077	767.9889	771.0130
780.3201	791.1052	824.0877
843.2399	847.5293	893.6591
894.7395	909.5565	977.7536
993.4770	1009.4215	1012.0916
1016.2283	1072.4564	1076.6945
1114.5441	1171.8507	1189.5858

1196.1783	1220.9815	1223.8703
1251.2047	1295.1255	1328.4327
1373.4677	1387.8658	1421.0023
1452.3743	1476.4918	1496.5633
1532.8983	1572.7653	1630.0472
1671.7325	1690.4926	1703.5446
1955.6590	3182.5932	3182.9963
3186.3813	3193.6459	3197.6720
3208.5331	3214.2214	3216.5330
3227.9797	3398.4274	3491.6325

i14 – i20

C	-2.588311	1.983166	-0.067092
C	-1.257910	2.165012	0.328637
C	-0.443558	1.039343	0.477720
C	-1.063172	-0.183937	0.313071
C	-2.313269	-0.394223	-0.244443
C	-3.119178	0.731125	-0.409241
C	-0.258637	-1.390212	0.299651
C	-1.092476	-2.362522	-0.427682
C	-2.302878	-1.800055	-0.685696
C	1.000414	0.791817	0.387425
C	1.298479	-0.661484	0.356995
C	0.693755	-1.552783	1.421548
C	1.968260	1.687401	-0.012110
C	3.184540	1.241519	-0.537770
C	3.418420	-0.137820	-0.728646
C	2.510089	-1.071731	-0.313292
H	-3.213377	2.860743	-0.191152
H	-0.868510	3.169960	0.449778
H	-4.114721	0.666851	-0.834175
H	-0.823577	-3.391968	-0.621418
H	-3.131818	-2.308114	-1.161546
H	0.442392	-1.100770	2.377882
H	1.173909	-2.523597	1.502574
H	1.748239	2.749848	0.005372
H	3.926659	1.961272	-0.861400
H	4.339892	-0.460284	-1.199978
H	2.713511	-2.131635	-0.420382

Frequencies[1/cm]

- 364.7144	87.1805	111.1704
203.6276	238.5202	254.0601
311.1493	370.7683	395.5737
455.1076	471.5537	477.2541
522.1030	555.8947	570.2405
585.5766	610.5213	643.4285

660.0412	679.3602	711.5706
739.2450	757.7630	763.5621
790.9394	817.4928	836.9837
839.0290	909.8247	919.4960
942.3711	945.0997	954.9124
976.9298	984.1645	989.3778
1031.2625	1056.3202	1075.3534
1077.0152	1111.6083	1119.3258
1132.9733	1148.7354	1180.8455
1192.2962	1236.3735	1268.9862
1298.7460	1316.5121	1320.4983
1354.8387	1363.4940	1409.2907
1423.5913	1458.1355	1487.9550
1496.8429	1517.7450	1552.1962
1562.3149	1607.3989	1663.9278
1679.8033	3107.9326	3183.2025
3184.4935	3188.3199	3196.0214
3197.6143	3202.6023	3208.0990
3216.4079	3217.9018	3240.9496

i20 – i21

C	-2.533274	2.103435	-0.021602
C	-1.157512	2.286486	0.188799
C	-0.353982	1.152114	0.302938
C	-1.003068	-0.059828	0.283122
C	-2.299097	-0.284386	-0.143033
C	-3.116146	0.849478	-0.236301
C	-0.121847	-1.235514	0.180824
C	-1.031661	-2.187163	-0.572641
C	-2.312743	-1.661954	-0.631992
C	1.084433	0.825301	0.141350
C	1.219688	-0.571952	-0.060294
C	-0.235105	-2.205405	1.312294
C	2.200219	1.645896	0.086291
C	3.446241	1.077841	-0.170344
C	3.576424	-0.292314	-0.365139
C	2.461213	-1.127874	-0.299148
H	-3.160188	2.983923	-0.113176
H	-0.743530	3.288460	0.193150
H	-4.154271	0.784811	-0.542125
H	-0.727448	-3.155779	-0.943347
H	-3.175510	-2.191489	-1.013608
H	-1.011812	-2.093053	2.055320
H	0.477661	-3.016430	1.391117
H	2.105200	2.715839	0.235299
H	4.324334	1.711754	-0.220089

H 4.553328 -0.715339 -0.569827
H 2.569528 -2.197670 -0.443443

Frequencies[1/cm]

-491.1805	101.2729	126.1857
150.9613	212.2160	246.7570
318.9248	350.6554	382.1422
428.0089	446.3343	476.9927
503.0187	528.8115	549.6891
566.5869	595.0399	609.1801
632.2909	634.3064	702.5360
708.0368	736.2346	769.3373
780.4368	785.0940	810.5271
840.2645	873.8453	875.9487
901.5990	906.8018	942.3274
969.9168	992.4515	1012.2827
1017.6606	1049.9192	1059.8649
1067.5568	1082.4185	1097.7670
1116.2488	1156.6930	1188.7379
1191.0305	1224.7544	1272.0438
1281.7933	1316.6082	1323.2111
1333.8105	1365.7963	1389.2299
1408.2558	1441.5368	1484.4405
1495.5162	1517.6475	1530.9777
1649.2454	1656.7186	1682.2253
1692.2741	3164.1119	3183.5518
3184.2515	3190.6516	3199.2946
3201.3568	3209.2834	3213.5184
3224.0406	3246.5165	3290.9319

i21 – i22

C 2.392156	-2.260511	0.016827
C 0.999261	-2.361615	0.123800
C 0.253431	-1.185941	0.212746
C 0.952743	0.005145	0.255781
C 2.308165	0.149183	-0.028789
C 3.052975	-1.033112	-0.104199
C 0.085477	1.164950	0.212820
C 1.402937	2.362054	-0.413820
C 2.513962	1.486438	-0.541147
C -1.168213	-0.805423	0.074527
C -1.257996	0.615627	0.002156
C 0.577392	2.396858	0.846541
C -2.316209	-1.576624	-0.006410
C -3.548099	-0.945627	-0.165800
C -3.635446	0.443114	-0.230476
C -2.493394	1.232559	-0.136620

H	2.974975	-3.172093	-0.054664
H	0.525781	-3.336459	0.088102
H	4.116115	-1.014968	-0.318258
H	1.246043	3.150920	-1.140407
H	3.324949	1.715361	-1.223009
H	1.115782	2.291732	1.789927
H	-0.137531	3.215861	0.868301
H	-2.258608	-2.657829	0.056557
H	-4.450588	-1.542102	-0.236317
H	-4.604334	0.913364	-0.354363
H	-2.567436	2.313763	-0.183492

Frequencies[1/cm]

- 739.1293	96.7598	125.2908
157.0975	203.2979	254.2813
288.3429	347.2610	406.1103
432.6015	452.8099	509.4280
522.4306	551.4962	559.4590
590.0484	606.6089	628.2191
660.0184	689.7796	722.5574
760.0242	766.0294	775.9092
789.9427	821.0305	845.1671
869.7526	896.2736	910.3292
939.2654	945.1915	967.6774
986.6070	1007.5266	1039.7103
1054.3515	1062.7347	1089.1564
1111.9291	1126.4118	1148.9712
1163.0351	1186.3607	1191.6938
1195.7246	1234.3954	1277.7783
1295.9494	1327.6770	1345.3226
1352.7422	1375.6473	1378.9660
1410.0969	1479.3193	1491.8611
1497.9593	1517.2508	1527.4690
1640.9734	1646.4896	1665.1642
1678.2360	3071.9787	3167.1396
3183.9590	3184.5603	3190.9419
3192.2743	3196.3557	3201.3189
3207.1000	3209.1287	3213.4774

i22 – p1

C	2.135816	-2.457800	0.027237
C	0.717377	-2.418270	0.027146
C	0.095324	-1.196659	0.008347
C	0.895949	-0.033612	-0.008576
C	2.288997	-0.041459	-0.016566
C	2.907620	-1.316732	0.004440
C	0.105044	1.134367	-0.037200

C	2.174134	2.379477	-0.077932
C	2.924587	1.234592	-0.061435
C	-1.304569	-0.729686	-0.004759
C	-1.295120	0.687028	-0.032132
C	0.741079	2.362314	-0.023482
C	-2.503376	-1.420910	0.008386
C	-3.696157	-0.698708	-0.002909
C	-3.686748	0.692463	-0.025297
C	-2.484241	1.397047	-0.039245
H	2.626328	-3.424670	0.042993
H	0.155674	-3.345892	0.040876
H	3.989758	-1.393106	0.001611
H	2.672097	3.341541	-0.113832
H	4.007301	1.295426	-0.090993
H	0.193228	3.287198	-0.163685
H	0.532402	2.815632	1.854182
H	-2.519423	-2.505116	0.029432
H	-4.642575	-1.227238	0.007841
H	-4.625733	1.234087	-0.030837
H	-2.483362	2.481429	-0.053730

Frequencies[1/cm]

- 820.7478	100.0733	122.4386
153.2811	205.6892	234.3649
298.3075	325.6374	333.6644
366.7308	439.3514	448.5774
480.3960	492.0464	498.0357
572.8003	575.5937	580.9932
631.1015	638.7514	669.8632
691.1627	767.6508	769.7087
782.8166	806.5199	811.3924
821.8321	853.4249	900.9828
918.1530	940.7618	970.5618
972.6232	993.7316	1002.9091
1010.9918	1013.2388	1034.1613
1056.0556	1066.5078	1115.1938
1139.5103	1167.5714	1188.7718
1191.4266	1216.2633	1237.9319
1262.4647	1303.9607	1323.6829
1347.5158	1410.6706	1418.7197
1453.8058	1472.3764	1486.7888
1508.3906	1522.9335	1544.4786
1651.6850	1656.1058	1682.5954
1689.2274	1694.4481	3185.3924
3185.8834	3187.7089	3192.7923
3196.3706	3197.2501	3202.8540
3209.7751	3211.8586	3214.8643

i22 – i23

C	2.102464	2.479359	-0.010572
C	0.711116	2.433202	0.007321
C	0.086057	1.183399	0.031972
C	0.893538	0.044969	0.056954
C	2.288147	0.061222	0.006483
C	2.891601	1.321696	-0.019569
C	0.084473	-1.147960	0.072188
C	2.222788	-2.395425	-0.080721
C	2.945131	-1.232345	-0.054311
C	-1.299086	0.714147	0.015738
C	-1.299394	-0.710131	0.020487
C	0.797278	-2.443172	-0.009204
C	-2.505488	1.404651	-0.014279
C	-3.695871	0.690390	-0.043055
C	-3.692158	-0.708463	-0.043801
C	-2.500623	-1.416610	-0.011932
H	2.595331	3.445075	-0.030469
H	0.135782	3.352136	-0.004290
H	3.972275	1.406016	-0.058141
H	0.396829	-1.860364	1.100319
H	2.746621	-3.342151	-0.147616
H	4.027457	-1.272705	-0.099131
H	0.245595	-3.365916	-0.125633
H	-2.517602	2.489320	-0.019302
H	-4.640563	1.221400	-0.069015
H	-4.633842	-1.244835	-0.073284
H	-2.507717	-2.501547	-0.015636

Frequencies[1/cm]

- 1794.9248	100.3990	124.5133
167.7184	204.1819	237.6276
289.8960	351.6475	398.5151
438.6056	472.6224	473.6830
495.0429	553.5771	564.4329
567.2053	610.9779	617.3615
623.9006	684.6175	712.7256
755.8668	770.4661	773.3755
784.8355	806.4250	810.7462
837.5367	884.3179	905.7094
908.8847	963.0086	965.4743
981.0713	986.8339	1001.5145
1023.4471	1053.2391	1076.1587
1095.1859	1118.1168	1131.5744
1164.7987	1184.2417	1185.4392

1205.5531	1245.8034	1266.1962
1314.5083	1327.2398	1336.2172
1364.6362	1388.4718	1408.0659
1451.4790	1465.7777	1488.8654
1517.6788	1535.4521	1555.5489
1627.5590	1633.7567	1673.9315
1676.6316	2174.4660	3181.4721
3184.0622	3187.9962	3192.1936
3196.1298	3199.6552	3208.6200
3209.4742	3212.9346	3231.8138

i23 – p1

C	2.149596	2.433745	-0.020585
C	0.733183	2.397270	-0.005389
C	0.108016	1.174892	0.037436
C	0.904811	0.016151	0.070999
C	2.294970	0.016358	0.013849
C	2.918046	1.290104	-0.018770
C	0.107699	-1.164553	0.118761
C	2.155172	-2.405454	-0.126283
C	2.920870	-1.260104	-0.056868
C	-1.293333	0.716083	0.014940
C	-1.300471	-0.696941	0.040948
C	0.743646	-2.382459	-0.080568
C	-2.485763	1.419240	-0.041340
C	-3.683734	0.709310	-0.078427
C	-3.687416	-0.682301	-0.058714
C	-2.493020	-1.397032	0.004515
H	2.642553	3.399027	-0.051020
H	0.172074	3.324627	-0.039542
H	3.999878	1.362108	-0.054351
H	0.038638	-1.244292	1.973543
H	2.652919	-3.363600	-0.225721
H	4.002750	-1.328395	-0.095481
H	0.184081	-3.308318	-0.147382
H	-2.489860	2.503551	-0.061223
H	-4.624218	1.246382	-0.124903
H	-4.630518	-1.215826	-0.090276
H	-2.501937	-2.481110	0.029330

Frequencies[1/cm]

- 1023.5632	103.5346	123.4773
167.2657	205.9051	252.5936
286.8952	351.4925	382.4489
440.8986	447.7388	464.1669
478.9922	492.6145	499.7596
572.8693	577.8880	580.1223

632.0445	634.9036	659.2483
692.6822	757.8765	769.9285
782.0900	796.6191	805.5341
822.5231	854.6179	899.9895
919.2700	922.5581	938.7052
971.4471	993.7050	998.5518
1006.7821	1011.7215	1050.6949
1056.9301	1076.7552	1116.2704
1140.4701	1165.4929	1188.7928
1189.3457	1215.7845	1240.5650
1260.8919	1305.5438	1323.4636
1348.4027	1399.1934	1413.3672
1448.3036	1464.2956	1483.6137
1508.1386	1521.8025	1544.8318
1646.6471	1655.1651	1678.7705
1691.5090	1692.1657	3185.5635
3185.9793	3186.7598	3193.1089
3196.9282	3199.8110	3203.1088
3209.9387	3211.6314	3214.9012

i23 – i24

C	2.124244	2.454143	-0.021548
C	0.728769	2.416625	-0.003295
C	0.095803	1.165414	0.010194
C	0.903221	0.017558	0.032929
C	2.304791	0.027453	0.001575
C	2.909343	1.302432	-0.025575
C	0.129232	-1.179124	0.070071
C	2.190550	-2.411843	-0.058833
C	2.946809	-1.240990	-0.032491
C	-1.273614	0.725476	0.034058
C	-1.290357	-0.721338	0.084496
C	0.796621	-2.426671	-0.023397
C	-2.485995	1.419409	0.000842
C	-3.674810	0.719342	-0.046727
C	-3.684239	-0.694904	-0.079489
C	-2.525060	-1.423548	-0.030034
H	2.618876	3.419255	-0.040458
H	0.158428	3.338335	-0.009321
H	3.990342	1.386515	-0.055066
H	-0.652676	-1.060566	1.181459
H	2.710887	-3.361630	-0.120674
H	4.029064	-1.296682	-0.061830
H	0.250548	-3.361456	-0.053567
H	-2.488181	2.504021	-0.014566
H	-4.615719	1.255342	-0.081948

H -4.633398 -1.213020 -0.158649
H -2.540016 -2.506729 -0.062030

Frequencies[1/cm]

- 1422.9114	103.6549	128.8637
182.7182	205.2667	239.5729
288.4728	353.1113	410.9303
445.8128	475.3367	490.8811
497.5414	560.0505	562.2945
572.0876	618.7468	629.1591
636.3936	676.4403	726.0881
752.3172	755.7378	770.5462
791.5032	818.8838	832.2752
848.1140	864.3006	899.2202
904.2815	965.6704	978.7747
982.3630	992.3786	997.3950
1034.7284	1038.5897	1081.2374
1090.3283	1122.5868	1123.5297
1159.5049	1181.3723	1190.5567
1196.4243	1248.2668	1249.6226
1304.9338	1338.7971	1346.1158
1361.6398	1395.9919	1409.2876
1454.8443	1472.9800	1484.2960
1514.1595	1543.3939	1577.3255
1587.7113	1623.3726	1653.6268
1661.2555	1878.0274	3183.6871
3185.8250	3186.7252	3192.9542
3197.7882	3203.1048	3206.6731
3209.6727	3214.6617	3216.6288

i24 – p1

C	2.169629	2.420900	-0.020155
C	0.751728	2.391301	0.025001
C	0.120918	1.173097	0.042446
C	0.912777	0.003176	0.020174
C	2.305643	0.001395	-0.031794
C	2.932368	1.275733	-0.050812
C	0.123032	-1.164662	0.048510
C	2.163296	-2.416858	-0.054390
C	2.929005	-1.274670	-0.070009
C	-1.278046	0.726614	0.058386
C	-1.287899	-0.703522	0.133161
C	0.744470	-2.382812	0.009236
C	-2.467666	1.426807	-0.014580
C	-3.666128	0.718445	-0.089136
C	-3.672348	-0.677736	-0.137371
C	-2.491720	-1.398405	-0.061004

H	2.666330	3.384668	-0.034272
H	0.196259	3.322530	0.041941
H	4.014266	1.344659	-0.091595
H	2.655986	-3.382206	-0.086941
H	4.010591	-1.345859	-0.114626
H	-1.275310	-0.809611	1.943285
H	0.185784	-3.311825	0.034402
H	-2.470708	2.510940	-0.042034
H	-4.604209	1.258122	-0.148608
H	-4.614516	-1.202726	-0.245560
H	-2.498816	-2.481522	-0.101966

Frequencies[1/cm]

- 1057.6808	105.0755	118.2232
165.1273	205.6458	253.6001
292.5018	355.6646	396.4209
436.1629	461.5949	471.3867
475.1394	497.1632	509.5080
574.1890	575.5722	580.5490
632.5641	639.3730	658.0295
687.1702	758.6145	766.1917
782.0289	802.6125	807.1569
822.6734	857.6211	892.3883
916.2067	935.3706	942.6938
968.0155	993.3614	1001.4922
1006.2580	1009.8330	1046.0198
1052.2695	1072.8950	1116.2726
1132.2719	1168.8934	1184.6356
1191.8767	1216.1185	1242.0244
1264.3247	1304.0366	1321.1458
1339.5586	1407.8556	1412.2203
1455.2538	1471.3161	1486.3823
1498.4456	1526.8175	1551.4139
1622.8041	1665.7411	1677.8264
1688.7117	1707.2481	3185.2456
3185.5080	3187.4923	3194.8847
3196.7073	3197.2441	3205.6070
3209.5866	3210.2542	3216.0860

i24 – i25

C	-1.866448	2.542170	0.313243
C	-0.493427	2.342356	0.004639
C	-0.052071	1.063594	-0.223525
C	-0.982989	0.008885	-0.122557
C	-2.328386	0.167349	0.183216
C	-2.764231	1.503073	0.402761
C	-0.357623	-1.229049	-0.379346

C	-2.505971	-2.240563	-0.025252
C	-3.100465	-1.025883	0.229353
C	1.244849	0.441120	-0.551039
C	1.055773	-0.923488	-0.650867
C	-1.124255	-2.365176	-0.335384
C	2.507441	1.128262	-0.629980
C	3.653214	0.660343	-0.087795
C	3.777215	-0.523194	0.757353
C	2.916992	-1.522906	0.855291
H	-2.214506	3.554642	0.485295
H	0.173870	3.196151	-0.044385
H	-3.804291	1.702270	0.638588
H	-3.109778	-3.140425	0.013106
H	-4.158598	-0.977783	0.464262
H	1.745213	-1.607745	-1.120915
H	-0.703424	-3.347123	-0.522582
H	2.515033	2.123204	-1.067925
H	4.541493	1.279249	-0.167675
H	4.654186	-0.532286	1.410510
H	2.883094	-2.411508	1.471053

Frequencies[1/cm]

- 238.1732	62.2496	96.0901
142.8093	163.6587	222.2194
235.9780	309.9091	346.0412
394.2572	428.9446	465.9745
481.6573	501.9096	540.0120
552.3596	592.0567	604.9748
632.2818	654.5811	683.1691
691.6923	750.9008	769.8189
776.6282	793.8420	807.7476
824.8036	835.4926	856.4592
899.5892	921.9991	939.2348
946.0895	983.0534	994.4004
1000.0747	1008.5609	1016.1699
1043.9206	1069.8763	1095.6278
1164.1912	1187.8376	1211.4533
1223.0885	1235.5203	1254.5099
1270.9973	1285.9755	1307.1877
1396.7727	1414.1717	1440.0248
1464.8245	1487.2047	1508.7365
1536.5840	1545.8809	1595.9591
1667.8813	1674.9174	1690.2311
1704.2952	3078.3827	3158.8357
3183.8493	3184.0982	3187.4705
3194.6641	3195.3879	3208.2223
3208.9951	3237.7137	3250.0846\

i25 – i26

C	-0.003640	2.461506	-0.583020
C	0.919777	1.365424	-0.701095
C	0.426076	0.093236	-0.454177
C	-0.930100	-0.063111	-0.129518
C	-1.842240	0.975332	-0.011195
C	-1.317845	2.287531	-0.236968
C	-1.231280	-1.434156	0.016596
C	-3.489137	-0.735931	0.455017
C	-3.171376	0.599453	0.302776
C	1.023049	-1.241904	-0.444311
C	0.031097	-2.150137	-0.198490
C	-2.531729	-1.772985	0.309827
C	2.454312	-1.497944	-0.567136
C	3.433509	-0.780122	0.007432
C	3.328599	0.344814	0.953795
C	2.439748	1.315043	1.038190
H	0.361426	3.461576	-0.788410
H	1.866107	1.519909	-1.204752
H	-1.974190	3.148655	-0.162937
H	-4.511792	-1.008003	0.691586
H	-3.939563	1.356397	0.421683
H	0.163792	-3.221047	-0.119928
H	-2.841478	-2.805613	0.430622
H	2.746331	-2.382564	-1.127156
H	4.449198	-1.137122	-0.140445
H	4.128880	0.352884	1.701210
H	2.318384	2.118639	1.752189

Frequencies[1/cm]

- 376.0195	68.7522	117.3283
173.3057	184.1488	221.3851
228.0096	289.8466	355.6690
374.9471	411.2364	466.7537
477.7567	513.4420	532.1528
556.2041	584.4359	593.8041
631.1525	655.1970	692.6339
704.2265	759.2961	777.5884
786.5287	796.6629	804.4558
816.6304	841.1853	860.0131
889.5046	900.0872	915.4015
943.8237	988.7393	995.3702
1002.1460	1002.9860	1019.9575
1037.3421	1064.2135	1093.9851
1160.2863	1181.1116	1210.1774
1216.5495	1249.6701	1253.3201

1277.7347	1289.4564	1349.5228
1396.5294	1414.6205	1437.5590
1454.5575	1490.7824	1501.4752
1533.3927	1580.8752	1631.0688
1670.9596	1684.4540	1688.0437
1704.8093	3063.3202	3155.2015
3177.2494	3183.3373	3183.8179
3193.5958	3199.5717	3208.1497
3210.5314	3230.1597	3234.9201

i26 – i27

C	0.251548	2.438031	-0.001014
C	1.148510	1.291783	-0.078139
C	0.467026	-0.025100	-0.086956
C	-0.955251	-0.051846	-0.063312
C	-1.785908	1.064795	-0.019212
C	-1.102657	2.352710	0.008274
C	-1.388521	-1.384612	-0.005606
C	-3.623215	-0.510291	0.062287
C	-3.155307	0.813668	0.036572
C	0.924202	-1.399275	-0.042785
C	-0.192442	-2.204350	0.001450
C	-2.768570	-1.609518	0.050735
C	2.310951	-1.816460	-0.026586
C	3.395997	-1.015460	0.041529
C	3.512412	0.435013	0.114381
C	2.578503	1.419072	0.072134
H	0.722982	3.414435	0.040849
H	0.858764	0.669382	-1.156195
H	-1.692983	3.261257	0.055157
H	-4.693221	-0.680612	0.106503
H	-3.862504	1.635302	0.073127
H	-0.171336	-3.285132	0.049900
H	-3.175582	-2.613730	0.092679
H	2.480599	-2.888698	-0.054245
H	4.355311	-1.524619	0.059262
H	4.537037	0.781396	0.210056
H	2.937268	2.442065	0.140387

Frequencies[1/cm]

- 1801.2217	89.9353	117.7208
195.2036	238.3935	260.9209
295.5734	371.1126	375.5316
404.4235	430.7052	487.1079
497.7267	511.6566	549.2280
570.8060	594.5364	626.3623
642.1219	653.3581	664.1680

729.3608	754.3155	763.5654
785.9401	796.2076	803.1346
831.5223	862.6728	875.8149
914.6468	916.1329	972.0178
981.4550	982.4891	989.8329
1004.7090	1036.8748	1041.4302
1072.7144	1102.3952	1158.8894
1186.1412	1193.7829	1200.3064
1244.0503	1259.8372	1269.8475
1301.2567	1339.2367	1361.4223
1380.4438	1429.6387	1434.3460
1445.0748	1465.8295	1480.7673
1514.9311	1537.4172	1575.1553
1608.8492	1639.7219	1675.0591
1684.3826	2148.0348	3158.9612
3168.7397	3182.6885	3184.0477
3185.0783	3191.6813	3195.5582
3204.0623	3209.1240	3229.2954

i27 – i28

C	-0.269345	2.428584	0.000015
C	-1.129122	1.298503	0.025031
C	-0.465015	0.027425	0.108631
C	0.936338	-0.039937	0.038272
C	1.776161	1.085421	0.007997
C	1.107889	2.356564	0.004540
C	1.369530	-1.381011	-0.007835
C	3.610920	-0.506184	-0.069314
C	3.144319	0.825011	-0.051077
C	-0.932596	-1.387529	0.109206
C	0.221288	-2.203543	0.030082
C	2.769007	-1.603053	-0.046051
C	-2.324376	-1.801375	-0.050462
C	-3.399486	-0.988563	-0.113256
C	-3.502286	0.457265	-0.055169
C	-2.546233	1.434480	-0.010432
H	-0.737832	3.407413	-0.038481
H	-0.793525	-0.682995	1.210497
H	1.693747	3.268711	-0.017681
H	4.682086	-0.672559	-0.110422
H	3.856504	1.642218	-0.089694
H	0.198472	-3.284046	0.038731
H	3.177247	-2.606953	-0.067995
H	-2.484050	-2.872033	-0.122107
H	-4.357131	-1.488664	-0.225699
H	-4.525901	0.818295	-0.084472

H -2.911569 2.458275 -0.013754

Frequencies[1/cm]

- 1423.3812	92.8410	125.1128
207.5716	240.8612	263.1461
299.3956	378.9838	392.6897
409.0976	436.8817	495.6872
505.4044	513.1894	551.0494
569.3014	615.0959	637.4831
644.4058	661.3209	685.0470
731.2404	757.0217	760.5178
786.3994	791.3738	823.1723
836.4694	839.5716	879.9921
903.7301	919.6931	960.6815
982.9018	984.8080	997.0469
998.3571	1057.2826	1074.0679
1079.7155	1111.5900	1133.8255
1170.7838	1190.7818	1203.4586
1242.1132	1258.9237	1270.6921
1325.3207	1342.2879	1362.3004
1371.9088	1397.7143	1426.1454
1464.2886	1471.1941	1478.4969
1493.8053	1529.8124	1556.1674
1581.8016	1620.0022	1663.0437
1670.7106	1929.8386	3157.6273
3167.3431	3178.5756	3182.9603
3184.0538	3196.3586	3197.1150
3202.3161	3209.2773	3240.8282

i28 – i29

C	0.230945	2.415189	-0.017145
C	1.083894	1.270615	-0.030632
C	0.447739	0.043747	-0.042143
C	-0.943580	-0.028906	-0.021763
C	-1.790586	1.077352	-0.004156
C	-1.143304	2.336928	-0.007665
C	-1.380813	-1.386773	-0.002460
C	-3.624325	-0.501311	0.044964
C	-3.186973	0.804482	0.027360
C	0.933066	-1.374071	-0.058674
C	-0.207760	-2.210037	-0.000582
C	-2.743907	-1.613511	0.033173
C	2.341019	-1.753733	0.026760
C	3.452801	-0.911044	0.103957
C	3.508208	0.509669	0.067803
C	2.529226	1.457121	-0.011713
H	0.700561	3.393523	-0.009235

H	-1.732769	3.247961	0.003762
H	-4.691479	-0.694280	0.071712
H	-3.900396	1.621060	0.043136
H	1.623500	-1.627997	-1.144397
H	-0.182957	-3.290061	0.027122
H	-3.150756	-2.618254	0.055404
H	2.513935	-2.823964	0.093092
H	4.408930	-1.419460	0.144735
H	4.520088	0.905307	0.101065
H	2.857449	2.491861	-0.028907

Frequencies[1/cm]

- 2135.5772	99.4929	115.0856
192.6808	251.8146	266.1422
299.7934	374.2498	384.7885
425.1804	434.5306	483.7522
496.1610	515.5176	557.4939
577.4590	601.7295	633.8813
645.5590	655.4630	680.3150
683.3509	745.9031	754.1510
773.7441	788.6784	803.0591
828.0572	858.1724	866.9738
889.1456	906.9327	933.8307
985.0350	991.9513	993.6662
997.7007	1036.6519	1063.8114
1081.1122	1112.3244	1157.7196
1174.5255	1191.7695	1212.9244
1246.1967	1261.0031	1265.0414
1287.5737	1331.0548	1355.9336
1399.2838	1421.2043	1427.7905
1457.8439	1469.5296	1482.4589
1499.2633	1524.2774	1545.0234
1602.7487	1641.2749	1672.1964
1690.9028	1863.8619	3157.7301
3176.1355	3179.8832	3182.9501
3183.1503	3197.3878	3199.0609
3202.3821	3208.3611	3238.7908

i29 – i30

C	0.203609	2.472587	-0.220612
C	1.103063	1.348243	-0.193461
C	0.510037	0.099483	-0.278115
C	-0.880020	-0.035183	-0.133671
C	-1.759240	1.033430	-0.089357
C	-1.158161	2.331846	-0.190437
C	-1.223152	-1.400829	0.056360
C	-3.496935	-0.631022	0.257410

C	-3.126107	0.695611	0.093703
C	1.076273	-1.219171	-0.272645
C	-0.003878	-2.144998	-0.007228
C	-2.570436	-1.692964	0.260153
C	2.405005	-1.500817	-0.862705
C	2.836974	-1.013216	0.465447
C	3.147031	0.354743	0.718318
C	2.462183	1.444132	0.250416
H	0.631714	3.470342	-0.214612
H	-1.788956	3.214679	-0.189113
H	-4.546464	-0.862554	0.402609
H	-3.881699	1.473745	0.118833
H	0.096022	-3.221117	0.033324
H	-2.914608	-2.708273	0.422890
H	2.677513	-0.872338	-1.709263
H	2.598044	-2.554470	-1.045404
H	3.145954	-1.758397	1.190256
H	3.969658	0.533662	1.405662
H	2.855346	2.433464	0.463371

Frequencies[1/cm]

- 454.9739	95.5847	149.7681
206.0025	261.9426	287.3512
307.2992	347.7082	421.9502
443.6550	454.2757	501.3326
528.5416	553.8500	564.6401
579.5165	587.4801	628.3669
670.2845	685.8664	706.4741
722.3569	753.7959	770.3405
793.4528	809.4976	829.4380
843.2186	858.6607	908.7653
944.4397	954.3986	966.7758
981.9150	985.6929	992.8091
1046.6095	1066.8571	1088.7077
1122.3308	1144.2828	1172.0412
1181.9279	1204.9115	1209.4126
1223.9757	1241.4254	1248.2284
1279.8040	1320.8706	1353.6186
1377.9891	1400.5464	1442.3476
1444.2930	1458.9702	1488.4820
1501.3865	1515.8864	1535.3461
1571.5180	1624.4696	1680.7055
1689.2485	3097.8973	3160.2904
3176.8964	3178.2621	3182.9012
3185.5707	3195.2635	3196.9858
3197.6343	3207.8002	3233.4317

i30 – i31

C	-0.299504	2.513660	0.145168
C	-1.174662	1.388205	0.075703
C	-0.571934	0.155504	0.133765
C	0.802999	0.009850	0.075152
C	1.681822	1.086622	0.112301
C	1.071985	2.371091	0.189180
C	1.152443	-1.355094	-0.167279
C	3.433665	-0.569524	-0.189313
C	3.064080	0.747850	-0.002203
C	-1.227615	-1.186229	0.064188
C	-0.060340	-2.089606	-0.298183
C	2.509012	-1.637885	-0.292970
C	-1.641211	-1.721278	1.396183
C	-2.575878	-1.050542	-0.575740
C	-3.208969	0.198429	-0.581344
C	-2.591379	1.389455	-0.220961
H	-0.726817	3.511321	0.132250
H	1.697578	3.256728	0.231239
H	4.489491	-0.800440	-0.283916
H	3.821857	1.522743	0.037187
H	-0.154881	-3.149927	-0.489896
H	2.866648	-2.642505	-0.486556
H	-1.560152	-1.129070	2.299840
H	-2.124294	-2.690136	1.433483
H	-4.245278	0.234960	-0.901579
H	-3.141835	2.322198	-0.260247
H	-3.109397	-1.938920	-0.893695

Frequencies[1/cm]

- 410.7411	93.6270	146.3704
176.8975	236.4320	263.7226
311.4365	337.2577	408.2327
418.1376	446.1496	474.0737
491.4670	524.0975	530.1981
544.9376	558.8270	584.9689
602.8113	617.0741	642.7087
663.6064	677.1178	691.3483
722.2247	765.1998	775.0287
797.2679	825.5489	835.8813
846.4418	890.5973	929.4729
961.7145	984.3845	993.3012
995.0053	1023.5051	1059.1520
1062.2542	1098.8457	1114.4561
1120.3367	1165.8886	1173.4184
1188.3380	1203.5937	1220.2833
1248.4214	1296.0159	1325.7928

1347.6818	1385.4078	1408.8618
1430.6398	1443.9842	1454.1396
1464.6712	1493.9359	1502.5754
1545.2376	1616.9476	1674.3538
1704.5036	3151.1203	3179.4363
3180.0885	3182.4863	3197.7589
3198.9314	3201.7926	3208.8998
3210.5313	3234.2823	3275.5888

i31 – i32

C	-0.438328	2.529231	0.165606
C	-1.281343	1.364891	0.077212
C	-0.657910	0.133074	0.219803
C	0.746155	0.031539	0.175102
C	1.574754	1.155630	0.181771
C	0.919518	2.432252	0.247879
C	1.193892	-1.268612	-0.150437
C	3.407311	-0.340740	-0.311518
C	2.953069	0.930722	-0.027688
C	-1.357998	-1.133182	0.168985
C	0.069224	-2.225807	-0.209062
C	2.532903	-1.447216	-0.410630
C	-0.806527	-2.283834	0.976848
C	-2.704603	-1.077015	-0.299550
C	-3.315865	0.157048	-0.488399
C	-2.662574	1.366862	-0.250823
H	-0.905202	3.508349	0.129297
H	1.524040	3.332638	0.285560
H	4.464454	-0.495766	-0.496577
H	3.645848	1.765581	-0.013304
H	2.925262	-2.418454	-0.691562
H	-4.355758	0.176791	-0.796304
H	-3.190257	2.305722	-0.375273
H	-3.277899	-1.990599	-0.411935
H	-1.480663	-3.134513	1.027772
H	-0.371404	-2.026800	1.941462
H	-0.008497	-2.972005	-0.989729

Frequencies[1/cm]

-583.0448	102.2683	164.4367
187.6420	247.9024	271.1140
363.6955	397.6510	410.6986
442.1425	488.5144	495.6616
505.2817	527.0987	546.2251
576.4627	592.4527	626.6886
652.3942	701.5576	706.9609
728.5348	760.9129	779.5943

802.2790	815.5537	827.4919
846.6159	860.5228	928.6100
955.8762	966.7162	973.9923
991.6587	1000.0221	1020.7256
1024.0320	1074.3909	1094.1735
1103.4165	1145.4862	1163.5189
1175.0570	1192.9081	1204.1851
1225.4949	1235.7361	1248.3571
1256.0658	1342.5142	1347.5107
1356.2290	1408.4657	1434.5499
1455.7531	1472.2165	1488.4781
1490.6664	1525.6274	1539.6547
1576.6405	1643.9178	1671.4055
1687.8152	3095.9970	3179.2826
3182.3910	3182.8366	3183.3861
3193.9173	3196.2076	3198.4384
3207.8865	3208.3303	3210.9959

i32 – p3

C	0.641945	-2.489111	0.030807
C	1.402016	-1.268281	-0.000962
C	0.706880	-0.033173	-0.007317
C	-0.721047	-0.018391	-0.002709
C	-1.441871	-1.237168	0.023529
C	-0.708180	-2.474420	0.046129
C	-1.420815	1.216681	-0.042537
C	-3.517539	0.007963	-0.020242
C	-2.839496	-1.201665	0.017915
C	1.431954	1.182857	-0.026850
C	-0.669248	2.435003	-0.079249
C	-2.818589	1.206137	-0.052864
C	0.695307	2.430159	-0.007125
C	2.824323	1.146868	-0.051940
C	3.500401	-0.066550	-0.053958
C	2.799346	-1.262067	-0.024896
H	1.181749	-3.430224	0.042245
H	-1.268093	-3.403455	0.070216
H	-4.601466	0.017290	-0.025512
H	-3.392299	-2.134938	0.040134
H	-3.354491	2.148884	-0.084335
H	3.332983	-2.206689	-0.020286
H	0.904247	2.830477	1.890632
H	-1.207529	3.375349	-0.126778
H	1.249431	3.353107	-0.137900
H	3.379010	2.079182	-0.061065
H	4.584134	-0.078038	-0.073743

Frequencies[1/cm]

- 817.6931	96.6428	148.2065
200.0361	239.8336	254.3968
308.6704	363.0552	373.5696
414.9618	429.5287	466.4512
502.9324	513.5455	516.0293
529.2945	556.3789	560.5933
593.3003	603.9907	695.1738
710.5310	739.3292	754.8408
774.9218	795.9109	820.6016
835.2419	841.8239	856.2236
875.4776	927.7642	938.1781
987.4835	999.4884	1005.6092
1009.3210	1015.5857	1027.5384
1106.7775	1129.1236	1130.4373
1160.5824	1175.3691	1208.1912
1218.3612	1238.6236	1270.4843
1272.1463	1273.8703	1341.2858
1365.4636	1411.7803	1440.1341
1450.6504	1475.4083	1480.7847
1501.7788	1546.1192	1554.4462
1613.7584	1662.3653	1667.7611
1674.3058	1710.5739	3181.9121
3184.2998	3184.5195	3186.6079
3192.2276	3192.5134	3201.8218
3203.4291	3210.4947	3210.8005

i33 – i34

C	-4.094781	-0.880334	-0.000141
C	-3.200253	-1.973168	0.000016
C	-3.623812	0.405455	-0.000138
C	-2.231485	0.672970	0.000017
C	-1.335834	-0.445665	0.000229
C	-1.847257	-1.762473	0.000209
C	-1.742243	2.018488	-0.000127
C	-0.401788	2.326461	-0.000053
C	0.018127	-0.055416	0.000400
C	0.427403	1.195378	0.000272
C	1.661370	0.349527	0.000127
C	2.386770	0.086320	-1.235549
C	3.623854	-0.499089	-1.215033
C	4.257273	-0.814716	-0.000261
C	3.624259	-0.498984	1.214697
C	2.387177	0.086411	1.235582
H	-5.162966	-1.065195	-0.000265
H	-3.592400	-2.983914	-0.000020

H	-4.316946	1.240758	-0.000256
H	-1.150537	-2.592512	0.000345
H	-2.477610	2.816958	-0.000324
H	1.900555	0.336436	-2.171433
H	4.127819	-0.712822	-2.151491
H	5.235411	-1.279730	-0.000404
H	1.901261	0.336571	2.171610
H	4.128541	-0.712628	2.151005
H	-0.045806	3.349090	-0.000251

Frequencies[1/cm]

- 364.4443	25.0480	68.5769
94.8255	162.5362	197.2053
277.6883	327.8870	355.7370
407.5490	408.4222	424.7591
491.8357	519.7839	532.7768
547.6446	611.9118	623.4580
649.9845	671.0005	688.0711
708.5127	764.9080	780.6362
791.7701	804.5096	839.2286
850.2334	855.7521	895.5661
910.8367	974.3820	982.6897
985.9149	992.3621	994.8514
1020.6993	1022.5213	1038.6494
1051.9541	1101.7057	1136.7310
1159.3683	1168.1570	1179.6909
1200.9310	1229.8223	1257.6896
1283.2411	1291.6230	1336.4370
1342.3480	1385.0042	1425.6376
1437.4927	1462.0404	1483.7162
1500.8568	1562.5740	1565.5003
1606.3432	1626.4764	1691.0868
1773.5016	3180.0101	3183.6918
3184.4612	3187.6392	3192.1951
3205.0736	3205.8749	3207.2796
3215.9111	3216.5887	3218.3986

i34 – i35

C	-3.733009	-1.356360	0.000233
C	-2.587099	-2.180233	-0.000057
C	-3.592400	0.002200	0.000199
C	-2.309225	0.608422	-0.000005
C	-1.146778	-0.224005	-0.000239
C	-1.334409	-1.631139	-0.000318
C	-2.186226	2.020498	0.000188
C	-0.952731	2.625418	0.000239
C	0.124548	0.418894	-0.000325

C	0.160210	1.790505	-0.000217
C	1.518447	-0.110106	-0.000404
C	2.413218	0.961007	-0.000387
C	3.776512	0.839051	0.000039
C	4.299109	-0.461496	0.000303
C	3.444439	-1.553179	0.000338
C	2.056207	-1.391884	0.000059
H	-4.719819	-1.804632	0.000424
H	-2.701955	-3.258243	-0.000117
H	-4.467170	0.644251	0.000330
H	-0.475989	-2.285875	-0.000742
H	-3.090767	2.620337	0.000367
H	1.510478	1.974457	-0.000496
H	4.431268	1.702872	0.000165
H	5.372933	-0.612283	0.000534
H	1.433333	-2.275758	0.000394
H	3.858035	-2.555265	0.000662
H	-0.855217	3.704579	0.000597

Frequencies[1/cm]

- 1950.9685	38.1827	69.0483
158.1265	159.3086	197.4599
263.0929	320.1146	344.7414
399.4900	412.0831	477.8275
484.6123	503.6301	543.0954
563.0758	579.5610	633.1931
654.5553	662.2577	715.9939
720.7234	749.9501	770.2905
805.2656	809.3981	819.4587
856.4492	868.8322	888.8744
951.6287	973.4169	975.0789
986.3956	1007.2694	1015.7367
1015.7870	1050.6158	1058.5564
1076.9428	1128.0262	1141.9939
1159.0121	1173.0635	1186.7985
1193.4427	1222.0479	1238.1763
1278.1291	1315.4915	1348.2981
1379.4373	1402.0282	1426.4403
1464.0063	1479.7851	1491.2105
1492.5820	1567.7943	1636.0782
1639.5316	1645.5526	1668.1006
1704.5935	1787.9215	3182.2946
3184.4269	3186.5625	3195.6246
3199.2970	3208.0249	3210.0029
3212.1269	3228.7021	3260.8789

i35 – i23

C	2.572376	1.221774	0.170593
C	3.787338	0.578193	-0.038548
C	3.835440	-0.789210	-0.293962
C	2.657232	-1.540107	-0.333400
C	1.473770	-0.864698	-0.162603
C	1.382375	0.494412	0.110183
C	-0.396706	2.318739	0.066895
C	0.010031	1.012702	0.234395
C	-1.762952	2.608560	-0.103720
C	-2.687775	1.596505	-0.202251
C	-0.520568	-1.364677	0.577517
C	-0.956708	-0.017000	0.308408
C	-2.295642	0.246626	-0.038181
C	-3.160409	-0.858545	-0.288570
C	-1.390086	-2.414082	0.267395
C	-2.687023	-2.147064	-0.203534
H	0.333283	3.116639	-0.012832
H	-2.074707	3.638218	-0.237212
H	4.708624	1.147655	0.005387
H	2.552922	2.284371	0.390854
H	4.790579	-1.275370	-0.461688
H	2.684751	-2.608907	-0.515776
H	-3.722356	1.820643	-0.439639
H	-4.187614	-0.667969	-0.580091
H	-1.098689	-3.435541	0.482651
H	-3.348110	-2.976502	-0.429443
H	0.197164	-1.535994	1.374090

Frequencies[1/cm]

- 532.957	84.3225	101.8623
159.1087	187.5819	254.0566
266.6770	351.5146	403.9561
420.3983	444.6390	474.7313
510.9119	521.7110	550.6412
570.6571	601.7877	618.8219
648.5849	692.7710	722.6858
757.9577	774.8746	780.9901
800.2935	808.2654	830.2555
869.9539	881.3297	888.2830
920.2284	962.9130	973.6288
990.6090	1000.0774	1007.1269
1012.7497	1051.9769	1064.2762
1090.3583	1127.8492	1150.6900
1164.4815	1180.1487	1186.4386
1212.2865	1232.7362	1254.8941
1271.0498	1325.0646	1331.2079
1372.3110	1394.1664	1417.8452

1452.6560	1474.2011	1484.2050
1505.4187	1540.4715	1603.6789
1626.8138	1641.6119	1658.0981
1680.5608	3152.6903	3179.3009
3184.3241	3185.0391	3185.5860
3195.1524	3196.8622	3198.7110
3210.3228	3210.6678	3211.3318

i24 – i36

C	2.252871	0.195808	0.074207
C	0.876501	0.014379	-0.098703
C	0.266965	-1.245872	-0.252677
C	1.050409	-2.368614	-0.241321
C	2.450628	-2.214172	-0.072722
C	3.042968	-0.982483	0.081071
C	2.697456	1.538006	0.217284
C	1.789299	2.569900	0.190434
C	0.395568	2.360060	0.028505
H	0.626844	-3.359823	-0.358696
H	3.072729	-3.102570	-0.065823
H	4.117919	-0.908077	0.207427
H	3.754078	1.744300	0.349618
H	2.147448	3.587577	0.303069
H	-0.281478	3.206717	0.030192
C	-0.059665	1.074446	-0.125487
C	-1.391582	0.489060	-0.311428
C	-1.214800	-1.043080	-0.403816
C	-2.624876	1.088791	-0.522600
C	-2.036694	-1.001388	0.814186
H	-1.681483	-1.509135	-1.274083
C	-3.772400	0.304327	-0.158650
H	-2.704330	2.137024	-0.787819
C	-3.468293	-0.757452	0.632154
H	-1.583384	-1.136215	1.790725
H	-4.784155	0.593843	-0.411164
H	-4.210309	-1.383930	1.113942

Frequencies[1/cm]

- 661.382	104.2179	131.8419
166.1250	194.0084	266.9516
319.3432	347.7730	394.5924
448.3580	477.4580	488.2989
512.9940	537.3959	564.4974
572.5327	620.0225	630.9585
656.8474	677.7593	701.3288
741.6674	770.6823	785.4044
798.0475	804.6569	820.0051

845.9799	883.2403	914.4204
930.8874	932.4227	967.4014
998.0989	1001.3184	1007.9303
1035.7699	1046.8369	1069.3609
1077.8066	1115.9707	1137.9875
1161.3835	1175.7772	1185.9945
1208.9909	1233.7551	1247.2287
1263.8868	1277.2210	1306.1319
1378.4773	1393.3649	1407.6920
1425.5169	1464.3523	1470.8080
1487.5752	1520.3955	1550.9781
1588.7257	1669.8114	1683.4332
1702.3837	3085.8612	3182.4791
3182.7485	3188.6668	3195.5732
3196.6299	3197.2426	3200.0183
3207.6461	3208.3718	3227.6988

i36 – i37

C	2.142411	0.419432	-0.129641
C	0.811319	-0.016355	0.083135
C	0.525495	-1.421173	0.132670
C	1.551789	-2.323501	-0.081235
C	2.861747	-1.884943	-0.343015
C	3.157146	-0.547549	-0.356918
C	2.423357	1.806108	-0.104144
C	1.424263	2.714344	0.130785
C	0.098488	2.285473	0.314123
H	1.341454	-3.386625	-0.029585
H	3.643608	-2.615573	-0.516541
H	4.171678	-0.208357	-0.537067
H	3.444110	2.137772	-0.262046
H	1.651045	3.773698	0.170512
H	-0.680615	3.018324	0.492506
C	-0.223340	0.945453	0.266849
C	-1.606990	0.444009	0.277526
C	-0.787094	-1.845184	0.561376
C	-2.644639	1.093686	-0.292911
C	-1.812167	-0.948812	0.685925
H	-0.915730	-2.874960	0.876410
C	-3.841348	0.315405	-0.571676
H	-2.566628	2.118702	-0.636237
C	-3.776163	-1.004755	-0.488584
H	-2.648895	-1.177350	1.340768
H	-4.754810	0.822791	-0.883020
H	-4.510858	-1.798256	-0.521304

Frequencies[1/cm]

- 510.916	77.0806	112.6332
169.5623	201.3165	218.9348
291.0050	313.2414	378.6622
436.2254	444.0024	467.6112
484.3230	495.4791	522.3425
550.2024	566.6627	597.7466
631.9792	651.7875	661.7725
722.6501	764.6897	771.7321
791.8905	797.9068	807.9320
823.1764	852.6881	860.7908
881.9980	900.3414	920.4579
925.2245	937.1544	960.0513
999.7734	1007.5596	1060.6001
1065.6931	1110.2491	1119.2901
1148.0639	1171.3528	1211.0811
1218.5290	1238.5673	1243.3098
1255.5449	1312.5142	1325.1475
1388.2563	1409.6424	1424.8916
1437.7671	1474.7521	1486.1206
1513.8467	1570.3033	1602.8405
1643.9562	1655.0399	1673.2902
1689.3430	3119.0949	3148.6316
3183.2525	3184.6906	3191.3391
3194.5413	3195.4207	3206.6055
3209.7300	3211.1639	3239.5908

i37 – i38

C	1.503936	1.203482	0.048010
C	0.752094	0.007882	-0.082582
C	1.411204	-1.251114	-0.002880
C	2.773436	-1.288154	0.251834
C	3.501699	-0.107602	0.433429
C	2.881747	1.117840	0.328248
C	0.845487	2.453390	-0.143154
C	-0.463314	2.500395	-0.517916
C	-1.224061	1.308533	-0.641170
H	3.277483	-2.247543	0.305466
H	4.564230	-0.160506	0.641565
H	3.452512	2.033045	0.445254
H	1.421643	3.366755	-0.037532
H	-0.935889	3.450459	-0.739125
H	-2.154964	1.338662	-1.190035
C	-0.646664	0.071238	-0.346525
C	-1.428805	-1.148288	-0.287012
C	0.634619	-2.450381	-0.234065
C	-2.755609	-1.178758	0.067174

C	-0.701483	-2.400649	-0.386121
H	1.155455	-3.401909	-0.255303
C	-3.529023	-0.109819	0.659897
H	-3.220780	-2.159869	0.104211
C	-3.249085	1.187943	0.665825
H	-1.274344	-3.314748	-0.504191
H	-4.398174	-0.446316	1.231528
H	-3.724237	2.046345	1.120203

Frequencies[1/cm]

- 267.7021	76.9384	126.1893
191.1050	208.2270	220.9614
267.6672	318.1952	390.4691
414.5044	440.7135	464.5573
479.0036	503.6479	524.2026
543.3165	562.0691	613.0791
624.0579	647.0178	670.4802
707.0740	761.1022	765.9995
787.1733	808.6353	808.8646
834.2919	843.0405	856.4200
870.4651	912.1485	926.5245
933.8392	981.1040	992.1504
997.6946	1004.9712	1066.3971
1088.4734	1114.6918	1130.3627
1163.6448	1178.1778	1212.6069
1213.5757	1248.6393	1260.9726
1273.5485	1285.0404	1365.0749
1396.7922	1403.8781	1441.2789
1452.5302	1472.3633	1498.6531
1515.4830	1548.9494	1621.4439
1639.3815	1646.3398	1662.0123
1692.9797	3081.5171	3171.0940
3179.5104	3182.4922	3184.4417
3190.2893	3199.9246	3203.7732
3209.5465	3218.8436	3242.2402

i38 – p3

C	1.423605	-1.229138	-0.022975
C	0.727404	0.007390	0.012755
C	1.450745	1.226304	0.011984
C	2.849319	1.187105	0.000917
C	3.521139	-0.023465	-0.019649
C	2.815961	-1.222557	-0.037528
C	0.661021	-2.454402	-0.073032
C	-0.682270	-2.448482	-0.020514
C	-1.426230	-1.204691	0.114815
H	3.404727	2.119088	0.005006

H	4.605005	-0.037940	-0.028719
H	3.350456	-2.166278	-0.066146
H	1.202258	-3.390818	-0.158172
H	-1.245030	-3.375014	-0.051808
H	-1.459975	-1.264959	1.855231
C	-0.694816	0.027839	0.024738
C	-1.391398	1.255295	-0.000616
C	0.718130	2.461980	0.015880
C	-2.792012	1.246508	-0.045236
C	-0.633394	2.476125	0.001787
H	1.277290	3.391776	0.021428
C	-3.495203	0.048056	-0.105901
H	-3.325395	2.190759	-0.068878
C	-2.831716	-1.162660	-0.058719
H	-1.173232	3.417209	-0.007119
H	-4.575384	0.064811	-0.195378
H	-3.382433	-2.095875	-0.097675

Frequencies[1/cm]

- 1143.896	94.6216	149.1962
210.6797	238.9718	264.6394
355.1558	397.0562	407.4779
447.6384	464.4170	498.0464
511.9598	512.2819	525.0530
540.8983	552.4228	567.7079
594.5149	605.3297	699.1897
705.8095	733.2451	754.7730
762.1769	791.9835	817.9902
823.2459	838.4037	867.1992
873.2476	915.6876	934.8577
986.4495	995.7628	1001.8673
1004.6591	1010.8814	1023.8233
1105.4294	1127.2052	1129.6949
1162.9938	1180.3205	1205.0024
1217.1021	1235.1998	1260.9858
1270.6677	1274.5554	1336.6893
1361.6373	1404.6972	1438.8428
1458.2944	1470.5521	1474.9743
1494.0182	1544.6996	1558.8507
1618.4187	1654.5396	1661.5402
1683.8038	1716.3652	3182.1406
3183.5139	3184.3692	3186.4456
3191.8409	3195.8585	3201.9367
3204.6581	3210.2812	3211.7735

Products

p1 fluoranthene(C₁₆H₁₀)

C	2.155541	2.418571	0.000027
C	2.921027	1.275799	-0.000062
C	2.295561	0.000018	-0.000199
C	0.902824	0.000016	-0.000091
C	0.107972	1.167401	0.000124
C	0.735199	2.385288	0.000250
C	0.107968	-1.167436	0.000006
C	-1.294582	-0.707986	0.000032
C	-1.294552	0.707975	-0.000034
C	2.921075	-1.275792	-0.000171
C	2.155603	-2.418554	0.000021
C	0.735203	-2.385271	0.000070
C	-2.488812	1.408499	-0.000105
C	-3.686602	0.695704	-0.000169
C	-3.686612	-0.695706	-0.000108
C	-2.488813	-1.408527	0.000202
H	2.649812	3.383719	0.000181
H	4.003607	1.346767	-0.000049
H	0.178012	3.315814	0.000483
H	4.003658	-1.346686	-0.000006
H	2.649788	-3.383745	0.000081
H	0.178125	-3.315862	0.000331
H	-2.496234	2.493040	-0.000002
H	-4.629252	1.231085	-0.000464
H	-4.629278	-1.231061	0.000262
H	-2.496222	-2.493063	0.000430

Frequencies[1/cm]

102.4419	122.8884	164.3336
208.2318	258.5078	301.2989
359.0163	439.1463	442.1522
470.6040	482.2362	497.8362
573.5710	576.1658	582.5915
632.2954	638.3298	659.9556
692.2855	761.4850	769.7575
783.9485	803.2074	808.7171
823.1019	855.5162	900.6511
919.9638	937.8114	944.2767
970.7668	994.9317	1000.7529
1009.3791	1010.7014	1044.8780
1056.5387	1071.9607	1116.5370
1142.1538	1168.6939	1188.9023
1192.0959	1218.0708	1242.0386
1264.8668	1305.8098	1323.9028
1349.8387	1410.3495	1419.2096

1459.5848	1475.3862	1492.1129
1509.6509	1527.5930	1551.1739
1653.9985	1680.7048	1691.4883
1691.9086	1707.6880	3184.4310
3184.4712	3185.0203	3191.7789
3195.4178	3195.6699	3202.0177
3208.7389	3209.3616	3214.2247

p2 acephenanthrylene

C	2.868118	-1.260499	-0.000000
C	3.864436	-0.312651	-0.000000
C	3.530123	1.047594	0.000000
C	2.209114	1.436352	0.000000
C	1.170259	0.490218	0.000000
C	1.508033	-0.893035	-0.000000
C	-0.235919	0.864378	0.000000
C	-1.147062	-0.174595	0.000000
C	-0.816556	-1.564668	0.000000
C	0.489945	-1.919156	-0.000000
C	-0.788101	2.165490	0.000000
C	-2.160017	2.340653	0.000000
C	-3.061775	1.255260	-0.000000
C	-2.543532	-0.020401	0.000000
C	-2.098511	-2.283039	0.000000
C	-3.106408	-1.381473	-0.000000
H	3.121206	-2.315841	-0.000000
H	4.904986	-0.615881	-0.000000
H	4.313575	1.796778	0.000000
H	1.966805	2.492579	0.000000
H	0.806622	-2.957758	-0.000000
H	-0.148447	3.040356	0.000000
H	-2.557762	3.349369	-0.000000
H	-4.130499	1.439692	-0.000000
H	-2.206290	-3.358953	0.000001
H	-4.163080	-1.612925	-0.000001

Frequencies[1/cm]

96.4836	103.8105	203.7542
241.1513	246.3766	281.0680
385.1106	401.3311	425.5956
456.2033	474.2901	512.5354
574.9770	576.6919	595.5810
621.2008	647.2649	672.7449
685.2020	737.1404	774.6388
777.3795	778.4096	797.4508
839.4913	845.6400	872.9676
888.8899	932.7049	936.0353

939.9413	966.5896	982.5585
998.9654	1015.2904	1066.3364
1071.1681	1083.7151	1098.8108
1120.4542	1167.0080	1187.4077
1203.5066	1219.0227	1242.2561
1253.4739	1307.3558	1338.2257
1358.3278	1373.0427	1400.7090
1432.4575	1477.4464	1498.0908
1521.4193	1530.7844	1583.0630
1604.9170	1682.8252	1685.7276
1692.9151	1716.5824	3182.1371
3185.3473	3187.2826	3193.2693
3200.6454	3206.5577	3213.2984
3217.9572	3225.1812	3246.9084

p3 pyrene

C	1.204913	-2.819027	0.000018
C	1.227488	-1.422810	-0.000062
C	-0.000000	-0.713231	-0.000316
C	-1.227488	-1.422810	-0.000062
C	-1.204913	-2.819027	0.000018
C	-0.000000	-3.507369	-0.000157
C	0.000000	0.713231	-0.000316
C	-1.227488	1.422810	-0.000062
C	-2.457115	0.675041	0.000239
C	-2.457115	-0.675041	0.000239
C	2.457115	-0.675041	0.000239
C	2.457115	0.675041	0.000239
C	1.227488	1.422810	-0.000062
C	1.204913	2.819027	0.000018
C	0.000000	3.507369	-0.000157
C	-1.204913	2.819027	0.000018
H	2.143144	-3.363947	-0.000173
H	-2.143144	-3.363947	-0.000173
H	-0.000000	-4.591428	-0.000372
H	-3.392560	1.224846	0.000605
H	-3.392560	-1.224846	0.000605
H	3.392560	-1.224846	0.000605
H	3.392560	1.224846	0.000605
H	2.143144	3.363947	-0.000173
H	0.000000	4.591428	-0.000372
H	-2.143144	3.363947	-0.000173

Frequencies[1/cm]

97.8726	152.6707	215.0911
250.8615	263.2555	363.3756
404.1181	415.6683	466.9862

503.8166	513.6339	514.4486
521.1224	542.0253	558.1547
593.9948	603.9005	698.4428
709.8884	734.7850	755.4879
768.6229	796.5348	821.3531
826.0036	842.1567	854.7895
871.9728	927.3851	938.6884
989.1554	997.6855	1005.2349
1005.3178	1013.4738	1028.0346
1106.5710	1128.5836	1132.8360
1162.4374	1181.6579	1208.8753
1219.1089	1242.7288	1272.2587
1276.0731	1276.9384	1340.6086
1367.0673	1415.5662	1442.3465
1461.4683	1476.5264	1481.1849
1505.1766	1556.6196	1562.1999
1630.8472	1672.8005	1675.4908
1686.2526	1724.0206	3181.0806
3181.1122	3183.2756	3183.3219
3191.1112	3191.3785	3200.9985
3201.2836	3209.4175	3209.7592

p4 phenanthrenyl (C₁₄H₉)

C	-2.947822	-1.435313	0.000002
C	-1.572891	-1.499476	0.000012
C	-0.771534	-0.337435	0.000005
C	-1.421427	0.926298	-0.000004
C	-2.812281	0.907505	-0.000012
C	-3.609367	-0.189127	-0.000011
C	-0.655565	2.139717	0.000012
C	0.692665	2.097794	-0.000002
C	1.400806	0.848661	0.000005
C	2.809789	0.828022	-0.000001
C	3.500756	-0.358794	-0.000004
C	2.795370	-1.570310	-0.000006
C	1.420041	-1.573540	-0.000002
C	0.684310	-0.370999	0.000007
H	-3.531094	-2.349772	0.000010
H	-1.105888	-2.475595	0.000034
H	-4.691450	-0.127917	-0.000021
H	1.271904	3.015148	-0.000000
H	3.344025	1.772572	-0.000005
H	4.584602	-0.360460	-0.000007
H	3.335156	-2.510363	-0.000014
H	0.903750	-2.524856	-0.000012
H	-1.188112	3.083228	0.000016

Frequencies[1/cm]

94.3448	101.1298	227.2302
240.9819	247.5622	407.5910
417.0155	450.3306	451.4373
502.1404	504.6161	557.1132
560.0422	592.8705	634.8467
716.4980	727.0984	731.6202
761.2385	769.5483	818.7380
841.3895	843.0962	893.5522
894.7951	899.6662	977.9166
990.8814	1006.8790	1016.4375
1016.5014	1070.3350	1075.4110
1116.0945	1172.1215	1189.7562
1198.0895	1216.6264	1224.6580
1251.0059	1298.2149	1330.0327
1368.6931	1388.4577	1421.4959
1452.0873	1475.4512	1498.3260
1529.5528	1571.8574	1628.7189
1672.7075	1691.9303	1703.9151
3183.7073	3187.5543	3188.1272
3195.3167	3204.0249	3210.3020
3213.6434	3218.8005	3230.7656

C₂H₂

C	0.000000	0.000000	0.598179
C	0.000000	0.000000	-0.598179
H	0.000000	0.000000	1.662063
H	0.000000	0.000000	-1.662063

Frequencies[1/cm]

690.7458	690.7458	785.0375
785.0375	2089.3899	3426.9485
3534.2365		

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