

Supporting Information

Infrared Photodissociation Spectroscopic Studies of $\text{ScO}(\text{H}_2\text{O})_{n=1-3}\text{Ar}^+$

Cluster Cations: Solvation Induced Reaction of ScO^+ and Water

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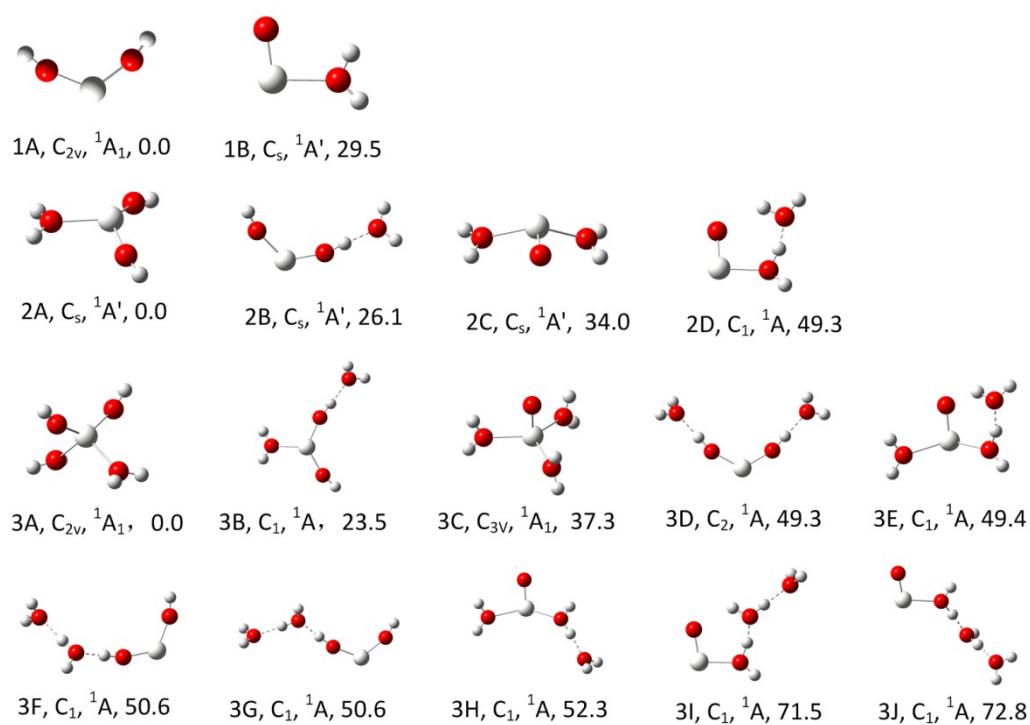


Fig. S1. Optimized structures of the minimum-energy isomers of $\text{ScO}(\text{H}_2\text{O})_n^+$ ($n=1-3$). The relative energies (with ZPE correction) are given in kcal/mol.

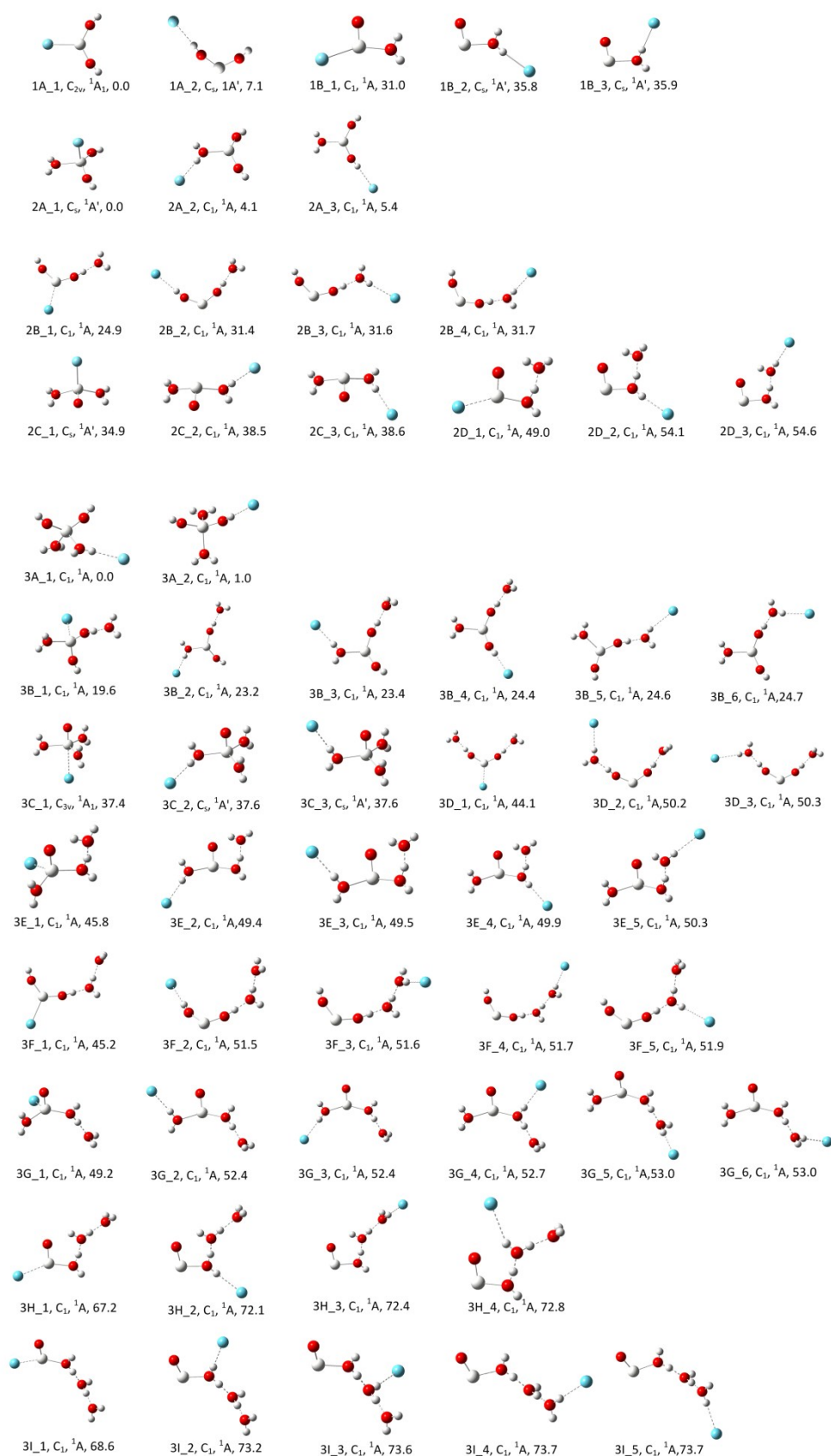


Fig. S2. Optimized structures of the minimum-energy isomers of ScO(H₂O)_nAr⁺ (n=1-3). The relative energies (with ZPE correction) are given in kcal/mol.

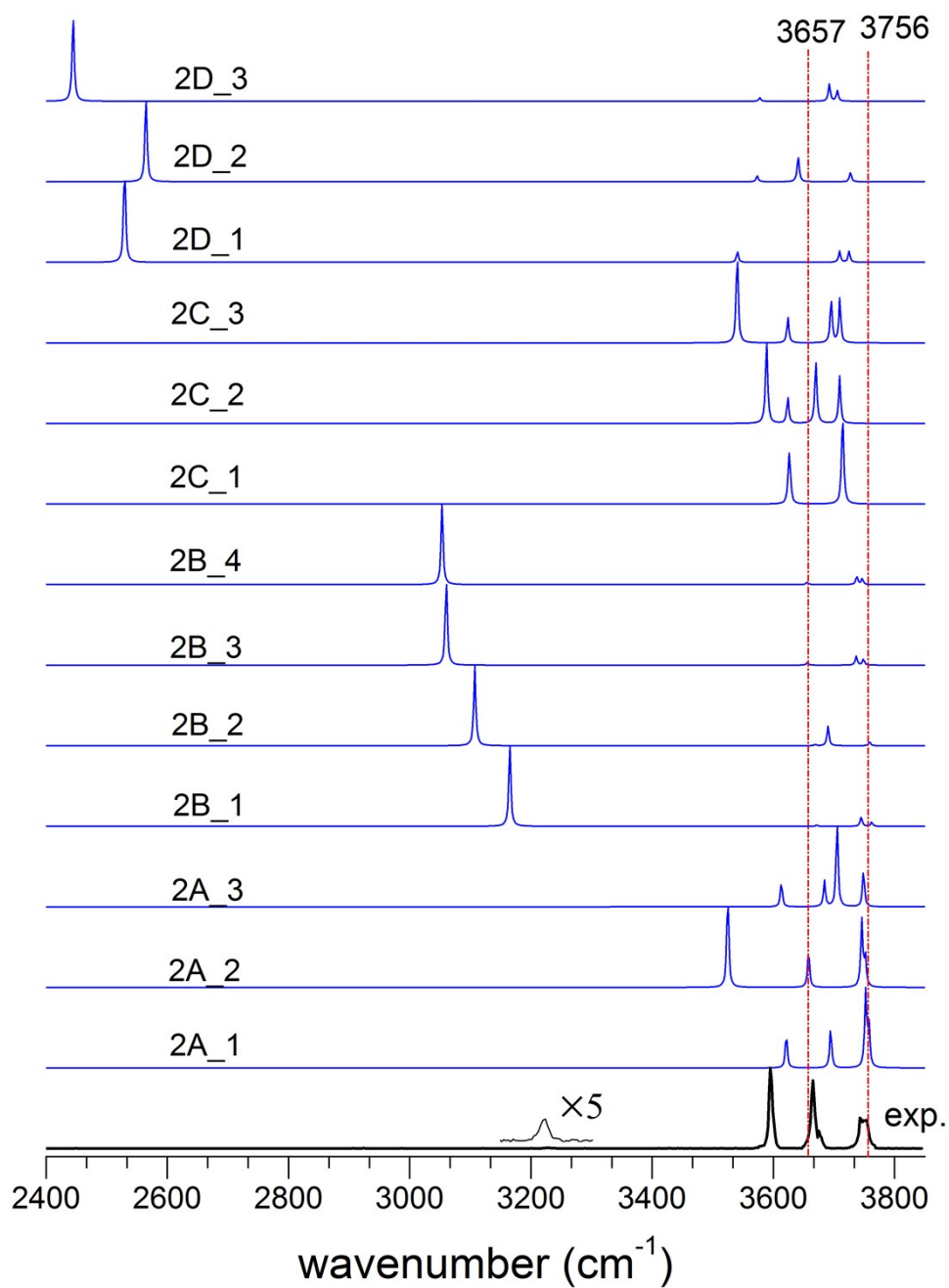


Fig. S3. Experimental infrared spectra (black) and simulated vibrational spectra (blue) of $\text{ScO}(\text{H}_2\text{O})_2\text{Ar}^+$ in O-H stretching frequency region. The two dashed red lines are corresponding to the symmetric (3657 cm⁻¹) and asymmetric (3756 cm⁻¹) stretches of the isolated water molecule.

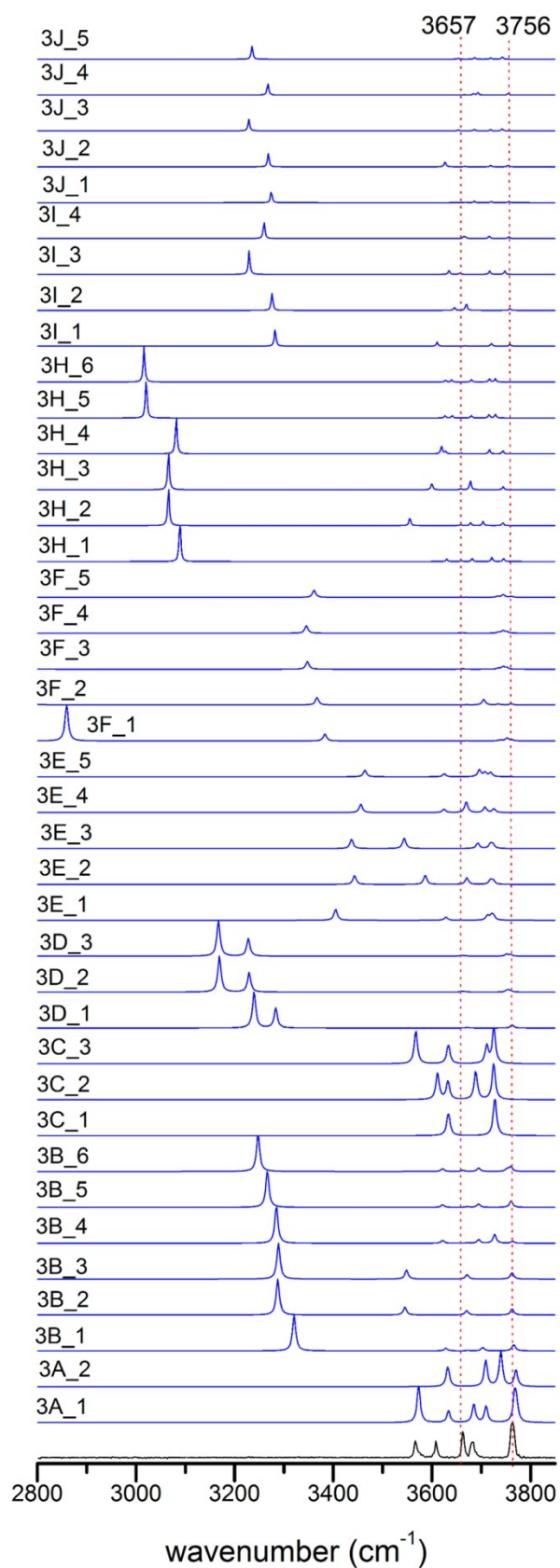


Fig. S4. Experimental infrared spectra (black) and simulated vibrational spectra (blue) of $\text{ScO}(\text{H}_2\text{O})_3\text{Ar}^+$ in O-H stretching frequency region. The two dashed red lines are corresponding to the symmetric (3657 cm⁻¹) and asymmetric (3756 cm⁻¹) stretches of the isolated water molecule.

Table S1. Anharmonic frequencies of isomers computed by DFT at B3LYP/aug-CC-PVTZ level (IR intensities are listed in parentheses in Km/mol).

isomer	Freq. (cm ⁻¹)	
1B_1	3617.970 (198.02)	fundamental Band
	3544.977 (128.92)	
	3137.008 (2.44)	overtones
	3616.768 (1.65)	combination band
	3543.991 (2.83)	
2A_1	3708.358 (190.67)	fundamental Bands
	3702.941 (347.15)	
	3608.856 (136.62)	
	3548.907 (151.04)	
	3177.926 (2.76)	overtones
	3762.083 (2.23)	combination Bands
	3625.891 (8.70)	
	3675.354 (2.44)	
	3617.929 (50.41)	
2B_1	3674.531 (217.00)	fundamental Band
	3687.732 (268.32)	
	3593.595 (41.99)	
	3023.915 (1662.35)	
	1573.601 (32.55)	overtones
	3108.346 (1.29)	
	3170.645 (92.57)	
	2147.169 (130.96)	
	2621.036 (4.13)	
	2681.055 (3.80)	
	3451.093 (2.62)	
	2784.496 (3.05)	
2C_1	3633.958 (299.93)	fundamental Band
	3628.388 (44.80)	
	3562.243 (61.91)	
	3557.826 (149.06)	
	3758.534 (4.36)	combination Bands
	3751.063 (1.57)	
	3744.876 (2.06)	
	3740.085 (4.56)	
3A_1	3758.973 (219.56)	fundamental Band
	3754.917 (337.00)	
	3642.028 (131.35)	
	3636.311 (123.46)	
	3579.044 (131.54)	
	3527.435 (378.17)	
	3197.151 (5.42)	
	3174.879 (1.57)	
	3199.450 (2.70)	
	2203.377 (10.37)	
	2112.678 (4.49)	overtones
	2149.645 (1.07)	
	4367.106 (4.34)	
	3722.785 (26.47)	
	3668.124 (70.89)	
	3781.425 (1.41)	
	3782.851 (1.75)	
	3717.008 (69.34)	
	3627.917 (1.40)	
		combination Bands

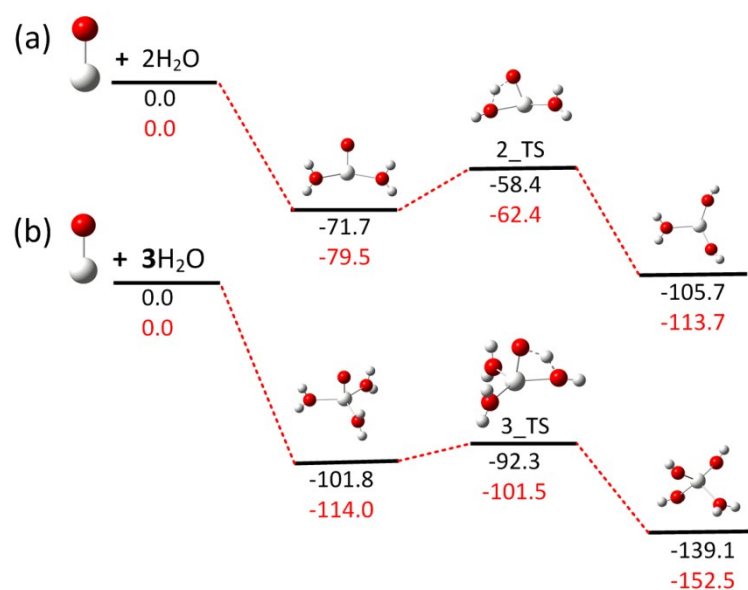


Fig. S5. Potential energy surfaces for the reaction of $\text{H}_2\text{O} + \text{ScO}^+ \rightarrow \text{HOScOH}^+$. The relative energies calculated at the B3LYP/ aug-CC-PVTZ (in black) and CCSD(T)/ CC-PVTZ (in red) level are given in kcal/mol.

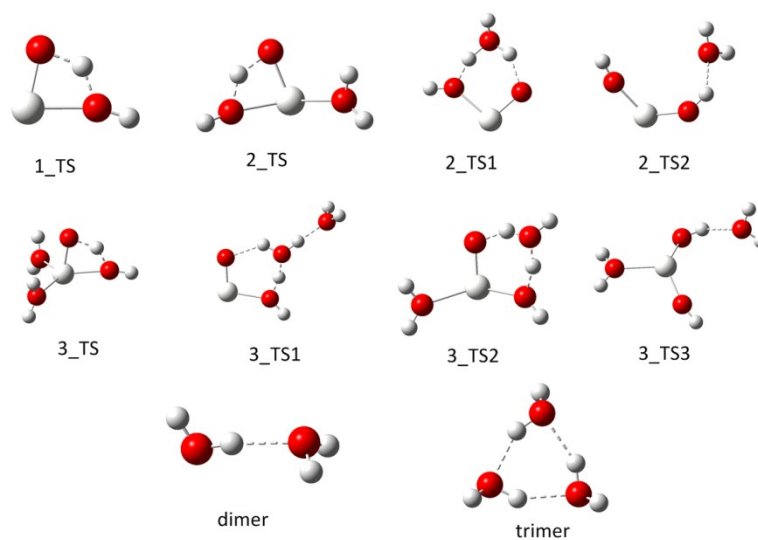


Fig. S6. Structures of transition states and reactants in potential energy surfaces.

Standard orientations and frequencies of [ScO(H₂O)_n]⁺ (n=1-3) isomers

1A Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
21	0.000000	0.000000	0.448869
1	0.000000	-1.563844	-0.447104
8	0.000000	1.563844	-0.447104
8	0.000000	2.236815	-1.136293
1	0.000000	-2.236815	-1.136293

Frequence s	IR intensity
155.8785	3.8157
396.7370	178.9095
487.2022	146.3928
493.4209	0.0015
500.6841	366.9070
806.9980	57.0643
830.1098	325.8224
3835.8216	499.5785
3844.8230	245.4500

1B Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
21	0.000000	0.635136	0.000000
8	1.497468	-0.034078	0.000000
8	-1.156908	-1.200901	0.000000
1	-0.631394	-2.015534	0.000000
1	-2.093090	-1.442481	0.000000

Frequencies	IR intensity
136.6891	42.4774
304.0806	22.8198
390.9289	43.6358
443.2987	258.0684
533.5747	47.5368
1043.8404	182.7139
1645.3130	120.4320
3731.3266	140.5887
3813.9327	226.4597

2A Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
21	-0.234747	0.168827	0.000000
8	0.143342	0.892295	1.633338
8	0.143342	0.892295	-1.633338
1	0.433641	1.471803	-2.343065
1	0.433641	1.471803	2.343065
8	0.143342	-1.967997	0.000000
1	0.311102	-2.510855	0.784125
1	0.311102	-2.510855	-0.784125

Frequencies	IR intensity
13.1378	5.1246
72.4880	1.5108
129.7759	5.4080
249.4791	0.0009
386.1323	4.1925
403.7782	143.4233
423.1016	168.0774
458.5776	188.0302
484.8889	441.9494
489.2049	10.0033
528.5421	25.3461
763.6576	82.8572
816.4039	363.2034
1654.4478	112.6291
3729.3084	189.0082
3801.3147	222.6700
3867.8175	458.2564
3873.8881	188.4679

2B Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
21	1.058064	-0.497503	0.003728
1	2.279663	1.957404	-0.037520
8	2.046241	1.024907	-0.023142
8	-0.724164	-0.437914	0.038073
1	-1.670925	-0.130791	0.032295
8	-3.229814	0.378944	-0.047778
1	-3.962184	-0.195871	-0.294045
1	-3.604019	1.089324	0.483767

Frequencies	IR intensity
16.8779	6.1005
63.1979	8.2934
110.8555	22.1884
182.7923	24.6157
187.9530	212.4546
225.8334	92.3241
336.0522	12.8120
437.5843	167.4621
484.9024	184.6079
794.5542	135.6376
848.6577	156.1009
871.8664	158.4949
973.4621	112.4244
1637.5693	45.0452
3190.5658	2680.840
3789.7446	37.7807
3859.0552	315.0021
3882.4435	136.0537

2C Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
21	0.265047	0.296773	0.000000
8	-1.299021	0.851784	0.000000
8	0.265047	-0.613006	1.994463
1	-0.578363	-0.512874	2.460067
1	0.871071	-1.106326	2.561780
8	0.265047	-0.613006	-1.994463
1	-0.578363	-0.512874	-2.460067
1	0.871071	-1.106326	-2.561780

Frequencies	IR intensity
26.5950	1.1499
97.6990	21.5124
146.0794	45.3490
279.5747	7.1876
292.4562	73.2009
328.5349	1.9162
406.0420	16.5077
423.0733	97.6341
432.8690	419.7862
503.5908	0.0198
516.4891	90.6523
1015.2567	194.5943
1639.5476	226.7439
1641.9873	25.9210
3741.6341	213.7366
3743.6902	38.2582
3829.7235	21.4422
3830.4261	388.9124

2D Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
8	-0.402660	-1.366891	-0.047314
21	-1.212754	0.069632	0.018145
1	0.661494	2.298080	-0.000713
1	1.308757	0.792235	-0.035088
8	0.446937	1.359761	-0.040047
8	2.282512	-0.356479	0.091240
1	1.763657	-1.171501	-0.005236
1	3.119618	-0.472214	-0.371045

Frequencies	IR intensity
102.0850	41.8580

125.6973	25.3667
195.2229	69.3127
248.2086	20.8924
334.1784	139.0094
338.3599	114.6266
429.6405	97.4430
473.7735	61.2210
534.7463	152.3444
798.4212	38.4015
990.0834	92.0458
1013.7231	183.5087
1609.0550	68.9875
1678.1099	90.6728
2593.1008	1688.8269
3687.4078	118.7766
3827.0167	199.2279
3846.4615	188.1432

3A Standard orientation			
Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
21	0.000000	0.000000	0.170563
8	0.000000	1.652779	0.987433
8	1.791380	0.000000	-1.094102
1	2.326178	-0.779350	-1.295220
8	-1.791380	0.000000	-1.094102
1	-2.326178	0.779350	-1.295220
1	2.326178	0.779350	-1.295220
1	-2.326178	-0.779350	-1.295220
1	0.000000	2.342908	1.652884
8	0.000000	-1.652779	0.987433
1	0.000000	-2.342908	1.652884

Frequencies	IR intensity
62.0894	0.0000
70.2949	7.4703
78.3635	4.3316
121.0481	4.7217
135.6633	0.9325
219.1622	0.0000
243.3115	11.1636
341.6147	12.5235
355.0643	112.5776
374.1606	274.5543
391.9306	0.3128
395.6029	142.8663
447.0748	207.9484
454.3518	0.0000
465.4338	406.5381
511.0002	0.0000
520.8439	47.1840
735.3203	94.1403
787.1101	360.0456
1644.6339	197.6170
1647.1763	32.4007
3750.2356	237.2478
3753.1610	63.3248
3829.7823	0.0000
3830.4489	390.2598
3892.1759	357.4198
3896.5801	175.4908

3B Standard orientation			
Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
8	-1.587651	1.700887	0.246099
8	1.054292	-0.162966	-0.190805
1	2.028968	-0.117459	-0.059753
21	-0.722237	0.161221	-0.258357
1	-1.481272	-2.531792	0.330331
1	-2.784549	-1.695252	0.504272
8	-1.861150	-1.648976	0.219975
8	3.720730	-0.103774	0.193298
1	-1.762016	2.590094	0.561503
1	4.185574	0.489957	0.791644
1	4.370502	-0.402557	-0.451033

Frequencies	IR intensity
24.2930	4.5524
34.9963	1.7535

48.7981	7.9038
74.7530	0.8465
106.4130	12.9252
152.4039	51.3151
165.7529	164.4051
199.4830	80.2933
257.7188	1.8700
309.2558	15.2373
384.5964	16.0945
397.0945	228.4860
432.1290	171.7456
473.3819	219.5704
524.9027	32.4703
763.1985	109.8220
792.7624	144.6218
842.2314	252.8696
905.2944	108.9960
1637.7371	54.7328
1651.2864	113.0245
3382.7094	2201.5882
3740.3483	160.8017
3793.6035	28.1495
3815.5487	215.0215
3884.0910	266.9775
3887.6069	130.4488

3C Standard orientation			
Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
21	0.000000	0.000000	0.099592
8	0.000000	0.000000	-1.572242
8	0.000000	2.203314	0.366405
1	0.000000	2.878395	1.054440
8	1.908126	-1.101657	0.366405
1	2.492763	-1.439197	1.054440
8	-1.908126	-1.101657	0.366405
1	-2.492763	-1.439197	1.054440
1	0.000000	2.652873	-0.490181
1	2.297455	-1.326436	-0.490181
1	-2.297455	-1.326436	-0.490181

Frequencies	IR intensity
55.9125	1.3769
55.9138	1.3765
96.8993	21.8141
132.5234	42.7652
132.5487	42.7501
238.5709	0.0000
270.7983	107.8610
270.7986	107.8708
305.1255	0.3190
374.2164	3.3364
374.2206	3.3357
379.9467	0.0000
422.8043	325.2060
422.8058	325.2558
482.2903	0.2916
482.2939	0.2929
509.3820	119.4545
984.3085	204.7878
1630.0267	192.4504
1630.0267	192.4390
1634.0486	12.7837
3752.1142	139.9950
3752.1142	140.0236
3755.0184	45.7881
3846.3031	27.3639
3846.3031	27.3602
3847.4481	503.3078

3D Standard orientation			
Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
21	-0.000508	-1.280962	-0.000997
1	2.232594	0.331177	0.035723
8	1.562940	-0.395782	0.037052
8	-1.570549	-0.406188	-0.032043
1	-2.238773	0.322110	-0.030444
8	-3.359146	1.581910	0.028394
1	-3.536434	2.174921	-0.709147
1	-4.178320	1.523002	0.531124

8	3.373048	1.570497	-0.037586
1	4.274971	1.429887	-0.344043
1	3.406280	2.315614	0.571179

Frequencies	IR intensity
26.9558	0.1508
61.9551	2.3489
75.4303	19.5140
76.0767	4.7510
86.2889	4.0092
129.0478	72.6229
192.5574	54.6695
199.0989	148.2445
201.1262	19.0637
222.4795	171.9858
233.4311	215.2009
316.3764	11.4372
321.3430	7.2374
802.3094	199.2012
816.6800	22.9047
839.7963	49.7694
859.5723	258.6480
931.8962	174.3804
946.4851	62.8253
1637.0270	78.6894
1637.6121	26.5384
3286.5226	3042.5045
3339.1835	1571.0726
3790.5888	32.0103
3791.3603	28.0389
3883.7068	124.1563
3884.8527	123.7885

3E Standard orientation			
Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
8	0.063492	-1.268413	0.409194
1	-3.308229	0.303734	-0.911396
1	-2.654426	-1.108928	-0.831674
8	-2.536415	-0.178928	-0.590261
21	-0.616124	0.259921	0.406142
1	1.883007	0.701373	-0.251447
1	1.407182	2.263376	-0.341923
8	1.119874	1.376477	-0.103086
8	2.623635	-0.617018	-0.460507
1	3.482972	-0.853365	-0.096810
1	1.963400	-1.261471	-0.138465

Frequencies	IR intensity
25.3150	1.6799
77.3669	5.1907
122.0217	39.6038
157.2904	4.2941
200.1198	85.6411
276.8399	3.4799
286.8706	19.3686
315.3676	151.9543
338.3709	105.1161
363.5184	42.6849
413.2843	221.2435
450.9011	134.4391
469.9730	36.2127
514.8952	38.2105
609.0269	221.3547
798.2701	24.6397
977.2822	185.8716
1006.2328	108.0217
1607.4755	83.2518
1643.0159	129.6415
1676.3528	85.3685
2623.8361	1513.2288
3569.1997	338.4989
3744.2552	130.4035
3829.5531	199.2139
3840.4649	187.8766
3847.0464	159.3052

3F Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
8	-0.269224	-0.816401	0.109372
21	-1.963799	-0.294177	0.209655
1	-2.411782	2.261659	-0.679742
1	4.551446	1.434614	-0.405580
8	-2.474060	1.369795	-0.328054
8	4.053180	0.948415	0.259696
1	2.892743	-0.289514	-0.192812
1	4.603518	0.936076	1.049525
8	2.217786	-0.940951	-0.479756
1	2.658190	-1.790482	-0.571990
1	0.724199	-0.861506	-0.092229

Frequencies	IR intensity
25.4918	1.4442
34.9219	4.4379
69.5972	11.8374
98.7186	24.1849
111.9195	33.4458
179.8850	48.5960
191.1528	65.3759
206.6796	43.6130
228.2173	192.5282
268.4818	30.7017
304.5744	78.5321
432.0237	173.3684
481.3440	180.2330
503.2688	17.2491
771.8624	110.4305
787.6608	169.6393
887.8052	153.7666
955.5051	97.0953
1103.2606	95.6058
1631.0642	78.9961
1660.3986	4.1182
2836.6718	3898.1732
3472.3232	787.6618
3790.3647	25.6488
3858.0297	109.5115
3867.8769	291.6155
3884.1702	118.1413

3G Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
21	-1.878494	-0.566051	-0.044477
8	-3.091737	0.759539	0.254683
1	-3.441857	1.640896	0.408724
1	2.975430	0.475848	-0.058287
8	-0.147254	-0.202466	-0.194382
1	5.031788	-0.233456	0.967674
8	4.458210	-0.420078	0.217146
1	5.021426	-0.806519	-0.461179
8	2.129780	0.963211	-0.157622
1	2.311372	1.752856	-0.674822
1	0.758220	0.255785	-0.206691

Frequencies	IR intensity
16.4401	0.5478
32.0186	6.3534
55.2172	0.4699
101.0467	51.7206
112.0773	22.1703
177.7518	17.5393
191.6298	76.9159
200.2069	79.9822
216.3434	203.2780
270.2030	30.5695
302.1051	46.3750
434.7251	165.6420
484.7404	170.3759
498.7346	34.2806
774.5222	113.3767
785.5584	175.7103
887.9883	146.1722
955.9343	104.0643
1103.4277	93.7285
1631.2254	73.5718
1659.0447	8.3996

2832.0836	4027.6378
3471.1570	826.2463
3791.6829	26.7509
3858.9416	90.9897
3866.8901	306.5307
3885.8154	117.7895

3H Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
8	-1.325715	-0.645036	0.189429
1	-2.217766	-0.202247	0.130451
1	-1.453540	-1.530274	0.553152
8	-3.619728	0.619100	-0.007382
1	-4.103154	0.953897	0.756436
1	-4.281383	0.407413	-0.675740
8	2.269501	1.411927	0.168722
1	3.086967	1.010901	0.497047
1	2.396911	2.367879	0.155413
21	0.724506	-0.116538	-0.266067
8	1.595610	-1.456024	0.170561

Frequency s	IR intensity
17.9950	4.1562
43.4868	4.9292
50.8550	10.2288
107.9987	11.3350
144.1408	22.3790
155.1809	29.3795
246.2931	54.3824
283.2112	53.7204
312.8609	229.6043
349.0195	11.5435
353.9776	23.1804
410.7887	85.7197
426.9494	244.2239
459.7669	72.8665
501.4472	35.2323
671.7983	34.8155
946.2698	115.9130
1008.1965	217.3375
1629.7520	150.4411
1635.5064	103.8642
1672.5128	17.5000
3157.4179	1851.5118
3746.6557	116.4191
3779.0291	46.4683
3799.1971	141.1857
3838.6052	195.9051
3867.2891	145.1712

3I Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
8	-1.417430	-0.153073	0.575489
1	-2.333391	-0.160415	0.208561
1	-1.014272	-1.024980	0.455187
8	-3.952543	-0.060801	-0.306212
1	-4.665923	-0.088470	0.340477
1	-4.317605	-0.410012	-1.125830
8	0.432165	1.357518	0.042081
1	0.263025	2.303952	0.083851
1	-0.468288	0.791783	0.246526
21	2.019887	0.030152	-0.133207
8	1.202661	-1.399275	0.012214

Frequency s	IR intensity
34.5850	10.0231
51.5061	17.3555
90.5890	6.6671
109.7777	35.6407
120.8071	16.5373
194.3761	61.9389
236.3866	135.2694
251.8965	128.6448
307.4207	29.4870
341.0112	153.6722
388.2011	78.8988
482.5798	64.7952
526.3083	82.1137

616.6910	174.3649
813.6182	47.7730
869.5155	31.2034
1005.0593	123.4469
1136.5894	93.6377
1571.7210	468.0387
1639.5507	263.5236
1666.8328	277.2886
1932.4272	2012.3756
3363.6316	1133.4524
3749.2639	211.0015
3789.1504	25.3633
3838.9115	179.5261
3881.4732	126.3784

3J Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
8	2.148580	0.981706	-0.081401
1	2.910125	0.353811	-0.068025
1	2.494407	1.856512	0.122508
8	4.168840	-0.798211	-0.087877
1	4.751954	-0.925944	-0.843819
1	4.660943	-1.096205	0.684611
8	-0.162301	0.283357	0.657698
1	-0.208652	0.124670	1.608439
1	0.794790	0.567515	0.415181
21	-1.912065	-0.024461	-0.494520
8	-3.061394	-0.512685	0.569834

Frequencies	IR intensity
28.7697	3.9631
39.4332	26.4055
60.2705	20.5436
70.1483	3.5717
122.6950	20.1216
144.7353	17.6882
227.2893	104.9867
249.9658	180.3633
304.6521	100.7597
306.5566	15.9031
343.7775	87.6460
434.6448	140.3779
508.1223	20.6356
532.3393	24.9868
736.7561	27.8856
845.8983	112.4069
1031.8504	231.5775
1134.1999	82.6617
1617.1665	100.4864
1643.8142	32.2397
1689.4026	8.9663
2635.0278	3191.4934
3364.9315	1000.3464
3787.5441	33.5226
3804.9904	138.0631
3841.5370	111.6458
3878.7846	129.2560

Standard orientations and frequencies of Ar-tagged isomers

1A_1 Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
21	0.000000	0.000000	0.576689
8	0.000000	1.586330	1.446669
8	0.000000	-1.586330	1.446669
1	0.000000	-2.274336	2.120112
1	0.000000	2.274336	2.120112
18	0.000000	0.000000	-2.194300

Frequencies	IR intensity
33.8005	15.6740
41.1489	2.5795
114.1336	1.2015
186.8259	16.1912

390.6410	166.7175
472.6635	157.2668
493.3850	0.0321
497.0867	351.6659
791.7199	82.0757
822.9820	312.9802
3848.5256	479.0483
3856.2448	254.3535

1A_2 Standard orientation			
Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
21	-1.800305	0.552716	0.000000
1	-2.733541	-0.991157	0.000000
8	0.000000	0.536305	0.000000
8	0.926850	0.267516	0.000000
1	-2.983267	-1.921390	0.000000
18	3.429508	-0.350797	0.000000

Frequencies	IR intensity
15.9174	0.7260
56.5321	11.6943
70.0183	14.0349
161.2499	6.8266
413.9619	169.6737
488.2175	166.7067
514.0852	120.1058
543.6741	154.2401
808.1139	70.9207
834.9186	311.9924
3770.9576	831.2947
3843.1058	340.3395

1B_1 Standard orientation			
Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
8	0.797065	1.599740	0.000602
21	0.451010	-0.001232	-0.000990
1	2.936590	-1.652941	0.000564
1	3.186810	-0.113117	0.002108
8	2.496756	-0.792974	0.000729
18	-2.330288	-0.259011	0.000415

Frequencies	IR intensity
15.7279	19.1889
54.1883	8.8121
114.8292	3.9548
161.0201	54.3167
302.9116	27.1934
388.4497	53.1835
445.6198	246.3574
525.9322	45.5276
1035.1385	183.4962
1644.3996	124.2047
3736.1491	140.8854
3820.2210	216.7415

1B_2 Standard orientation			
Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
8	-2.887039	0.691249	0.000067
21	-1.800338	-0.528337	-0.000022
1	1.000639	0.429998	0.000041
1	-0.060621	1.579797	0.000144
8	0.048054	0.617429	0.000066
18	3.309943	-0.076897	-0.000044

Frequencies	IR intensity
32.5409	21.4082
41.0195	21.2532
73.1548	5.4073
153.0392	51.5430
380.5422	10.6714

405.2295	42.3859
472.5153	229.7994
561.1137	41.8387
1043.2059	189.7993
1645.5821	90.5370
3675.6989	492.1583
3775.6405	275.7329

1B_3 Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
8	1.199346	-1.417446	-0.000218
21	1.897623	0.059250	-0.000159
1	-0.037056	2.288831	-0.000043
1	-0.723632	0.884114	-0.000080
8	0.138448	1.338897	-0.000077
18	-2.766207	-0.210489	0.000324

Frequence s	IR intensity
21.5009	2.5759
49.7944	30.6334
94.2195	43.5087
150.4866	20.9796
315.5843	66.5953
402.9810	46.1519
520.2727	158.0441
561.9636	40.7893
1041.7862	176.3865
1648.3141	91.2017
3624.5179	508.2846
3800.3129	240.1859

2A_1 Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
1	-1.165687	-1.550729	2.309107
8	-0.872400	-0.945078	1.624618
8	-0.871275	-0.962279	-1.615283
1	-1.163568	-1.575409	-2.293507
21	-0.484880	-0.199376	0.000807
1	-1.675988	2.268672	-0.791005
1	-1.676736	2.276018	0.768023
8	-1.343210	1.806481	-0.009135
18	2.253309	0.198630	-0.000620

Frequence s	IR intensity
42.1247	3.4729
57.9695	0.3120
79.9150	1.2651
87.8021	3.4581
131.7340	6.0382
164.4882	8.2363
253.7959	4.8243
385.5100	5.4809
392.2841	151.8492
397.3394	182.1159
456.2682	169.1832
457.1782	19.5186
466.8005	388.6057
529.6107	24.6815
759.4987	87.5219
800.7123	321.4323
1650.5603	115.6245
3741.0817	172.9473
3816.5937	205.7927
3876.2626	398.7333
3881.7135	211.3562

2A_2 Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
1	-3.869744	-1.220806	-0.002229
8	-2.952567	-0.936102	-0.001283
8	-1.247315	1.881008	-0.000322
1	-1.422535	2.825199	-0.002206
21	-1.423214	0.062670	0.000953

1	1.333556	-0.733950	0.000096
1	0.496514	-2.051947	-0.000267
8	0.426255	-1.086714	0.000311
18	3.529928	0.055550	-0.000281

Frequencies	IR intensity
8.7627	9.9670
22.9835	1.6810
37.3892	0.1060
62.9761	3.2782
112.2089	6.8041
134.9977	10.0168
319.2016	28.7764
397.6594	143.5934
399.4229	1.2409
454.2088	191.7570
471.8659	145.6289
481.5534	1.2868
498.8402	391.3551
561.5809	17.6993
762.8527	91.0009
815.0974	356.4506
1656.2988	89.6046
3641.2126	599.8936
3778.9304	243.0381
3869.6317	444.7739
3875.6709	193.0725

2A 3 Standard orientation			
Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
1	2.433480	2.585111	0.538772
8	2.238170	1.692684	0.242465
8	-0.417589	-0.172697	-0.164630
1	-1.369755	-0.094023	-0.048414
21	1.373209	0.156912	-0.234762
1	2.205603	-2.532119	0.279908
1	3.479718	-1.654333	0.467075
8	2.549964	-1.631109	0.198842
18	-3.919489	-0.039490	0.082180

Frequencies	IR intensity
28.4954	2.0526
31.6098	0.6955
50.6078	7.0799
66.9604	8.3652
83.3021	0.6510
141.2758	7.3091
255.8085	1.4601
389.4630	9.0682
411.6199	201.7383
422.3564	157.7043
475.5725	228.5778
493.3006	137.3534
518.2421	146.1247
532.8613	27.7061
767.6465	79.0033
816.8383	361.7324
1653.4512	114.7416
3732.6762	192.0780
3806.0964	208.7686
3827.5283	676.8585
3872.5595	288.8695

2B 1 Standard orientation			
Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
21	0.244182	0.488985	0.006083
1	0.267563	3.239340	-0.026923
8	0.458806	2.297993	-0.015592
8	-1.365604	-0.295225	0.034293
1	-2.337565	-0.487609	0.027757
8	-3.966719	-0.830347	-0.046336
1	-4.337533	-1.718704	-0.033470
1	-4.678046	-0.231584	0.203119
18	2.496995	-1.136083	-0.004286

Frequeencie s	IR intensity
25.9146	4.7433
30.5806	0.4359
48.9066	3.8800
62.2309	16.0151
98.3218	0.8833
118.4523	1.8859
159.1105	246.0392
192.1418	39.7642
216.5658	63.0906
320.0603	14.1272
425.8287	166.3435
481.4112	179.2774
784.4629	139.4157
832.4691	112.7953
857.5587	207.0870
934.6319	107.4321
1637.0029	46.2643
3269.6857	2570.034
3792.9396	34.5978
3868.6871	310.5546
3886.5886	132.4022

2B_2 Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
21	0.978263	-1.417920	0.001533
1	-1.603294	-0.498483	0.005763
8	-0.787745	-1.011395	0.006533
8	2.211879	-0.128467	-0.037341
1	2.662838	0.757501	-0.032511
8	3.399569	2.231810	0.045272
1	4.301322	2.355515	0.359772
1	3.212977	2.966960	-0.547923
18	-3.761500	0.858847	0.003722

Frequeencie s	IR intensity
12.7116	0.1243
35.2939	4.2392
50.8927	2.6028
53.1106	2.4439
63.0669	17.0060
107.5926	36.9983
183.9636	26.4187
195.5087	175.9712
226.3093	122.5357
333.1631	10.8700
478.4889	132.5041
524.7741	142.6050
801.7469	113.9176
841.9760	182.7122
867.9987	154.5293
967.6505	113.6890
1638.0617	47.0387
3210.0985	2619.8539
3790.3445	39.0393
3812.1029	629.3703
3882.9389	132.9181

2B_3 Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
21	-2.597557	-0.608380	0.041627
1	-4.418273	1.421321	-0.252845
8	-3.952020	0.587539	-0.145362
8	-0.894243	-0.084543	0.049596
1	-0.040759	0.430448	0.054337
8	1.373390	1.237111	0.138967
1	2.236842	0.814643	0.065206
1	1.498802	2.165597	-0.081926
18	4.614170	-0.332049	-0.055808

Frequeencie s	IR intensity
9.2908	2.1837
21.7034	4.2466
38.6325	1.0001
65.0315	10.9980

81.5804	29.4913
111.8761	47.3133
182.5680	30.4538
216.1532	85.3762
234.9192	138.9508
349.6145	13.0176
437.8451	167.8791
487.4213	184.0432
792.4898	154.2802
863.4374	108.5406
873.6725	191.6713
975.9019	105.5006
1637.5620	31.4085
3161.4851	2920.7899
3776.7711	97.1260
3860.3079	307.5671
3872.5206	198.6339

2B 4 Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
21	-2.687700	-0.144918	-0.198440
1	-2.696843	2.455628	0.670167
8	-2.897857	1.578617	0.331778
8	-1.091402	-0.934952	-0.127951
1	-0.130169	-1.137685	0.043594
8	1.419505	-1.494147	0.402935
1	1.763496	-2.393430	0.403929
1	2.170149	-0.911050	0.240704
18	4.216283	0.657426	-0.113625

Frequency s	IR intensity
10.8479	0.8031
27.5012	4.3400
51.7431	5.7513
65.9658	3.6563
106.4478	17.7063
137.9439	53.7512
179.3823	26.7671
223.7904	61.3231
257.5747	171.2410
359.7720	15.2217
439.2516	167.0822
488.2844	182.4767
794.6965	140.3855
859.3049	177.8686
873.7937	121.8360
984.2178	107.6460
1639.6899	33.2304
3154.2618	2862.3321
3776.4742	92.0144
3861.2190	301.3933
3870.5186	207.0015

2C 1 Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
8	0.826982	0.004655	1.585547
1	1.462423	-2.532940	-1.293524
1	1.727427	-2.383139	0.237301
8	1.326024	-1.955646	-0.532730
21	0.435530	0.000590	-0.024627
1	1.666894	2.416015	0.239697
1	1.398401	2.560382	-1.291025
8	1.276379	1.979309	-0.530721
18	-2.379797	-0.016625	-0.086225

Frequency s	IR intensity
26.3800	0.7499
40.5682	5.7468
64.8070	10.9074
101.8681	12.5473
141.7040	32.2872
142.6447	43.9269
279.4600	20.3955
296.6258	82.8588
338.4145	1.1332
389.5490	0.0750

409.2897	139.9448
423.2636	360.7082
496.0706	0.0716
511.9225	82.5791
1006.1873	192.1077
1634.5413	202.3020
1637.1178	57.6141
3745.4701	174.7904
3747.6100	71.0493
3836.3068	57.1338
3837.2652	334.5029

2C_2 Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
8	-2.258909	-1.396374	0.238590
1	1.549444	-0.433956	0.105102
1	0.673202	-1.633511	0.586501
8	0.640317	-0.762673	0.165559
21	-1.400322	-0.102482	-0.326265
1	-3.617979	1.162381	0.650892
1	-2.892126	2.461099	0.183010
8	-2.818066	1.499736	0.222326
18	3.843749	0.326144	0.017459

Frequencie s	IR intensity
24.2363	8.1891
33.7601	16.7931
38.3386	5.0120
63.1363	2.3246
107.8068	22.1842
151.2380	48.6172
284.6811	42.5263
333.8213	1.4366
364.3647	0.6274
412.6987	34.0539
425.9440	182.8600
446.7616	316.3695
507.6871	26.7596
538.3993	54.5788
1013.8556	198.8100
1639.5118	167.2469
1644.8586	63.9281
3707.3718	380.9023
3743.6085	112.6713
3791.3703	285.8535
3831.8346	206.1810

2C_3 Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
8	-0.662707	-1.291504	-0.424675
1	0.722441	2.359868	0.162470
1	1.327767	0.925269	0.058939
8	0.499191	1.432874	0.014715
21	-1.307789	0.227505	-0.343366
1	-3.315420	-1.221930	0.817158
1	-4.013578	0.163782	0.973651
8	-3.221512	-0.274826	0.639723
18	3.323476	-0.329831	0.186687

Frequencie s	IR intensity
19.4927	1.7156
22.8889	3.8182
48.2173	5.5215
77.2678	23.7543
115.4669	30.8582
149.4599	33.4375
284.0966	10.4991
298.8759	96.7730
334.1754	2.7468
410.5139	63.5518
423.0290	216.3044
491.0278	175.5836
508.9541	29.6036
538.8515	57.7775
1013.7745	188.9451
1640.0535	158.5194
1646.2678	65.6066

3657.2808	438.8843
3743.7649	123.0895
3817.4236	211.3522
3832.1582	214.0336

2D_1 Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
8	-0.546515	-1.298374	0.086944
21	0.125988	0.214830	0.039962
1	-1.963049	2.259147	-0.033595
1	-2.452079	0.696713	-0.003728
8	-1.654556	1.348760	0.025041
8	-3.283848	-0.564124	-0.151093
1	-2.652735	-1.294013	-0.030225
1	-4.098887	-0.785308	0.311435
18	2.911130	-0.071003	-0.042790

Frequency s	IR intensity
-8.2299	1.8285
38.7004	1.9456
101.6374	38.6287
111.4019	12.9620
142.9722	19.2575
206.0706	85.9300
258.3498	17.3150
335.2988	116.3271
339.2624	147.9424
430.9815	93.6646
470.6735	56.9475
554.7685	177.0374
796.2518	31.2476
993.3520	100.5637
1004.2990	178.1268
1606.5830	75.6664
1677.5757	89.7642
2613.0998	1648.3212
3657.6460	177.7770
3831.7475	193.0547
3848.0426	185.6571

2D_2 Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
8	-2.732410	0.138671	0.023387
21	-1.638512	-1.097392	-0.014527
1	1.086515	-0.077412	0.032941
1	-0.117956	1.032790	0.050128
8	0.127089	0.034223	0.060436
8	-0.884473	2.342595	-0.087201
1	-1.825728	2.119516	-0.007160
1	-0.728028	3.170766	0.378553
18	3.550683	-0.184686	-0.006798

Frequency s	IR intensity
25.5827	6.8810
43.6613	8.7677
56.1693	5.9739
105.5191	45.3757
125.7565	27.9136
195.5727	80.8156
241.1249	29.8279
334.2125	74.6186
418.7726	193.4608
422.1813	22.2547
477.7903	73.0582
533.7357	128.0737
814.3925	32.1947
982.5281	86.8329
1013.3867	189.6500
1608.6868	74.8570
1678.5165	97.7712
2649.4955	1631.0297
3691.3095	120.1222
3761.2780	512.8527
3850.4733	179.1626

2D_3 Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
8	-1.761973	-1.388752	0.039060
21	-2.696647	-0.048023	-0.191862
1	-1.110626	2.374885	0.058551
1	-0.317610	0.952715	0.281889
8	-1.210270	1.417072	0.034561
8	0.713695	-0.043748	0.710282
1	0.332516	-0.924064	0.565171
1	1.640969	-0.065024	0.444326
18	4.119596	-0.067034	-0.199558

Frequencies	IR intensity
18.5264	4.4881
35.8152	6.8203
55.0021	3.8690
108.2976	36.5590
129.4376	28.7755
202.1906	51.3248
290.2528	10.7759
337.1595	145.6255
349.5857	108.4072
444.5453	101.8315
476.5201	70.6098
535.2647	140.4229
803.1306	37.3407
1007.4309	116.6229
1016.4673	148.0756
1610.5488	47.5073
1679.4574	91.8487
2525.2961	1912.5167
3695.8136	74.0183
3814.3733	373.3215
3827.9412	214.8973

3A_1 Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
21	-1.210069	-0.060337	0.175364
8	-0.694156	1.072617	1.536210
8	0.625010	-0.924216	-0.633837
1	0.689903	-1.820047	-0.989645
8	-2.105243	1.266209	-1.324756
1	-2.049527	2.230706	-1.307533
1	1.527787	-0.612313	-0.463607
1	-2.832176	1.027095	-1.914641
1	-0.598552	1.478815	2.399155
8	-2.374074	-1.486112	0.295766
1	-2.989680	-2.135852	0.638894
18	3.780634	0.092816	-0.057353

Frequencies	IR intensity
13.9989	1.1519
25.2377	2.3575
58.6794	2.6785
74.2503	3.8235
79.9724	1.9827
107.9249	8.1903
120.2781	5.2981
136.9037	1.5385
233.6799	3.9232
283.0775	28.5731
352.4599	128.0799
366.5161	9.1838
383.4439	143.9369
391.5250	16.9363
417.3300	116.6961
435.6376	98.4374
441.1658	182.8010
457.1676	399.0997
517.0630	16.4115
543.8052	22.5854
734.5343	95.8042
785.6646	354.0680
1645.6580	157.1110
1649.7993	52.4075
3691.2108	452.3504
3753.7018	142.8575
3806.8309	226.1655
3832.4860	198.4971
3892.3416	347.2888
3896.7094	175.9114

3A 2 Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
21	1.175014	0.000060	0.119307
8	-0.624764	-0.002586	-0.271719
8	1.960737	1.791156	-0.872176
1	2.695625	2.327117	-0.545917
8	1.963066	-1.791234	-0.869830
1	1.477350	-2.326613	-1.511087
1	1.475122	2.324408	-1.515270
1	2.698942	-2.325566	-0.543109
1	-1.581043	-0.001857	-0.186234
8	1.961800	0.001875	1.788035
1	2.086361	0.005031	2.738517
18	-4.200798	0.000141	0.047954

Frequency s	IR intensity
12.8318	3.2518
26.0722	0.2980
41.7696	4.6147
68.2082	0.0402
72.9742	6.7312
83.6808	2.6792
123.8572	7.1135
138.4712	1.8506
227.8731	0.0613
251.6047	10.6215
349.2184	12.6140
357.0113	55.3918
379.3558	332.3731
393.7638	0.5351
406.3846	167.8452
453.7784	180.6544
465.2456	158.2879
489.9808	189.1075
512.0932	2.2327
521.5568	49.5000
737.0581	91.5424
789.2585	366.8218
1645.0778	197.3647
1647.5213	33.7836
3751.5256	233.8170
3754.3570	68.3981
3831.0859	1.2608
3831.7380	377.3895
3863.2959	524.3252
3894.9811	244.1503

3B 1 Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
21	0.263874	-0.463834	0.172944
1	0.820563	-1.612615	2.627412
8	0.821420	-1.258476	1.736270
8	-1.420768	0.116592	-0.153599
1	-2.375724	0.337490	-0.096325
8	-4.070813	0.688173	-0.056458
1	-4.672603	0.425645	0.647427
1	-4.480053	1.441628	-0.493903
8	0.790219	-1.787612	-1.490772
1	1.398029	-2.538247	-1.451965
1	0.254664	-1.888716	-2.289305
18	1.919628	1.750328	-0.158816

Frequency s	IR intensity
27.8481	0.6352
39.7361	2.6332
43.8314	3.4308
59.8851	5.6399
66.7685	10.5508
75.6226	0.2459
106.7036	2.0804
141.7033	3.5355
168.3174	149.3585
175.6702	37.3511
197.4548	111.1157
253.6560	5.3108
291.3604	13.8927
378.4999	145.5894

385.8951	86.9893
424.0675	165.4593
459.0814	218.2273
523.3377	29.6232
755.7380	111.6680
782.3851	125.4125
827.9468	250.3451
881.3085	98.0063
1636.4284	56.8794
1648.4897	115.0414
3430.3931	2060.1862
3748.0361	153.1045
3793.9896	25.7061
3825.5610	202.9103
3888.1229	101.5910
3890.9793	279.4568

3B 2 Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
21	0.644378	0.473305	-0.315841
1	0.172631	3.060683	0.546781
8	0.148519	2.165409	0.203097
8	2.277235	-0.289062	-0.161835
1	3.219429	-0.494076	0.033143
8	4.841739	-0.907778	0.408522
1	5.405787	-1.465060	-0.137192
1	5.430876	-0.390039	0.966547
8	-0.956262	-1.007115	-0.225672
1	-1.904068	-0.840423	-0.088249
1	-0.826302	-1.965086	-0.202632
18	-4.195564	-0.418725	0.206743

Frequence s	IR intensity
11.5943	1.5717
18.0741	1.3636
31.0861	2.6767
41.6403	2.6824
49.0029	3.4615
69.4466	5.2849
93.5056	4.4705
110.2669	15.4248
144.4155	168.2223
158.3354	73.8605
196.8942	57.4713
301.0257	16.1161
310.9891	39.1728
394.9628	12.5166
428.9384	174.2363
457.0335	32.6113
471.6924	335.6975
553.1085	25.6099
762.8038	107.3705
791.1854	129.4533
838.8318	276.8913
895.0305	101.3903
1636.4885	54.6847
1652.4349	86.0358
3396.2551	2244.2309
3662.3204	499.2728
3791.4917	249.3106
3793.5979	26.2462
3886.3726	243.4328
3887.9141	145.6964

3B 3 Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
21	1.045415	-0.925377	-0.242660
1	2.937811	-2.696578	0.726803
8	2.176899	-2.242981	0.358580
8	1.328916	0.860503	-0.209943
1	1.682464	1.769374	-0.081388
8	2.233001	3.377010	0.166630
1	2.896287	3.637616	0.813728
1	2.228928	4.063631	-0.508002
8	-1.057843	-1.443288	0.018652
1	-1.404214	-2.309337	0.273556
1	-1.803535	-0.819914	0.028128
18	-3.663291	0.632120	0.065093

Frequence s	IR intensity
13.8147	0.8784
21.0361	3.3560
39.8310	1.8116
44.5108	0.9935
64.1894	2.9559
79.0063	7.0663
109.4803	13.8947
114.1807	13.1883
154.7762	22.0127
175.8446	147.5024
201.7348	127.2046
308.9236	26.4667
309.7013	22.5211
395.4579	9.9120
429.9943	168.8981
460.9602	68.9887
475.7366	304.7558
552.7173	22.0606
761.2913	111.0576
785.4718	152.2905
840.2283	250.1127
898.7186	107.1543
1637.9417	55.5374
1653.3846	91.7622
3397.7009	2123.6026
3665.7519	526.9826
3792.4976	245.5349
3794.1037	17.9998
3885.7860	264.9143
3888.2624	131.4595

3B_4 Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
21	-0.798114	-0.755619	-0.339559
1	1.869357	-0.067000	-0.072216
8	1.009741	-0.480050	-0.189767
8	-2.113693	0.472335	-0.159705
1	-2.643734	1.289047	-0.017953
8	-3.614306	2.674275	0.264718
1	-3.318265	3.478318	0.703362
1	-4.380841	2.920128	-0.263079
8	-1.429367	-2.695463	0.463663
1	-0.854982	-3.428358	0.725297
1	-2.324399	-2.910347	0.761038
18	4.310792	0.823190	0.125723

Frequence s	IR intensity
17.3870	0.1616
19.0288	1.8730
37.7449	2.8916
42.2860	5.8124
50.8845	1.9254
59.0663	12.6340
77.7139	0.8475
105.8543	12.9491
155.6143	53.7980
168.9712	155.6805
198.6641	90.9515
256.8971	1.4734
300.9380	14.0439
386.5933	38.9677
395.5148	236.3351
464.5133	134.0397
501.2162	165.2320
522.7920	33.8068
766.7277	94.5046
793.8312	146.7483
840.5314	272.3932
901.9852	106.0770
1636.3705	55.1536
1650.6736	114.1935
3393.2834	2192.6793
3741.5100	165.8957
3793.6638	27.8343
3816.9598	210.2081
3850.4421	527.9579
3887.7337	121.5158

3B_5 Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
21	-2.426291	-0.097657	-0.239015
1	-3.808913	-2.209612	0.891397
8	-3.507308	-1.398589	0.476922
8	-0.622700	-0.124727	-0.337184
1	0.325732	-0.382230	-0.271449
8	1.958202	-0.847408	-0.119245
1	2.282730	-1.752257	-0.164367
1	2.732002	-0.278737	-0.191889
8	-3.162780	1.923929	0.183511
1	-4.028614	2.156314	0.546761
1	-2.624183	2.727358	0.186918
18	5.486113	0.298017	0.132772

Frequency s	IR intensity
9.7364	0.7546
15.2635	3.5496
34.1988	0.4832
38.4908	2.5706
55.2681	10.4066
68.6572	26.6315
79.2837	14.8787
100.8648	11.6296
158.2871	21.1061
178.1056	163.1914
205.7110	43.1279
253.1186	3.3977
307.5996	15.7506
384.2371	16.9106
393.1315	233.4170
429.0686	173.8236
473.3318	217.7680
522.1439	32.0811
764.2911	118.0348
800.4459	122.2571
842.2911	264.6205
906.0292	99.2462
1638.5465	59.7060
1650.6185	112.6159
3374.4257	2331.6791
3741.3201	158.7485
3793.0100	51.4453
3816.6172	214.3997
3884.4791	196.1625
3884.8974	222.1017

3B 6 Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
21	2.128884	0.239539	-0.287869
1	2.102230	2.921165	0.389632
8	2.304397	2.017759	0.137791
8	0.601282	-0.724566	-0.292679
1	-0.333601	-1.025225	-0.205488
8	-1.929564	-1.570055	0.008817
1	-2.701994	-0.996097	0.060468
1	-2.249063	-2.427338	-0.290107
8	3.798166	-0.963609	0.467418
1	4.632030	-0.632009	0.828337
1	3.762197	-1.912697	0.650676
18	-4.895145	0.498092	0.113387

Frequency s	IR intensity
9.8184	1.8727
16.3117	0.9732
33.1530	2.4743
40.3770	4.6635
69.0144	2.9341
73.8279	1.2840
103.6979	7.4949
111.3416	51.1981
159.2085	24.7726
199.8906	32.8395
234.2772	160.6987
253.0779	2.7515
323.0891	15.0088
384.3344	20.5998
393.3635	223.2453
428.0557	176.0965
468.0213	220.9956

522.3390	32.3220
763.5655	125.1741
815.6412	108.5671
840.9793	272.7282
914.0228	95.5667
1638.8859	46.1872
1650.5022	112.8011
3354.9208	2339.6650
3741.2977	160.7735
3783.0755	67.6977
3816.6477	213.2046
3876.7519	162.9729
3884.3146	283.2549

3C_1 Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
21	-0.693657	-0.000530	-0.000424
8	-2.368704	-0.004194	-0.003444
8	-0.489765	0.803181	2.058420
1	0.169433	1.059219	2.712965
8	-0.484441	1.383394	-1.722903
1	0.176227	1.824182	-2.268558
8	-0.480305	-2.184391	-0.334169
1	0.180405	-2.877734	-0.440296
1	-1.365654	0.951753	2.440991
1	-1.359523	1.638944	-2.046261
1	-1.355363	-2.591758	-0.397270
18	2.705944	0.001256	0.001339

Frequency s	IR intensity
24.4107	10.6703
25.7777	10.6912
43.1975	3.7331
56.9199	0.7253
57.1860	0.6622
96.6505	18.7369
133.7406	41.5837
134.9400	43.6030
248.2413	8.1881
277.0503	113.9841
284.7285	119.7084
304.1175	0.3309
373.0049	2.2233
373.6741	1.3142
382.8492	0.3434
422.7993	297.1865
423.8686	293.5601
476.3856	1.2144
477.5916	1.5267
506.6458	129.6508
978.6504	245.8004
1624.2274	206.6672
1624.6468	206.6279
1628.8140	23.2416
3752.6685	126.2564
3753.0351	126.0567
3755.4720	67.6664
3849.5840	62.4978
3850.3014	37.2742
3851.2443	424.9869

3C_2 Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
21	1.206579	0.000055	-0.011760
8	2.031265	0.000023	1.443220
8	-0.850449	0.000865	0.803803
1	-1.772123	0.000681	0.512306
8	2.044479	-1.906790	-0.780386
1	2.000722	-2.501511	-1.537513
8	2.046840	1.905511	-0.781242
1	2.004302	2.499980	-1.538635
1	-0.846022	0.001009	1.770803
1	2.660362	-2.286862	-0.138521
1	2.663117	2.284863	-0.139322
18	-4.123644	0.000212	-0.231407

Frequency s	IR intensity
22.5762	1.7272

27.0911	12.0225
54.4852	0.1270
59.6076	0.4291
60.4754	1.0703
100.1947	23.0378
131.9990	37.9023
137.4227	44.0438
257.1082	28.7351
278.1151	113.0407
308.6120	0.0905
352.2386	13.2783
371.3749	5.1107
378.0946	21.9325
383.3840	0.2689
420.3373	312.3471
424.7967	350.9461
477.0103	0.6556
489.0919	29.4871
521.5224	82.0821
983.0629	207.4953
1627.4723	194.0661
1629.5769	121.0115
1636.5026	60.2722
3730.8149	280.3826
3751.8207	134.9497
3753.8483	62.0729
3810.7138	296.1090
3847.7956	30.5922
3848.5696	345.0744

3C_3 Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
21	1.124747	-0.000442	0.161275
8	0.367297	-0.004124	-1.329454
8	-0.664426	0.004422	1.467978
1	-0.886071	0.007015	2.405886
8	2.227504	1.906863	-0.112076
1	2.838629	2.497748	0.342044
8	2.238203	-1.902268	-0.106358
1	2.851308	-2.488595	0.351029
1	-1.498046	0.002384	0.970155
1	2.033172	2.289303	-0.979086
1	2.046838	-2.289206	-0.972034
18	-3.575230	-0.002695	-0.270305

Frequence s	IR intensity
16.8680	1.2980
19.9558	0.9878
51.7160	7.2283
59.2486	0.7032
67.1104	6.7619
104.6355	33.8390
136.3632	47.1920
137.9864	26.3905
245.8025	1.8158
274.5302	113.4433
280.3342	112.0792
307.5969	0.7892
372.6461	3.1338
376.3798	9.6545
390.9632	67.5011
421.0505	315.8076
461.7765	192.9849
483.4857	11.5057
493.2190	24.6726
521.6612	92.8987
983.1680	199.5499
1629.1206	192.2958
1631.4842	108.2555
1639.4905	70.0845
3685.2797	357.2785
3752.6674	135.0456
3754.6074	77.7640
3833.8892	188.2857
3848.1296	34.2098
3848.9369	353.6988

3D_1 Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
21	-0.303043	-0.048807	-0.071945
1	0.927099	2.421233	-0.037395

8	0.324102	1.642792	-0.071387
8	0.767851	-1.498313	0.009717
1	1.562366	-2.080303	0.038434
8	2.948634	-3.076187	0.015788
1	3.644725	-3.058247	0.680467
1	2.952368	-3.964313	-0.355784
8	1.981662	3.758321	0.085967
1	1.714787	4.609044	0.449146
1	2.705804	3.939081	-0.521985
18	-3.073402	-0.414137	0.052071

Frequence s	IR intensity
5.2265	1.1877
12.2199	10.1912
24.6256	0.1656
25.7902	0.2020
45.9615	7.0201
79.3309	9.6256
81.1763	2.5572
115.2742	2.6868
124.9068	48.5675
180.7474	57.4254
187.0759	249.0279
205.2301	39.1642
210.6544	112.7161
222.0276	170.8265
309.8843	12.9654
315.4917	5.9397
789.4389	198.8224
802.0303	8.2393
824.2297	53.9204
853.0466	276.9090
905.7255	164.6794
920.4787	65.7525
1636.9548	71.3565
1637.7710	36.3253
3346.5282	2886.5946
3391.8938	1574.7113
3792.8149	31.5841
3793.0861	23.7589
3886.7957	127.0638
3887.0372	112.8074

3D_2 Standard orientation			
Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
21	2.253527	-1.175384	-0.123451
1	-0.450303	-1.673410	0.100373
8	0.532584	-1.675248	-0.015153
8	2.738847	0.555076	-0.043975
1	2.683732	1.538564	0.032328
8	2.542848	3.219096	0.158442
1	2.687908	3.693879	0.983538
1	2.808086	3.818200	-0.547231
8	-2.099766	-1.724058	0.373347
1	-2.616898	-2.535085	0.338705
1	-2.718734	-0.997818	0.238729
18	-4.412999	0.991100	-0.129737

Frequence s	IR intensity
6.1264	1.4948
11.7719	0.2018
25.2955	0.0627
51.1661	4.1693
64.3558	4.2784
79.1765	5.9056
81.6440	11.7238
99.0633	36.9346
129.1620	80.3752
196.8674	47.7742
203.4595	71.2190
210.6588	67.9723
227.4656	149.1239
235.8607	207.5679
324.7629	9.7106
332.2355	10.7325
799.3634	141.6515
829.7163	48.0991
838.5859	86.1482
862.1939	262.6735
936.2775	104.7757
946.7083	113.2506

1637.1573	42.7754
1638.8969	49.3519
3274.0541	3042.4455
3336.0413	1670.5375
3782.6088	72.6656
3790.1740	29.7092
3876.6490	184.3987
3883.1469	122.3065

3D_3 Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
21	1.751824	-1.314196	-0.001926
1	-0.633515	0.064339	-0.080532
8	0.109755	-0.589013	-0.065864
8	3.232055	-0.294199	0.050007
1	3.833480	0.489732	0.053763
8	4.843273	1.842806	0.002267
1	4.993847	2.424201	0.754842
1	5.651146	1.863953	-0.521323
8	-1.901394	1.158212	-0.039421
1	-2.827297	0.891567	-0.009294
1	-1.882224	2.032077	-0.442357
18	-5.344070	0.160545	0.039413

Freque s	IR intensity
13.8435	1.1380
15.6058	0.8597
22.9576	0.7419
50.8871	3.0968
63.0603	1.3878
81.8198	2.4245
85.3492	15.6812
112.1409	31.4409
128.2830	90.3558
195.2222	61.9528
202.7787	46.3208
210.7457	50.2441
229.8116	198.9429
250.6716	183.7705
319.8848	7.9802
341.6311	10.5633
805.1175	148.6446
826.9743	53.4160
842.1315	68.5453
860.3407	276.5786
932.7415	142.4047
946.7823	76.1922
1637.6896	63.3555
1639.0205	28.8578
3272.0220	3210.2498
3334.4643	1608.1368
3780.6132	82.8280
3790.3988	29.2560
3875.5339	182.8547
3883.5920	122.7911

3E_1 Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
8	0.707054	0.222886	-1.314321
1	-0.849274	3.213972	0.694956
1	-0.154255	2.967616	-0.679411
8	-0.487449	2.531039	0.117350
21	-0.091566	0.359483	0.155817
1	2.169406	-0.823301	0.764858
1	1.592788	-0.774837	2.293307
8	1.373565	-0.592617	1.374447
8	3.086976	-0.854970	-0.459546
1	3.554521	-1.623468	-0.801556
1	2.459560	-0.542495	-1.144278
18	-2.460613	-1.134297	-0.119082

Freque s	IR intensity
22.1383	1.0796
36.8703	2.4868
46.9251	4.2680
81.5024	4.0439
108.4417	4.5800
148.6667	42.4529

174.1988	9.4215
206.7035	95.2807
268.6872	18.7890
289.9785	23.4696
306.3855	124.5492
343.8210	127.1852
365.6392	37.8216
401.1172	203.0306
449.9457	136.0244
474.2927	28.8951
509.1201	35.8810
636.4659	230.1554
806.4683	27.4765
967.9651	184.6769
1008.6572	102.9656
1607.8238	85.8306
1639.5471	131.6945
1677.9377	83.2661
2635.7177	1467.4122
3517.4479	445.3795
3748.2421	127.8542
3835.4941	188.4242
3843.9299	182.5789
3848.3080	149.7050

3E_2 Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
8	-1.763507	-1.358210	-0.103943
1	2.092002	-0.484200	0.181647
1	1.153277	-1.660837	0.596051
8	1.178748	-0.805523	0.144249
21	-0.770431	-0.104417	-0.595971
1	-2.929354	1.118950	0.252094
1	-2.107999	2.479389	-0.130898
8	-2.079161	1.518267	-0.168654
8	-3.886564	0.117445	0.896651
1	-4.830204	0.033576	0.726555
1	-3.453538	-0.728744	0.667147
18	4.369930	0.314378	0.226465

Frequencies	IR intensity
17.0474	1.6323
26.6775	8.0694
38.0473	2.1644
58.8480	1.5309
91.9178	10.6269
128.8709	35.7572
161.2985	1.7039
203.9798	86.2740
286.1751	10.2489
316.1115	137.6628
340.1251	118.8284
354.9593	7.3570
373.5903	26.4884
441.3719	196.8857
453.7443	150.2623
472.8085	43.8941
540.0427	30.5369
619.1438	223.2565
800.2874	23.7731
977.0232	193.6879
1008.9143	104.9729
1607.5959	86.0909
1645.8747	101.7599
1677.1092	85.8170
2629.6984	1512.7768
3556.8512	377.1123
3704.9781	388.7147
3792.1557	280.8403
3841.5736	176.0767
3847.5687	160.3904

3E_3 Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
8	0.540971	0.729000	-0.820758
1	-1.514866	-2.327111	0.703920
1	-1.859864	-0.872221	0.260631
8	-1.144943	-1.529975	0.305059
21	0.835483	-0.859661	-0.384632
1	2.932400	0.423383	0.522206

1	3.391115	-1.048418	1.067627
8	2.727161	-0.585236	0.547406
8	2.745924	1.929204	0.350141
1	3.382100	2.543541	-0.029759
1	1.931069	1.952748	-0.190508
18	-3.597778	0.724279	0.149353

Frequence s	IR intensity
15.8617	0.0640
27.2157	3.3776
39.5805	0.2967
63.7416	4.5386
107.9721	27.0663
134.7664	29.7558
161.6392	3.0749
205.7349	91.7323
282.7774	15.9011
287.8786	26.1042
319.2535	167.1796
340.9606	113.8636
372.1902	35.3344
451.0146	131.6430
468.3111	0.8712
488.4432	172.5758
539.9216	33.5712
620.9883	221.6727
800.3337	23.8302
976.5534	182.6939
1011.3769	103.4337
1606.3349	81.9203
1648.7972	100.6880
1677.0287	87.6278
2623.9250	1477.3069
3550.6589	384.4510
3660.8736	436.2785
3815.1130	222.4445
3841.6922	180.4307
3846.5159	161.3509

3E 4 Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
8	-2.269378	0.939573	-0.233780
1	-2.601679	-2.834824	0.871549
1	-3.440963	-1.525878	0.981159
8	-2.629072	-1.904815	0.614722
21	-1.351493	-0.443842	-0.439943
1	0.446676	1.379822	0.103142
1	1.501804	0.138148	-0.035491
8	0.574857	0.388511	-0.128297
8	-0.239866	2.702370	0.489470
1	-0.031644	3.581087	0.156617
1	-1.172067	2.503605	0.274586
18	3.899272	-0.607022	0.052797

Frequence s	IR intensity
22.1956	3.2634
27.7469	2.2956
36.8972	7.6321
54.6383	3.3028
84.4744	4.1127
123.4560	42.1636
159.1136	4.3190
201.0213	90.2760
272.7534	4.3055
286.3313	44.9486
337.3834	94.8125
362.5692	26.7017
392.4141	92.7079
410.1037	244.5300
448.4280	127.9116
473.5646	44.2689
511.8882	40.7147
617.1199	204.0807
812.6451	26.9752
976.9931	182.2882
997.6449	113.3075
1608.1028	86.7401
1641.5717	130.7746
1675.8218	84.8835
2680.6860	1476.5403

3570.1760	336.3192
3744.2590	137.4786
3790.7915	430.4835
3830.0348	213.3398
3848.9816	150.1690

3E_5 Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
8	1.094642	-1.212435	-0.221856
1	4.804389	-0.142910	0.612683
1	3.920944	-1.419551	0.750320
8	3.934197	-0.511301	0.415806
21	2.018115	0.163141	-0.450732
1	-0.278284	1.105287	0.388737
1	0.467557	2.558651	0.261649
8	0.570387	1.616318	0.096137
8	-1.207029	-0.016622	0.804778
1	-2.129155	-0.113475	0.540968
1	-0.713065	-0.801717	0.498943
18	-4.643909	-0.201107	-0.130380

Frequeencie s	IR intensity
17.1908	4.4554
24.6731	3.3683
27.0121	1.7740
57.1252	3.0780
84.8514	1.9107
126.0885	35.1770
161.4840	9.8246
202.7782	76.7814
276.8394	12.0088
307.7122	59.4424
321.5008	75.4575
356.3442	90.5139
366.6264	86.7847
410.3877	221.4223
461.8415	122.3005
483.3893	36.3320
515.2907	39.1116
614.4520	226.9603
803.3757	22.5238
978.5318	188.2029
1020.6282	94.8435
1608.7521	66.0757
1642.9795	129.2939
1677.1484	86.6011
2569.6641	1685.3484
3578.7181	315.1871
3744.8107	132.5632
3818.4121	330.2629
3830.2506	188.0301
3842.0549	192.2676

3F_1 Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
8	0.529741	-0.461893	0.036564
21	-0.974835	0.494660	0.015423
1	-0.677618	3.228743	-0.077622
1	5.786126	0.369292	-0.707295
8	-0.990174	2.321681	-0.041967
8	5.188866	0.284964	0.043192
1	3.764793	-0.759824	-0.024417
1	5.718590	0.461781	0.827278
8	2.959629	-1.311122	-0.111235
1	3.198452	-2.209786	0.131508
1	1.485368	-0.780321	0.006650
18	-3.350482	-0.964822	0.005977

Frequencies	IR intensity
-3.4513	0.2391
22.0480	5.5871
22.8162	0.5532
34.9696	2.1590
71.3021	7.0043
94.9869	20.4522
103.6888	51.0412
120.4824	2.5962
169.3652	47.9996
178.2131	58.7071
206.2231	36.8037

222.0733	204.2973
263.6707	31.1454
294.2868	67.1948
426.9954	173.3674
481.6754	167.6526
488.0462	17.4976
755.2728	119.1290
778.1458	171.2625
876.9186	150.3750
933.5168	99.7720
1059.8936	95.1723
1630.6896	82.2211
1658.4545	4.8259
2953.8798	3770.1538
3494.9335	738.6681
3791.7183	24.5704
3862.2974	104.7219
3876.1113	293.3228
3886.0618	114.5106

3F_2 Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
8	-1.392903	-1.272661	0.212281
21	0.174820	-1.985975	-0.229196
1	2.270908	-0.219060	-0.165163
1	-4.143520	3.231081	-0.527260
8	1.692165	-0.983088	-0.254072
8	-4.231293	2.288899	-0.705621
1	-3.565656	1.083460	0.390818
1	-5.034070	2.189620	-1.227635
8	-3.136966	0.438447	0.992396
1	-3.773844	0.218782	1.678241
1	-2.101026	-0.609188	0.504029
18	3.845999	1.779889	0.122235

Frequencies	IR intensity
10.4812	1.1900
19.2112	0.0857
33.7711	0.9595
45.8812	7.3488
53.2323	3.3732
71.2190	15.4466
112.0924	27.7909
122.4237	36.3678
186.7318	31.9249
191.7722	71.9248
217.9415	52.0156
237.1504	202.2562
272.3891	25.1317
301.3234	80.2336
482.0222	137.4436
502.7313	15.9183
529.6198	142.1030
769.4013	101.3579
792.2775	159.7286
882.3592	180.3122
944.8248	88.4132
1106.3158	98.6399
1631.5167	80.3138
1660.5556	4.6628
2859.3762	3813.8844
3478.3574	777.3312
3791.1429	25.4292
3827.4700	587.4866
3858.1157	104.6378
3885.0231	116.8324

3F_3 Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
8	-1.923775	0.525310	-0.675814
21	-3.421455	-0.409869	-0.489299
1	-4.010088	-1.062119	2.108232
1	2.621382	1.120595	1.978584
8	-3.992762	-0.948585	1.154416
8	2.323087	0.759195	1.137475
1	0.979547	1.480101	0.280228
1	3.098135	0.358066	0.729227
8	0.184435	1.869089	-0.144293
1	0.482653	2.574475	-0.725370
1	-1.071708	1.043337	-0.481911

18	5.390153	-0.808182	-0.299333
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Frequencies	IR intensity
6.9265	1.0676
19.3483	0.8734
24.6213	0.8507
30.5930	8.6064
41.1908	3.0088
68.7350	6.6679
112.5266	18.1664
143.2664	53.0737
182.6602	25.3449
196.4444	63.7053
224.6474	57.2315
257.3154	162.0202
286.0565	23.2197
307.3166	92.5694
432.6443	172.1511
484.4294	180.2216
506.5467	18.4528
781.9520	96.8673
787.6362	172.6584
888.5699	153.2171
958.5425	97.8952
1111.0387	95.4971
1631.2393	69.1658
1660.8672	3.5282
2815.5308	3968.0527
3458.2392	844.7015
3783.0358	52.4458
3858.2470	108.3242
3868.2904	286.4850
3875.8233	166.9555

3F_4 Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
8	-2.116831	-0.911541	-0.148908
21	-3.563049	0.095878	0.066602
1	-3.083643	2.795201	-0.019834
1	3.145451	-0.526044	0.588405
8	-3.463230	1.915085	0.045472
8	2.395142	-1.019317	0.938860
1	1.043010	-1.467004	-0.072639
1	2.736944	-1.539964	1.672752
8	0.274133	-1.660455	-0.651753
1	0.445305	-2.500123	-1.087406
1	-1.165117	-1.222252	-0.321623
18	5.277131	0.880922	-0.201537

Frequencies	IR intensity
14.2539	1.4251
26.0328	1.5100
29.6470	0.3639
35.8235	6.9980
59.1223	1.9248
68.4433	9.9104
111.3639	14.4475
154.1513	78.4961
182.3974	36.1469
197.7995	52.7924
221.4903	63.6499
271.3043	99.8552
304.8241	11.4194
310.2330	129.6830
431.2663	174.7621
482.0318	179.8448
505.3903	18.3914
782.7677	102.3122
786.3029	170.4886
889.1326	152.9698
958.7668	96.9839
1112.7991	95.1217
1632.5896	65.5635
1660.8339	5.3784
2814.0325	4003.8191
3455.9021	847.5703
3781.8090	65.4783
3858.1332	108.5065
3867.8045	284.0693

3876.0771	171.2961
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3F 5 Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
8	1.133917	-0.359815	0.313864
21	2.762121	-0.948996	-0.079628
1	4.641336	1.027302	-0.376585
1	-1.600400	4.205331	-0.010467
8	4.155205	0.200465	-0.321976
8	-1.584615	3.341616	-0.435928
1	-1.142901	1.897287	0.461642
1	-2.231730	3.382572	-1.147544
8	-0.842271	1.119651	0.978572
1	-1.618462	0.732999	1.393829
1	0.338524	0.225721	0.550574
18	-4.404933	-1.442090	-0.193084

Frequency s	IR intensity
7.1113	3.1311
9.7954	1.1512
22.3889	0.1939
29.5159	1.7627
35.3133	7.3751
70.8617	8.6713
109.6607	10.7712
121.6334	46.8830
180.6534	41.6924
193.5329	57.3603
223.3954	76.5494
239.2705	177.1965
274.0421	28.1362
305.3225	89.2487
431.7791	172.3276
486.3120	179.9994
505.4529	17.4347
773.1383	111.6022
785.3216	173.0428
888.8910	152.2051
959.5711	105.8256
1108.0432	92.5143
1631.8195	77.5352
1660.8613	6.0134
2819.9038	3940.0135
3472.2430	774.6484
3790.9970	25.5151
3856.7803	109.8684
3868.1719	292.7304
3884.8861	117.5062

3H 1 Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
8	1.727427	-0.222089	0.693637
1	2.569503	0.088623	0.262704
1	1.931348	-0.486831	1.599237
8	3.899364	0.618935	-0.539416
1	4.611340	0.029539	-0.812670
1	4.308765	1.472667	-0.358994
8	-1.180571	-1.980860	-1.275463
1	-1.717924	-2.631129	-0.801391
1	-1.169614	-2.227912	-2.207231
21	-0.348838	-0.485697	0.132383
8	-1.021158	-1.126522	1.509856
18	-1.700461	1.979942	-0.198367

Frequency s	IR intensity
20.6389	0.6021
30.8322	3.3541
41.7568	7.2234
50.8294	0.3139
75.7596	11.9033
109.0799	6.3389
131.6931	3.1228
142.3079	18.5077
146.5333	50.9697
246.1028	72.0349
269.5773	64.1940
298.6777	222.4266

339.3773	11.3197
355.3147	16.5908
405.3643	76.2566
427.3862	226.7157
453.3650	70.1945
494.8490	32.2811
664.4150	33.2966
930.3096	115.3688
999.6605	210.5927
1629.0527	208.5580
1630.7443	54.1292
1670.0077	18.2567
3191.1892	1779.5122
3749.8712	112.4257
3780.3006	44.4042
3803.2185	139.2379
3844.4791	187.1696
3869.1124	140.9966

3H_2 Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
8	2.551410	0.608091	0.306197
1	3.420607	0.122655	0.360775
1	2.665010	1.474861	0.715974
8	4.792445	-0.763917	0.386900
1	5.153197	-1.141161	1.197264
1	5.546607	-0.570527	-0.181476
8	-1.048443	-1.303756	-0.384172
1	-1.920355	-0.929225	-0.174844
1	-1.158320	-2.257593	-0.473383
21	0.568620	0.201169	-0.468364
8	-0.292052	1.573513	-0.120753
18	-4.093035	-0.101946	0.382554

Frequency s	IR intensity
4.8737	0.2699
19.2440	2.0002
32.8431	0.7480
39.9867	0.1525
60.1788	15.6148
79.2146	22.7857
123.5321	7.2676
143.6100	22.4704
148.2103	26.2190
246.9486	60.1010
289.4999	75.7030
304.5100	227.9919
345.6357	12.9120
359.6675	19.4836
417.6963	110.3695
459.5847	55.3954
486.2627	162.2368
522.8022	33.6710
669.0257	35.4538
940.9494	115.3078
1007.4700	211.5029
1629.2676	133.6994
1641.8395	95.4318
1671.9581	18.1644
3167.4284	1861.6325
3672.7833	393.7947
3778.9988	46.3249
3800.0813	142.0944
3826.3015	211.3107
3867.5192	144.1407

3H_3 Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
8	-2.648342	0.185782	0.151414
1	-2.945887	1.136479	0.108964
1	-3.389622	-0.347015	0.465816
8	-3.324231	2.722060	0.001569
1	-3.465740	3.276449	0.777303
1	-3.894252	3.074349	-0.691366
8	1.354714	-0.975900	0.148180
1	1.652550	-1.847407	0.444628
1	2.128528	-0.395619	0.120118
21	-0.821753	-0.914977	-0.233321
8	-1.205747	-2.478817	0.156857
18	4.097783	1.038459	0.000562

Frequency s	IR intensity
16.4536	3.1028
29.2639	3.4593
30.1181	9.8780
44.0076	4.5299
54.9365	9.4045
63.8212	5.8275
116.2074	8.1929
145.4195	24.2255
147.4808	32.7344
246.5255	56.3180
307.5901	225.6230
347.1818	12.0502
356.7971	5.7491
362.8180	16.5335
422.0949	19.6381

430.5159	327.2579
463.1295	73.7883
525.5911	32.4120
669.9721	34.2915
942.5357	115.0440
1007.6362	220.1685
1630.0696	136.5828
1640.0678	91.9807
1672.9060	18.4952
3167.3929	1811.0216
3718.8737	308.1074
3779.5209	46.3234
3799.1750	273.1976
3800.2034	170.7700
3868.0037	143.8634

3H_4 Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
8	-0.475440	0.797878	-0.097417
1	-0.816759	1.732105	-0.043037
1	-1.230448	0.197025	-0.018247
8	-1.256066	3.310900	0.024377
1	-1.561896	3.729325	0.837103
1	-1.724754	3.746325	-0.696709
8	3.479910	-0.138414	0.602658
1	3.766915	-1.038811	0.811642
1	4.173039	0.465387	0.894423
21	1.467830	-0.117270	-0.328770
8	1.185867	-1.749994	-0.308303
18	-3.161372	-1.340647	0.186026

Frequency s	IR intensity
15.4616	2.2157
19.9853	1.9504
33.9203	6.7769
42.7047	7.2217
58.0185	1.9822
66.6420	18.3983
113.1629	18.1484
143.8013	17.9351
145.6016	32.7149
248.9137	48.3419
285.9068	51.9564
308.7611	233.8550
342.8557	13.0548
354.6354	21.4971
415.2973	186.9980
460.8032	78.5766
480.1192	104.4679
500.8970	36.4257
690.6124	28.0988
937.9070	110.7321
1006.7053	211.3156
1630.2426	137.6361
1635.1682	103.9367
1673.9118	17.4894
3183.4540	1778.0805
3739.2260	382.4284
3747.5160	107.4328
3779.2701	43.8514
3839.5740	194.8368
3867.3710	141.0033

3H_5 Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
8	-0.363816	-1.067556	-0.102153
1	0.550228	-0.955980	0.286806
1	-0.328084	-1.775887	-0.757125
8	1.978522	-0.688760	0.999713
1	2.734752	-0.309416	0.534286
1	2.341635	-1.291490	1.658327
8	-3.325087	1.831932	0.164742
1	-4.097421	1.827266	-0.418643
1	-3.250932	2.714787	0.545826
21	-2.294113	-0.130944	0.166392
8	-3.288708	-0.913184	-0.902992
18	5.012161	0.513393	-0.367677

Frequency s	IR intensity
8.8163	3.5715
17.2451	6.1333
31.7698	12.9928
43.0722	12.6511
47.6533	4.8548
70.6768	0.3112
110.1230	15.9176
147.8562	25.5307
189.0326	38.1485
255.8979	47.0929
280.9722	57.5473
345.8005	162.4704
355.5083	25.4861
374.5455	28.1259
410.9636	81.9250
426.4931	245.7709
462.3272	72.7661
500.2395	34.3375
677.1645	35.2107
961.0419	107.4477
1007.3168	220.6338
1630.2396	151.4494
1634.9798	98.4316
1674.8441	15.4346
3120.5976	2030.0763
3746.3945	117.9699
3761.3146	122.0882
3801.5332	140.2724
3838.7807	194.3146
3852.1629	195.2349

3H_6 Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
8	0.282350	-0.481951	0.711235
1	-0.581212	0.015456	0.791769
1	0.209420	-1.297049	1.223342
8	-1.931536	0.905234	0.839178
1	-2.190278	1.404128	1.622124
1	-2.751641	0.617577	0.418008
8	3.827049	1.308067	-0.351494
1	4.678564	0.893939	-0.150963
1	3.984609	2.248497	-0.496034
21	2.174064	-0.166814	-0.286004
8	3.077871	-1.496762	0.113594
18	-5.058371	-0.125343	-0.439015

Frequency s	IR intensity
20.2161	2.1726
22.0896	8.6332
27.8421	7.4561
48.9128	7.2659
53.5614	7.5622
75.4769	5.7877
113.2478	10.4666
147.0852	25.6757
196.0738	44.0262
256.5553	49.4512
282.3297	56.0153
348.4195	124.3693
357.3889	40.8171
385.7444	49.0614
413.1489	76.6282
428.5085	247.7739
462.7324	73.1876
500.8012	34.3426
679.7109	35.2298
963.3634	108.6382
1007.5021	220.1787
1630.1124	151.5449
1634.4614	95.0065
1675.0834	15.4741
3116.0086	2026.9249
3747.1877	120.4790
3760.1306	123.1389
3801.7191	140.0639
3839.5079	194.2486
3851.9965	200.6351

3I_1 Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
8	2.531997	-0.148836	-0.588653
1	3.425863	-0.249640	-0.186749
1	2.045318	-0.982925	-0.507434
8	5.034861	-0.297825	0.404725
1	5.771736	-0.342665	-0.213962
1	5.335573	-0.726732	1.212541
8	0.774880	1.471551	-0.035731
1	1.004663	2.405680	-0.034444
1	1.638584	0.863346	-0.240659
21	-0.889255	0.214587	0.049783
8	-0.145974	-1.255790	-0.136379
18	-3.672972	-0.201454	0.098532

Frequeencie s	IR intensity
9.3822	0.2880
28.7724	0.6286
37.1653	10.1612
58.2585	14.4361
88.5425	7.0578
100.5979	28.6213
113.8062	10.1510
128.1339	10.1624
202.7394	82.5775
236.0179	99.3404
252.9273	155.4512
302.6428	26.7074
338.0273	150.0310
384.8881	84.8530
498.4685	52.0785
520.8658	101.6530
615.7585	194.6118
805.3624	52.0457
860.3013	26.8220
997.8347	131.1704
1129.3804	92.4955
1595.9344	159.3108
1641.1430	228.3434
1666.8427	309.8275
1993.9005	2236.7619
3390.6136	1096.3809
3729.8628	255.1197
3789.6706	25.2018
3843.5323	175.3569
3882.2625	123.2494

3I_2 Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
8	0.878767	-1.665758	0.544094
1	0.636466	-2.556131	0.197945
1	1.828945	-1.524398	0.432263
8	0.077626	-4.098638	-0.287984
1	-0.102010	-4.777679	0.371124
1	0.316191	-4.564351	-1.096211
8	-0.095580	0.527300	0.008502
1	-1.057016	0.602940	0.022974
1	0.210758	-0.479162	0.206273
21	1.590327	1.733218	-0.121185
8	2.776936	0.591805	0.017823
18	-3.574011	0.781307	0.008390

Frequeencie s	IR intensity
8.8472	2.9187
28.2651	19.3187
40.9891	6.1936
42.7368	12.7813
56.6353	3.0907
87.4843	3.7413
99.9151	33.1696
116.0910	20.9338
188.8981	62.7421
232.6436	146.8802
249.1137	114.1693
301.1112	30.2956
386.1682	63.5564
409.6171	121.4462
469.7428	63.6513
522.4985	89.1221
607.4206	145.9990

812.2165	58.3361
871.6452	25.5394
1007.3126	146.9429
1106.1634	90.8231
1604.1918	50.0998
1643.9060	155.4491
1678.4332	303.9436
2046.5264	2408.2864
3384.2249	1069.1981
3766.2857	192.8161
3789.1684	30.0176
3791.1280	425.2945
3881.5582	123.7839

3I_3 Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
8	-0.062339	-0.093235	0.039780
1	0.743709	0.146145	0.558861
1	-0.447616	-0.907954	0.392318
8	2.186891	0.626779	1.295198
1	3.028755	0.414961	0.875075
1	2.359536	0.671196	2.241216
8	-2.025946	1.274676	-0.456141
1	-1.876626	2.164629	-0.790222
1	-1.087061	0.781383	-0.224449
21	-3.569964	-0.088826	-0.202630
8	-2.717695	-1.372935	0.395026
18	5.177848	-0.271516	-0.499359

Frequeencie s	IR intensity
6.6102	3.0165
16.0569	3.0465
26.5896	7.9856
54.6165	17.4977
69.9596	12.3791
88.6422	3.0672
117.7770	29.2962
143.8947	45.3643
196.1173	69.9349
248.1057	50.0255
285.8405	153.5379
336.0073	12.4869
339.8875	173.5190
391.6982	85.2395
479.9614	61.3093
528.2172	79.5200
616.5769	177.3219
817.8752	42.8374
882.1964	33.9105
1003.7006	119.8412
1132.6647	95.3011
1555.5877	647.4629
1640.2173	266.5106
1667.1766	264.8233
1911.4753	1960.0207
3336.1009	1215.5561
3754.7217	217.1365
3776.9578	61.6618
3839.9048	176.7376
3871.5004	185.0028

3I_4 Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
8	0.567967	1.087407	-0.446972
1	1.279952	1.683725	-0.114482
1	0.765575	0.177366	-0.189859
8	2.441529	2.848915	0.330440
1	3.086905	3.159133	-0.313917
1	2.865248	2.921658	1.192063
8	-1.857064	1.415102	-0.243334
1	-2.174610	2.302224	-0.438969
1	-0.785396	1.375082	-0.312233
21	-2.627025	-0.486869	0.101885
8	-1.232450	-1.355054	0.257766
18	2.820556	-1.853662	-0.063633

Frequeencie s	IR intensity
19.5819	0.7837
24.9871	4.5130

32.2272	8.6008
42.0874	14.6718
51.3882	12.6077
80.0843	1.9088
112.3937	48.3152
116.9063	5.5758
186.2864	58.8176
237.7089	99.3282
257.8894	159.5211
301.0418	24.8261
339.5702	150.6268
387.7284	74.2897
442.5596	86.5037
530.6434	69.7332
601.8353	131.7834
806.3372	48.5340
866.6356	33.8009
1010.3267	144.8161
1107.6729	89.7764
1600.1322	86.9237
1644.1189	179.1483
1688.6752	266.7366
1996.6869	2594.2606
3367.4998	1087.1582
3785.7276	139.1777
3790.0363	69.1646
3838.9865	174.6919
3880.1343	123.6321

3J 1 Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
8	2.934784	0.395077	0.950834
1	3.697461	0.516192	0.337581
1	3.283485	0.418515	1.847528
8	4.963948	0.738596	-0.795517
1	5.310049	1.604778	-1.035398
1	5.671150	0.108758	-0.970777
8	0.955425	-1.070792	0.350691
1	1.196203	-2.004133	0.309640
1	1.786447	-0.528146	0.598674
21	-1.061429	-0.540921	-0.069465
8	-1.836724	-1.953003	-0.404212
18	-3.044124	1.464686	-0.024602

Frequence s	IR intensity
8.1383	2.6921
21.1246	10.5119
31.7707	0.9293
37.8311	21.5652
69.1299	1.8297
71.2074	14.2871
107.3746	17.5673
116.8149	3.3785
154.4478	26.4606
224.8275	130.6902
241.2994	154.4508
301.8518	65.7357
302.3642	54.8346
338.6714	81.1306
434.4643	136.9251
499.8745	28.1838
524.6766	24.2514
726.4793	27.3823
836.4532	113.1562
1023.9434	223.3991
1114.8751	82.3381
1620.1867	111.8227
1644.3264	28.0635
1689.2845	9.6016
2706.1968	3042.3228
3382.7381	967.2352
3788.4717	32.6157
3807.7370	138.9899
3843.3269	108.4051
3880.0753	127.0365

3J 2 Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
8	-2.423450	-0.560037	0.985255
1	-3.168776	-0.400917	0.358939
1	-2.726015	-0.299847	1.861110

8	-4.415775	-0.187136	-0.794024
1	-5.141303	-0.811420	-0.901899
1	-4.746004	0.663761	-1.101545
8	-0.002464	-0.272467	0.298547
1	0.249293	0.655598	0.191162
1	-0.987102	-0.320767	0.574630
21	1.438210	-1.779463	-0.044883
8	2.825197	-1.007387	-0.462737
18	1.024968	3.005474	-0.014232

Frequence s	IR intensity
15.4616	1.3284
20.3790	4.4314
25.8258	3.3272
39.9801	31.4651
45.0892	11.4207
70.2034	1.8224
78.4481	23.8962
116.7435	23.5409
146.8831	16.0364
226.0748	105.3844
246.9308	178.0779
295.9721	81.6299
301.8774	32.7824
343.9677	84.3660
490.6270	101.7831
507.8766	26.9160
525.9652	24.9124
758.7113	24.8505
840.9300	112.0112
1029.9086	224.6012
1119.7058	80.0080
1618.7231	90.9854
1643.8390	36.3693
1689.7859	7.8771
2692.9069	3069.8991
3376.4190	970.4472
3746.5027	361.2884
3787.3674	32.9000
3841.9477	109.2096
3878.7383	127.6550

3J_3 Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
8	-1.168610	0.733171	-0.323277
1	-1.536458	1.633397	-0.157818
1	-1.906370	0.113116	-0.312617
8	-2.078436	3.237342	0.096521
1	-2.447447	3.779131	-0.609235
1	-2.458963	3.569713	0.916529
8	1.085767	0.050090	0.565978
1	1.078310	-0.073293	1.522940
1	0.141950	0.327099	0.258556
21	2.903554	-0.249921	-0.471327
8	4.005931	-0.670738	0.669410
18	-3.811270	-1.716652	0.011692

Frequence s	IR intensity
14.2315	2.1882
29.2662	1.1761
35.3916	8.3061
41.4032	32.2551
44.7117	12.7761
69.6549	9.1438
78.0807	4.8353
115.3650	20.7899
148.9595	17.1229
227.2151	93.0723
252.4274	184.4900
304.9069	23.7776
336.4139	91.2264
370.5138	88.0011
433.8142	136.9597
515.1212	19.4354
547.3983	23.6350
740.3022	27.5201
843.4248	105.8365
1030.9691	235.7985
1149.8546	80.6316
1616.1312	85.1911
1643.8016	36.2224

1690.8036	10.8152
2582.5507	3314.3142
3375.4693	999.7653
3787.3192	36.1354
3805.7345	131.6501
3815.2474	230.0574
3878.6630	126.3648

3J_4 Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
8	0.246360	1.531934	0.717292
1	1.078399	1.420946	0.194951
1	0.480023	1.974268	1.539542
8	2.444057	1.205311	-0.782314
1	2.789158	1.898030	-1.355492
1	3.194522	0.641916	-0.559423
8	-1.621619	-0.160420	0.628289
1	-1.395602	-0.995361	1.055685
1	-0.823556	0.482906	0.703890
21	-3.511832	0.047502	-0.296970
8	-4.281797	-1.385161	-0.079034
18	5.229417	-0.886309	0.043519

Frequence s	IR intensity
14.8156	0.5958
24.5404	4.6009
34.0107	30.4934
39.8662	7.1060
61.4765	17.4573
67.1979	2.7722
75.9512	0.6734
144.5887	12.1218
170.1001	48.1367
236.8071	73.8123
288.1426	170.0670
305.4165	88.5495
333.0822	15.0860
351.4426	92.1755
435.9145	141.8171
509.7440	23.0527
538.4689	23.2534
739.2917	30.4890
864.1189	106.0096
1031.2021	234.0269
1137.8773	81.2762
1615.5816	87.7755
1645.8042	27.0937
1691.3383	8.7178
2625.7357	3223.9696
3335.4985	1085.8235
3773.7192	85.6031
3807.8518	139.5858
3841.7579	108.7261
3866.0631	188.7660

3J_5 Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
8	-0.297061	1.341052	0.850045
1	-1.091360	1.291386	0.264144
1	-0.480398	1.997112	1.529942
8	-2.409393	1.105743	-0.788291
1	-3.189240	0.585134	-0.562370
1	-2.704162	1.772683	-1.417370
8	2.032215	0.965344	-0.042824
1	2.357908	1.694886	-0.583613
1	1.086578	1.188259	0.291138
21	3.224744	-0.764891	0.209569
8	4.595619	-0.506730	-0.654687
18	-5.281665	-0.872779	0.064624

Frequence s	IR intensity
13.3922	3.7520
24.7075	12.7607
31.4169	0.6855
38.8537	23.8242
57.9544	10.5809
62.4342	19.1106

80.7787	3.8408
145.7652	17.5523
162.8938	42.8209
235.9083	74.1917
286.3268	152.1535
307.0851	87.1739
331.2591	41.5959
350.9909	81.6088
430.3185	142.2842
506.2302	22.8466
537.4735	26.0372
738.9206	32.4661
857.3041	107.7552
1031.0134	236.6394
1134.0972	81.6192
1614.2283	77.4465
1645.4078	35.4974
1690.4383	7.9921
2634.5956	3217.8082
3342.2466	1068.9682
3774.0983	86.6625
3808.5720	140.8749
3842.1276	111.3888
3866.5749	188.9520

Standard orientations and frequencies of transition states

1 TS Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
21	-0.497021	-0.487771	0.000022
8	-0.515490	1.220893	0.000024
8	1.428430	-0.054621	-0.000237
1	2.390105	-0.067518	0.001277
1	0.743803	0.980544	-0.000031

Frequencies	IR intensity
-1649.0815	1198.6038
241.4698	182.9326
414.5291	86.2794
605.5207	204.5896
728.0018	94.9267
966.5539	210.5260
1069.9379	48.8471
1925.0923	112.7093
3848.5145	319.4839

2 TS Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
21	0.024250	-0.132094	-0.481234
8	-0.546495	1.356760	0.176496
8	-1.703861	-0.664011	0.384407
8	2.039303	-0.227081	0.361941
1	-2.399574	-1.116506	0.866763
1	-1.475834	0.532410	0.534387
1	2.302788	0.512540	0.930248
1	2.751802	-0.879811	0.391749

Frequencies	IR intensity
-1571.0775	1432.7484
52.1724	2.1515
105.9644	14.5272
208.7289	160.4663
256.3150	24.1252
366.5442	6.0807
417.2592	181.8464
443.2176	186.0573
529.4291	34.8841
593.8563	247.7505
719.5988	88.6307
941.6306	222.5381
1089.5560	45.8210
1649.2364	118.4776
1933.5808	98.2471
3728.1591	157.7518
3808.8922	229.8076
3872.3467	259.9399

2 TS1 Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
21	-1.065026	0.052938	-0.081553
8	-0.119497	-1.342304	-0.055293
8	0.461378	1.348242	-0.061123
8	2.190784	-0.324523	0.185308
1	0.599679	2.299601	-0.024726
1	1.553180	0.592001	0.039200
1	1.458300	-1.028202	0.080702
1	2.888763	-0.445131	-0.472572

Frequencies	IR intensity
-444.4340	203.8441
146.5827	62.7047
258.7296	16.9115
397.6442	145.8866
421.2396	92.0883
476.3556	263.1015
551.2078	39.2350
581.6075	91.4230
657.6104	68.6187
836.7687	15.7553

966.5854	77.3611
1184.1824	1399.0861
1325.0045	121.7622
1647.9049	723.6470
1850.9504	167.5951
2856.9317	1140.5002
3787.5228	182.9335
3840.7744	176.6972

2 TS2 Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
21	0.895198	0.375276	-0.280457
8	1.403485	-1.278975	0.248673
8	-0.486282	1.223341	0.505258
8	-2.514509	-0.579022	-0.156005
1	1.449126	-2.126547	0.700303
1	-1.389518	1.009332	0.783501
1	-3.262599	-0.335593	-0.713705
1	-2.817711	-1.350737	0.336094

Frequencies	IR intensity
-143.0698	3.5645
54.3997	6.7982
141.8763	21.6095
147.3878	9.0663
221.4148	4.9525
246.8585	37.1042
354.3287	115.9371
415.1385	152.2230
455.4656	111.2791
478.2447	395.1119
624.3925	134.3126
802.2033	72.9431
822.5093	318.4729
1648.5546	78.8144
3733.4538	463.4677
3775.4752	10.1179
3859.0721	254.2760
3861.3330	180.2673

3 TS Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
21	0.005722	-0.061595	-0.203914
8	1.957815	-1.077680	-0.118382
1	2.442317	-0.945719	0.709335
1	2.541306	-1.552678	-0.723121
8	-0.022262	0.650238	1.384932
8	-0.102820	1.931504	-0.578675
8	-1.855790	-1.235883	-0.112334
1	-0.076951	1.699118	0.608911
1	-2.408788	-1.741569	-0.720818
1	-2.347440	-1.140764	0.716207
1	-0.086144	2.829665	-0.912656

Frequencies	IR intensity
-1489.2559	1592.0148
45.2195	42.7921
61.3450	3.6912
96.8190	11.8787
109.6773	60.3357
121.6527	64.9232
227.8320	23.7947
247.4722	60.4596
326.1569	0.0481
375.2407	30.1309
389.5470	185.6482
407.7134	104.3861
445.6737	268.3236
506.5119	0.5240
519.5476	77.1257
586.7885	288.7320
719.8370	77.5153
917.9250	235.3021
1094.9370	41.8625
1642.5795	208.2036
1645.3611	36.7617
1943.5737	84.6789
3742.0210	210.6593
3744.3424	62.1228
3828.4132	19.1937

3829.2500	396.8307
3892.7444	220.0945

3 TS1 Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
21	1.943357	-0.003654	-0.172566
8	-3.766291	-0.066834	-0.373735
1	-4.070317	-0.527190	-1.163149
1	-4.521746	-0.020977	0.222647
8	0.453199	1.367916	0.043814
8	1.039877	-1.383066	0.059412
8	-1.342205	-0.092666	0.689808
1	0.333522	2.321737	0.067145
1	-0.534582	0.754455	0.341125
1	-2.232707	-0.121778	0.249068
1	-0.861317	-0.932314	0.552661

Frequencies	IR intensity
-323.8767	939.7528
40.5420	2.9667
65.7445	17.7997
81.2242	36.6155
135.0835	33.9467
215.5424	3.1188
248.3962	179.9051
259.1585	352.1147
312.0434	157.7890
339.8877	28.5883
364.6173	160.8820
574.9223	33.6580
606.0666	98.9446
630.4409	182.5098
751.2164	767.0687
854.3149	63.3216
927.9362	236.5386
1021.6141	889.6043
1269.2611	115.1667
1633.6439	218.8962
1663.0832	100.7214
1793.5055	140.8465
3238.9025	1397.1413
3587.5043	372.8099
3785.9738	34.2299
3847.1929	164.6481
3877.2594	134.3769

3 TS2 Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
21	-1.399512	0.208821	-0.438824
8	1.975592	-1.648074	-0.390825
1	2.058232	-2.322180	0.294295
1	2.449945	-2.008056	-1.149558
8	-2.020914	-0.774084	0.962457
8	0.073599	1.196854	-0.286781
8	2.477068	0.992787	0.631821
1	-2.096575	-1.141767	1.846672
1	3.269625	1.529324	0.532897
1	2.664030	0.106165	0.282961
1	1.001741	1.311406	0.074655

Frequencies	IR intensity
-69.8149	9.6895
45.2142	6.4257
48.2012	1.7075
113.2624	18.5242
155.8425	8.6442
170.3924	17.9747
206.0842	71.1769
251.1843	33.0010
277.2263	39.7313
287.7650	90.2702
387.0366	44.4154
418.2764	163.9355
442.5415	180.7440
476.4145	195.0912
607.8668	122.4368
786.3890	133.4291
866.2662	237.9971
901.4702	108.6716
1027.6741	160.8263
1613.4666	55.7329
1644.8543	69.3636
3057.9619	2383.7759

3662.2209	278.6932
3770.1121	23.3709
3857.3480	87.8274
3857.7356	170.4422
3869.3123	299.8371

3 TS3 Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
21	-0.456757	0.078538	-0.132413
8	-2.499146	-0.697174	-0.199666
1	-3.315418	-0.179454	-0.237876
1	-2.747963	-1.614926	-0.019461
8	-0.413601	1.877907	0.211648
8	0.633596	-1.209114	0.565116
8	3.131559	-0.122886	-0.272562
1	-0.156989	2.747520	0.525450
1	3.693847	0.503589	0.196755
1	3.725704	-0.577486	-0.880320
1	1.573444	-1.318410	0.759828

Frequencies	IR intensity
-110.7772	3.0262
27.0515	4.9507
53.6696	6.6251
73.8364	1.0630
126.2314	7.2467
133.2046	14.1342
218.3250	3.2293
231.7390	34.8742
252.4803	2.9335
334.2861	129.7091
382.8409	13.9887
399.4575	199.1162
409.9714	171.4183
450.1242	31.9247
467.7489	467.1181
529.7505	30.5706
605.4398	138.9550
763.0484	95.9119
804.4702	352.0711
1646.5913	86.3279
1651.3823	107.8277
3736.7693	203.0951
3774.3184	261.8613
3785.4100	122.2209
3811.8799	217.8117
3868.3723	93.5153
3884.7293	288.3178

Dimer Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
8	1.516760	-0.000038	-0.121144
1	0.561306	-0.001272	0.044667
1	1.926815	0.000231	0.747760
8	-1.391153	-0.000145	0.110016
1	-1.744208	0.767423	-0.351146
1	-1.748767	-0.764919	-0.352262

Frequencies	IR intensity
137.7332	138.3577
159.9150	55.0812
161.6584	28.3382
190.9884	224.5296
364.9784	51.7966
626.7590	94.2503
1628.1306	91.9623
1647.2456	38.6997
3675.6375	334.7100
3791.6592	10.4116
3870.8697	85.3834
3890.6322	84.4232

Trimer Standard orientation

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
8	-1.470131	-0.671358	-0.085701
1	-0.592192	-1.093972	-0.042620
1	-2.007083	-1.089320	0.592687
8	1.323317	-0.926270	-0.093771

1	1.967313	-1.181544	0.572020
1	1.221774	0.041861	-0.021583
8	0.145189	1.603622	0.110727
1	0.069916	2.239149	-0.606333
1	-0.646732	1.035872	0.055789

Frequencies	IR intensity
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175.6589	25.1259
183.2043	18.7994
193.3767	106.3079
214.3796	49.2182
216.3724	88.1531
254.6720	38.4228
354.5871	68.4117
366.2022	49.0476
456.0717	122.9033
585.5008	169.8877
672.9544	292.0974
875.0360	8.9979
1636.5324	87.8277
1638.6918	71.8852
1660.6308	14.2793
3528.0578	13.6211
3590.2329	586.7822
3600.5068	543.7942
3862.7631	90.7967
3866.6336	98.2005
3867.7998	45.8582