



Supporting Information

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Towards Absolute Configuration Determination of Complex Molecular Systems: Matrix Isolation Vibrational Circular Dichroism Study of *R*-2-amino-1-propanol

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Table S1 HF/6-31G*, MP2/6-31G* and G2 energies in (in kJ mol⁻¹) as determined for the interconversion reaction of conformer g'Gg' to the various other conformers.

Conf. ^a	$\Delta_r G_0^\circ$ (HF) ^{b,c}	$\Delta_r G_0^\circ$ (MP2) ^b	$\Delta_r G_0^\circ$ (G2) ^c	$\Delta_r G_{298}^\circ$ (G2) ^c	% ^d
g'Gg'	0.00	0.00	0.00	0.00	40.2
gG'g	1.62	0.92	1.55	1.85	19.1
gGt	5.76	9.45	5.43	4.30	7.2
gGg'	6.97	9.29	6.33	4.80	5.9
tGt	7.37	10.75	7.16	5.71	4.1
gGg	7.61	10.07	6.53	5.81	3.9
tGg	8.31	10.08	7.66	6.50	3.0
g'G'g	8.45	9.64	8.75	7.47	2.0
tGg'	12.11	14.83	9.40	7.52	2.0
g'G't	8.85	11.59	8.95	7.76	1.8
tG't	9.65	12.62	10.10	8.74	1.2
gTt	9.79	15.36	10.52	8.78	1.2
tG'g'	10.77	12.10	10.18	9.17	1.0
tTt	11.84	16.26	11.06	9.33	1.0
gTg'	10.90	15.30	11.08	9.65	0.8
gTg	11.36	15.96	11.40	9.73	0.8
g'G'g'	11.79	13.18	10.55	9.75	0.8
g'Tt	10.59	15.55	11.62	9.76	0.8
tG'g	14.03	15.85	11.48	9.84	0.8
tTg'	12.10	15.03	11.36	9.85	0.8
tTg	13.01	16.06	11.49	9.87	0.8
g'Tg'	11.01	14.92	12.32	10.64	0.6
g'Tg	13.26	17.39	13.12	11.46	0.4
g'Gt	22.37	27.46	20.47	17.41	0.0
gG't	21.72	26.25	20.06	17.69	0.0

^aThe first letter of the conformational labeling denotes the configuration around the *lp*-N-C-C(OH) (*lp*: lone pair) dihedral angle, the second the letter defined by the N-C-C-O, while the last letter by the C-C-O-H dihedral angle. (g and G = *gauche*; t and T = *trans*.) See also ref. [8].

^bFrom ref. [8].

^cPresent work.

^dCalculated from $\Delta_r G_{298}^\circ$ (G2).

Table S2. Observed and calculated VCD rotatory strengths of *R*-alaninol together with original assignments of ref. 8. and some examples of alternative reassignments based on the signs of the observed and calculated VCD rotatory strengths.

Frequency / cm ⁻¹		Observed VCD strength x10 ⁴ ^b	Assignment of ref. 8.			Alternative assignment		
Ref. 8.	This work ^a		Conf.	Vibr. Mode	Calculated VCD strength ^c	Conf.	Vibr. Mode	Calculated VCD strength ^c
3542	3544	+1.1(sh)						
3539		+2.4	gG'g ^e	νOH	-0.4			
3534		+1.1(sh)						
3529		-0.3	g'Gg'	νOH	+0.2			
Non obs.	3525	+0.7				gG'g	νNH ₂ as	+0.6
Non obs.	3519	+0.8				g'Gg'	νNH ₂ as	+3.4
2995	2993 ^d	-0.3	gG'g	νCH ₃ as				
2991			gGg'	νCH ₂ as	-6.3			
2978		sh	gGt	νCH ₃ as	+0.1			
2975		+2.2	g'Gg'	νCH ₂ as	-0.3			
2971		+sh	gGg'	νCH ₃ as	-6.3			
2967		-1.5	gG'g	νCH ₂ as	+2.3			
2952		+0.9	g'Gg'	νCH ₂ as	+8.6			
2945		sh	gG'g	νCH ₃ as'	-0.4			
2938			gGg'	νCH ₃ as'	+14.3			
2936	2937 ^d	+0.7	g'Gg'	νCH ₃ as'	+0.7			
2913		-0.5	gGt	νCH ₂ as	+0.1	gGt	νCH ₂ s	-14.8
2855		-0.8	g'Gg'	νCH ₂ s	-15.3			
1474		+1.6	g'Gg'	δCH ₂	-0.9			
1458		+0.7	g'Gg'	δCH ₃ as'	-6.5			
1454		-1.2	g'Gg'	δCH ₃ as	-4.1			
1419		-1.3	g'Gg'	ωCH ₂	-4.4			
1413		-2.3(sh)	gGg'	ωCH ₂	-0.3			
1409		-3.7	gG'g	ωCH ₂	34.5			
1403		-2.0(sh)	gG'g	δCH ₃ s	-11.4			
1399		+1.0	gGg'	δCH ₃ s	+7.7			
1392		+1.8	g'Gg'	δCH ₃ s	+3.9			
1384		+3.6	g'G'g	ωCH ₂	34.4			
1381		+1.8(sh)	g'Gg'	δCH	-5.7			
1373		+4.9	gG'g	δCH ₃ s	-7.8			
1364		-0.1	gG'g	δCH	9.8			
1362		+0.7	gGt	δCH	-0.2			
1355		-0.7	gGt	γCH	-13.6			
1342		-2.4	g'Gg'	δCOH	-27.8			
1335		+0.2	g'G'g	γCH	-9.4			
1327		-0.1	gGg'	γCH	-3.6			
1316	1318	-0.4	g'Gg'	γCH	+8.7	gG'g	δCOH	-3.6
1264		+1.0	g'Gg'	γNH ₂	+17.8			
Non obs.	1253	+0.5						
1186		+1.8	gG'g	twCH ₂	+53.4			
1177		-0.9	g'Gg'	twCH ₂	-27.1			
1158		+0.6	g'Gg'	νCN	-13.8			
1151		+1.5	gGg'	νCN	-10.8			
1141		-0.2	gGg'	γCH ₃ '	53.5			
1138		+0.2	gG'g	νCO	-18.7			
1087		-1.8	gG'g	νCN	56.2	g'Gg ^{re}	νCCas	-23.8

1078	sh	$g'Gg^{re}$	$\nu CCas$	-23.8	$gG'g$	νCN	+56.2
1074	+2.4						
1065	1063 +4.0	$g'Gg'^e$	νCO	-33.6			
1063	1060 -8.5						
1053	1052 +1.3	gGg'	δCOH	-20.9			
Non obs.	1050 +1.0						
1024	1026 -1.4	$gG'g$	γCH_3	-83.2			
1014	+5.1	$g'Gg^{re}$	γCH_3	+53.4			
1010	+6.0						
987	+1.4(sh)	$gG'g$	$\gamma CH_3'$	+52.9			
954	+1.4(sh)	gGg'	γCH_3	+53			
950	+2.1	$gG'g$	γCH_2	-0.9			
931	-1.9	$gG'g$	$\nu CCas$	-40.7			
921	+2.7	$g'Gg'$	$\gamma CH_3'$	+8.5			
839	+2.1	gGt	ωNH_2	+114			
836	+2.6	gGg'	ωNH_2	-8.5			

^aListed only if the deviation from ref. 8 is larger than 1 cm^{-1} , or if it was not reported in ref. 8.

^bsh=shoulder

^cNon-Boltzmann weighted BPW91/tz2p rotational strengths from this work.

^dNot resolved in the present study.

^eSite splitting.

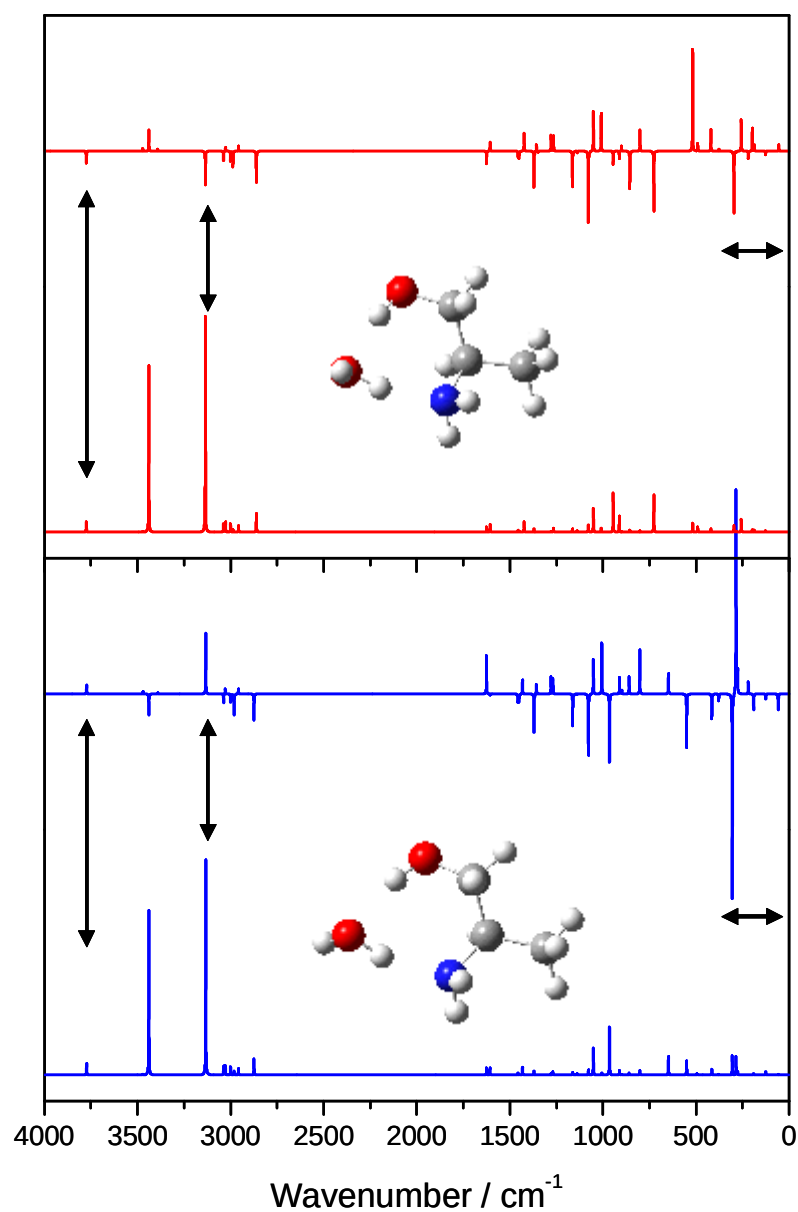


Figure S1. Calculated (BPW91/TZ2P) structures and IR and VCD spectra of two possible conformers of the R-alaninol·water complex differing only in the steric alignment of the complexed water. Region of intermolecular vibrations is marked by horizontal arrow, stretching vibrations of the complexed water labeled by vertical arrows.

Optimized geometries, vibrational frequencies, infrared intensities and VCD rotatory strengths of the 10 lowest energy conformers of $\underline{S}$ -alaninol as obtained at the BPW91/tz2p level of theory

Conformer g'Gg'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.757914	-0.762426	0.209566
2	1	0	-0.643918	-0.877241	1.307151
3	1	0	-0.790458	-1.770997	-0.224338
4	6	0	0.445773	0.019705	-0.339771
5	1	0	0.341331	0.049698	-1.434953
6	6	0	1.777239	-0.646171	0.024849
7	1	0	1.910058	-0.685626	1.115638
8	1	0	1.826317	-1.676321	-0.354867
9	8	0	-1.982074	-0.115193	-0.108471
10	1	0	-1.770738	0.837300	-0.026644
11	7	0	0.299175	1.415389	0.122650
12	1	0	0.608900	1.509377	1.091360
13	1	0	0.864769	2.053555	-0.433900
14	1	0	2.625520	-0.092570	-0.398094

Frequencies --	142.7530		217.2472		249.4080
IR Inten --	6.5535		0.0535		3.7040
Rot. str. --	-10.4390		0.6062		0.4541
Frequencies --	264.8007		349.0843		433.9213
IR Inten --	9.7988		5.3013		0.2648
Rot. str. --	26.4168		7.6357		1.3304
Frequencies --	498.4954		577.6583		803.3682
IR Inten --	7.8951		97.0109		61.3413
Rot. str. --	11.6078		-81.8397		-27.7516
Frequencies --	836.0605		899.6625		905.9279
IR Inten --	67.4768		7.8669		5.3427
Rot. str. --	5.2577		-8.4808		19.9298
Frequencies --	1001.3898		1041.4737		1065.8422
IR Inten --	8.4292		114.2942		5.1133
Rot. str. --	-53.3739		33.5777		23.7664
Frequencies --	1142.6734		1157.9023		1245.8421
IR Inten --	17.9383		8.9867		12.2557
Rot. str. --	13.8095		27.1413		-17.8096
Frequencies --	1278.6149		1318.5432		1356.3150
IR Inten --	1.9034		16.0224		1.1000
Rot. str. --	-8.6605		27.8127		-3.9330
Frequencies --	1367.5977		1398.8659		1448.4141
IR Inten --	8.7191		68.9526		2.4514
Rot. str. --	5.7458		4.3748		4.0617
Frequencies --	1451.4602		1463.7250		1610.9854
IR Inten --	7.0264		2.7807		25.7841
Rot. str. --	6.5295		0.9094		-14.6323
Frequencies --	2867.0589		2957.8857		2972.2552
IR Inten --	71.5572		20.7449		21.8086
Rot. str. --	15.2868		-4.3902		11.6718
Frequencies --	3005.3451		3027.6042		3036.0598
IR Inten --	24.0826		44.4347		27.5717
Rot. str. --	6.1181		0.3269		-8.5797
Frequencies --	3414.3752		3504.7330		3560.9635
IR Inten --	0.5906		2.6016		83.3405
Rot. str. --	-2.1371		-3.3533		-0.2223

Conformer gG'g

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.977270	-0.215456	0.644665
2	1	0	1.157402	-1.210795	1.072889
3	1	0	1.405292	0.529228	1.344282
4	6	0	-0.534349	0.042355	0.501548
5	1	0	-0.962545	0.088443	1.520889
6	6	0	-1.243206	-1.067586	-0.275299
7	1	0	-0.808593	-1.180978	-1.275550
8	1	0	-1.148562	-2.025661	0.250093
9	8	0	1.640667	-0.161898	-0.612890
10	1	0	1.200899	0.573986	-1.083936
11	7	0	-0.678402	1.322291	-0.225259
12	1	0	-1.627834	1.444730	-0.572917
13	1	0	-0.475901	2.115554	0.382829
14	1	0	-2.314975	-0.851234	-0.384134

Frequencies	--	135.6351	196.5360	252.7378
IR Inten	--	6.7848	2.2834	6.3774
Rot. str.	--	14.6398	-18.5041	-24.6348
Frequencies	--	275.8269	359.8913	394.9790
IR Inten	--	3.8610	3.5533	0.1225
Rot. str.	--	14.5385	-9.6485	-1.4101
Frequencies	--	553.0773	630.9007	783.4509
IR Inten	--	112.3953	23.8619	4.7244
Rot. str.	--	68.2379	2.7768	13.6740
Frequencies	--	822.2257	912.1743	936.4339
IR Inten	--	91.1922	6.2755	27.0980
Rot. str.	--	5.4351	40.6895	0.9873
Frequencies	--	974.8475	1009.0912	1056.6302
IR Inten	--	14.0070	25.0948	36.6109
Rot. str.	--	-52.9306	83.2524	-56.1807
Frequencies	--	1121.7853	1171.7481	1236.0365
IR Inten	--	7.9271	27.2914	1.2131
Rot. str.	--	18.6909	-53.3966	-3.1272
Frequencies	--	1294.4413	1318.1773	1349.3402
IR Inten	--	16.3354	9.9750	4.5985
Rot. str.	--	9.3109	-9.8485	7.8043
Frequencies	--	1373.1954	1393.3881	1447.5950
IR Inten	--	11.3958	55.7328	7.7445
Rot. str.	--	8.8213	-34.4711	-1.5159
Frequencies	--	1454.1227	1463.8374	1609.4395
IR Inten	--	3.3089	2.0269	31.4176
Rot. str.	--	-2.4919	-2.1940	-7.2751
Frequencies	--	2877.6502	2895.6782	2972.0805
IR Inten	--	40.0987	119.5327	24.1205
Rot. str.	--	-41.5070	21.8620	4.2763
Frequencies	--	3006.3071	3038.7643	3058.2801
IR Inten	--	31.3790	25.4441	18.8678
Rot. str.	--	-2.3400	0.4207	-4.1215
Frequencies	--	3426.8884	3509.0057	3577.2061
IR Inten	--	0.2732	1.6547	64.3933
Rot. str.	--	-0.6643	-0.6493	0.4665

Conformer gGt

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.756958	-0.687003	0.241757
2	1	0	-0.691412	-0.686878	1.342878
3	1	0	-0.763929	-1.731249	-0.115236
4	6	0	0.458820	0.037657	-0.326162
5	1	0	0.338165	0.046081	-1.428317
6	6	0	1.746025	-0.714883	0.015286
7	1	0	1.879116	-0.780572	1.103037
8	1	0	1.735666	-1.729522	-0.403769
9	8	0	-1.939151	0.004280	-0.197584
10	1	0	-2.691947	-0.323242	0.314986
11	7	0	0.504145	1.391640	0.245414
12	1	0	1.246503	1.938904	-0.188994
13	1	0	-0.375320	1.870323	0.050422
14	1	0	2.620031	-0.194191	-0.397521

Frequencies	--	140.5314	211.0076	215.0445
IR Inten	--	2.8783	57.1172	46.9049
Rot. str.	--	0.3703	-47.0794	-6.5413
Frequencies	--	241.9791	290.5956	362.0846
IR Inten	--	13.7658	25.0473	5.1152
Rot. str.	--	-8.1240	25.7132	12.2448
Frequencies	--	451.4480	488.3077	808.8148
IR Inten	--	9.0610	18.6573	49.8671
Rot. str.	--	-5.6957	10.9458	81.7985
Frequencies	--	835.2857	918.2814	929.4430
IR Inten	--	73.8025	5.7058	3.0556
Rot. str.	--	-113.9655	-11.4112	17.9712
Frequencies	--	1003.1858	1016.0393	1083.1544
IR Inten	--	0.9287	104.2346	17.2960
Rot. str.	--	12.1980	1.6939	27.6760
Frequencies	--	1116.8348	1198.3725	1225.1079
IR Inten	--	14.0581	1.6487	22.5899
Rot. str.	--	-23.4699	-4.0590	9.4800
Frequencies	--	1245.4447	1330.4877	1337.6169
IR Inten	--	2.6450	3.4572	16.6269
Rot. str.	--	-6.2268	13.5813	0.2222
Frequencies	--	1363.5681	1398.6078	1447.2601
IR Inten	--	8.1643	0.8606	2.2369
Rot. str.	--	-5.4319	14.5743	-0.7550
Frequencies	--	1452.7161	1458.7714	1605.7574
IR Inten	--	7.1982	4.2684	34.9735
Rot. str.	--	-4.9720	-3.6835	9.5625
Frequencies	--	2866.6850	2918.8187	2963.2055
IR Inten	--	52.7217	56.6142	45.2281
Rot. str.	--	18.2208	14.7982	-0.1343
Frequencies	--	2968.5465	3037.4687	3044.7399
IR Inten	--	27.3759	27.7998	28.1689
Rot. str.	--	5.7970	-1.8130	-0.0843
Frequencies	--	3422.6197	3501.9492	3749.2780
IR Inten	--	2.8954	2.7732	26.6988
Rot. str.	--	-8.1554	3.2637	-3.9614

Conformer gGg'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.752527	-0.764806	0.154022
2	1	0	-0.622892	-0.957090	1.233803
3	1	0	-0.821673	-1.731654	-0.361964
4	6	0	0.460669	0.024435	-0.361324
5	1	0	0.411138	0.034010	-1.465889
6	6	0	1.761513	-0.652868	0.066144
7	1	0	1.859854	-0.646145	1.160378
8	1	0	1.792494	-1.695899	-0.273275
9	8	0	-1.992173	-0.094142	-0.090317
10	1	0	-1.992250	0.688255	0.484915
11	7	0	0.391011	1.393224	0.191586
12	1	0	1.314349	1.823544	0.207166
13	1	0	-0.193152	1.984643	-0.397585
14	1	0	2.634505	-0.139657	-0.359174

Frequencies	--	63.3467	138.5322	216.1763
IR Inten	--	70.2928	10.1697	1.4367
Rot. str.	--	10.6307	-5.6514	14.2933
Frequencies	--	243.5049	351.0549	439.8287
IR Inten	--	1.8724	0.6863	38.7982
Rot. str.	--	-3.2933	4.0887	5.0381
Frequencies	--	458.4922	495.9840	801.2891
IR Inten	--	53.6886	14.0140	43.9726
Rot. str.	--	38.5802	-29.3000	-15.5060
Frequencies	--	828.9089	898.1785	928.2792
IR Inten	--	59.7868	4.7522	11.2959
Rot. str.	--	8.4940	-16.1108	20.2575
Frequencies	--	989.7425	1020.2626	1066.2550
IR Inten	--	6.6154	112.5320	7.5151
Rot. str.	--	19.9620	20.9014	-2.2693
Frequencies	--	1139.0531	1187.9615	1217.7732
IR Inten	--	6.9994	12.9187	1.9335
Rot. str.	--	10.8413	16.5941	-2.9109
Frequencies	--	1299.1191	1335.9181	1351.0956
IR Inten	--	1.9043	16.1498	8.5700
Rot. str.	--	3.5959	-7.8851	40.0947
Frequencies	--	1361.8848	1372.4054	1441.4395
IR Inten	--	10.7889	25.9681	0.0987
Rot. str.	--	-7.6636	-2.0083	0.3334
Frequencies	--	1450.1539	1456.3437	1611.9577
IR Inten	--	8.3765	2.8703	31.1694
Rot. str.	--	-1.8157	2.9099	-14.1233
Frequencies	--	2897.7414	2923.8034	2965.9069
IR Inten	--	31.2744	66.5909	25.9749
Rot. str.	--	-0.0725	29.7417	-2.5037
Frequencies	--	3016.1501	3033.1300	3044.2185
IR Inten	--	27.8273	29.0977	27.4322
Rot. str.	--	6.2840	-14.3147	6.2907
Frequencies	--	3434.3459	3510.0656	3697.1376
IR Inten	--	0.3486	2.3841	20.5366
Rot. str.	--	-3.6773	0.0731	5.9253

Conformer tGt

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.755255	-0.695413	0.244665
2	1	0	-0.674184	-0.720799	1.347188
3	1	0	-0.778780	-1.736787	-0.123175
4	6	0	0.459253	0.037972	-0.339026
5	1	0	0.335456	0.038663	-1.434026
6	6	0	1.753829	-0.697727	0.007736
7	1	0	1.913923	-0.722969	1.095879
8	1	0	1.735838	-1.734245	-0.352080
9	8	0	-1.938772	0.009485	-0.161580
10	1	0	-2.705160	-0.414669	0.250118
11	7	0	0.559282	1.445437	0.069681
12	1	0	-0.336884	1.907985	-0.085673
13	1	0	0.747416	1.506869	1.072276
14	1	0	2.610616	-0.186985	-0.445882

Frequencies	--	128.5091	210.2201	215.1113	
IR Inten	--	12.2345	0.6750	89.8777	
Rot. str.	--	5.5844	14.0254	-35.9112	
Frequencies	--	238.6853	266.8835	358.2350	
IR Inten	--	13.5315	27.7702	3.5269	
Rot. str.	--	-16.5812	5.7794	-6.6728	
Frequencies	--	435.5561	494.0976	800.5056	
IR Inten	--	5.1961	22.3371	30.2117	
Rot. str.	--	3.4669	-3.3443	25.0569	
Frequencies	--	856.1575	907.2026	915.8067	
IR Inten	--	126.8579	2.7253	7.9200	
Rot. str.	--	-6.9885	6.3946	-8.3494	
Frequencies	--	987.3185	1027.5757	1091.9862	
IR Inten	--	20.6700	69.2827	29.0007	
Rot. str.	--	-44.4786	16.3338	-32.8248	
Frequencies	--	1118.1297	1193.8985	1208.0904	
IR Inten	--	10.1117	5.8300	26.8893	
Rot. str.	--	-7.1930	3.4671	72.4039	
Frequencies	--	1248.8412	1310.6225	1354.4660	
IR Inten	--	1.7550	10.7387	3.1760	
Rot. str.	--	-9.1119	38.1375	-12.1268	
Frequencies	--	1372.6843	1385.1062	1446.1301	
IR Inten	--	6.4222	0.4009	3.3367	
Rot. str.	--	17.8796	-8.0371	1.1882	
Frequencies	--	1455.2963	1459.2552	1617.3076	
IR Inten	--	6.8998	4.4966	25.8548	
Rot. str.	--	2.1232	-2.7638	-2.2882	
Frequencies	--	2896.0065	2932.2840	2957.8181	
IR Inten	--	60.1053	33.8527	24.9058	
Rot. str.	--	15.9036	-8.3044	32.5256	
Frequencies	--	2966.6088	3032.2007	3058.7994	
IR Inten	--	44.5479	37.8556	17.4029	
Rot. str.	--	-30.3398	0.3923	-0.2847	
Frequencies	--	3402.1716	3486.3465	3748.3173	
IR Inten	--	2.1319	2.2976	26.7337	
Rot. str.	--	0.5964	-0.5173	-0.6506	

Conformer gGg

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.758301	-0.676887	-0.275915
2	1	0	0.687791	-0.652729	-1.371236
3	1	0	0.770743	-1.730664	0.048682
4	6	0	-0.455580	0.037796	0.324141
5	1	0	-0.322432	0.031273	1.428540
6	6	0	-1.747419	-0.715344	-0.001161
7	1	0	-1.894594	-0.772601	-1.087301
8	1	0	-1.727492	-1.733710	0.408999
9	8	0	2.001244	-0.029707	0.040629
10	1	0	2.176598	-0.167567	0.984117
11	7	0	-0.513273	1.396439	-0.227879
12	1	0	-1.211286	1.959997	0.255378
13	1	0	0.389398	1.856188	-0.106710
14	1	0	-2.617579	-0.200993	0.427256

Frequencies	--	142.0982	212.0921	237.5457
IR Inten	--	4.2066	0.8852	3.5998
Rot. str.	--	-7.0906	-7.9652	-3.1499
Frequencies	--	279.7057	311.9767	364.6711
IR Inten	--	20.6085	95.8457	22.6045
Rot. str.	--	-11.6110	-23.1267	3.8901
Frequencies	--	456.4002	494.7249	800.8968
IR Inten	--	25.2228	14.1212	89.9234
Rot. str.	--	-36.9290	19.1653	46.1057
Frequencies	--	832.2458	897.2139	922.5912
IR Inten	--	34.2468	19.7922	1.6207
Rot. str.	--	-4.8363	-33.2440	5.0784
Frequencies	--	998.7285	1016.2551	1060.0977
IR Inten	--	25.5611	83.7700	5.5450
Rot. str.	--	46.8908	-38.2662	-1.7426
Frequencies	--	1132.6282	1161.9537	1241.8260
IR Inten	--	5.2645	14.9348	4.7818
Rot. str.	--	7.9759	-23.1348	9.0194
Frequencies	--	1299.0484	1329.2312	1350.3967
IR Inten	--	1.2805	17.2719	12.8492
Rot. str.	--	-7.4409	-14.7737	-7.5413
Frequencies	--	1363.0229	1370.5499	1440.7359
IR Inten	--	19.9072	10.1920	0.3859
Rot. str.	--	-3.6005	39.8726	-1.4097
Frequencies	--	1447.8222	1456.8508	1605.1312
IR Inten	--	7.3938	3.7740	32.4170
Rot. str.	--	-10.6787	1.5272	15.5602
Frequencies	--	2822.0263	2940.2964	2968.8205
IR Inten	--	93.8159	49.9489	29.1576
Rot. str.	--	23.0124	-1.0104	4.9731
Frequencies	--	3022.0941	3037.3900	3045.9352
IR Inten	--	17.0777	28.1330	29.1553
Rot. str.	--	-1.2897	1.8499	0.3909
Frequencies	--	3422.6815	3503.9737	3721.1451
IR Inten	--	3.3721	3.2455	16.8809
Rot. str.	--	-8.5010	4.4349	-8.6490

Conformer tGg

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.756674	-0.689102	0.273869
2	1	0	-0.671310	-0.689708	1.370258
3	1	0	-0.785145	-1.741159	-0.061847
4	6	0	0.454752	0.035724	-0.340550
5	1	0	0.323956	0.017745	-1.437878
6	6	0	1.755319	-0.693570	-0.002827
7	1	0	1.925660	-0.706905	1.083977
8	1	0	1.733275	-1.734344	-0.349931
9	8	0	-2.000985	-0.032580	-0.010053
10	1	0	-2.202865	-0.167446	-0.948860
11	7	0	0.556038	1.449227	0.045120
12	1	0	-0.363910	1.886276	-0.030474
13	1	0	0.827157	1.522724	1.027645
14	1	0	2.608407	-0.189443	-0.471261

Frequencies	--	141.4076	211.7311	224.7344
IR Inten	--	3.0863	0.4036	19.8629
Rot. str.	--	-0.0096	-2.4057	39.0960
Frequencies	--	259.0331	303.1163	350.8506
IR Inten	--	58.3228	74.9314	2.2892
Rot. str.	--	64.1603	-154.4252	-0.5898
Frequencies	--	443.3591	499.1796	806.4422
IR Inten	--	1.6891	5.1090	35.9299
Rot. str.	--	2.3853	4.3174	30.8947
Frequencies	--	858.0802	889.6794	913.4138
IR Inten	--	113.5282	18.9863	13.4107
Rot. str.	--	29.1665	3.4107	-29.2854
Frequencies	--	985.9088	1016.5539	1064.0060
IR Inten	--	4.7067	109.5262	5.1411
Rot. str.	--	-24.9152	-16.6415	-30.1969
Frequencies	--	1135.5546	1171.1150	1236.8567
IR Inten	--	6.9929	11.2438	1.1076
Rot. str.	--	26.3364	11.0041	-6.6789
Frequencies	--	1291.2033	1339.1909	1348.7267
IR Inten	--	8.5390	3.6662	12.0945
Rot. str.	--	33.7367	-24.7224	24.2061
Frequencies	--	1362.8604	1367.4001	1441.3715
IR Inten	--	21.9805	6.8962	0.1127
Rot. str.	--	-6.0666	14.7625	-0.4045
Frequencies	--	1449.0203	1457.2947	1617.8618
IR Inten	--	7.5014	4.3367	27.0608
Rot. str.	--	-3.2026	2.8341	-5.1179
Frequencies	--	2912.7984	2918.6963	2964.0271
IR Inten	--	33.4886	59.9385	26.7698
Rot. str.	--	23.6430	-11.4239	5.7441
Frequencies	--	2998.7605	3031.9065	3056.3440
IR Inten	--	33.4152	37.7015	18.0420
Rot. str.	--	-10.5454	-0.0492	-0.0741
Frequencies	--	3398.1939	3477.5685	3719.2268
IR Inten	--	1.4118	2.6014	18.4197
Rot. str.	--	-1.1943	-1.6402	-6.8927

Conformer g'G'g

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.977458	-0.215868	0.644440
2	1	0	1.157172	-1.211710	1.071784
3	1	0	1.405781	0.527992	1.344743
4	6	0	-0.534254	0.042193	0.501580
5	1	0	-0.962190	0.088075	1.521005
6	6	0	-1.243258	-1.067562	-0.275467
7	1	0	-0.808741	-1.180707	-1.275805
8	1	0	-1.148511	-2.025772	0.249665
9	8	0	1.640830	-0.161322	-0.612930
10	1	0	1.200779	0.574689	-1.083415
11	7	0	-0.678698	1.322389	-0.224828
12	1	0	-1.627897	1.444307	-0.573247
13	1	0	-0.476748	2.115673	0.383350
14	1	0	-2.315068	-0.851276	-0.384167

Frequencies	--	135.3775	196.6085	252.5502	
IR Inten	--	6.8029	2.2782	6.3870	
Rot. str.	--	14.6932	-18.5202	-24.7344	
Frequencies	--	275.5577	359.9161	394.8935	
IR Inten	--	3.7903	3.5594	0.1145	
Rot. str.	--	14.5724	-9.6119	-1.3880	
Frequencies	--	552.5889	630.8692	783.2994	
IR Inten	--	112.4019	23.9123	4.6916	
Rot. str.	--	68.5619	2.6320	13.5979	
Frequencies	--	821.6651	912.1453	936.3254	
IR Inten	--	91.2530	6.2850	26.7902	
Rot. str.	--	5.4734	40.6821	1.0876	
Frequencies	--	974.8440	1009.0629	1056.7122	
IR Inten	--	13.9653	25.1524	36.9140	
Rot. str.	--	-53.0664	83.1942	-56.1240	
Frequencies	--	1121.8550	1171.7996	1236.0090	
IR Inten	--	7.9507	27.2408	1.2291	
Rot. str.	--	18.8973	-53.4616	-3.1717	
Frequencies	--	1294.3521	1318.1554	1349.3087	
IR Inten	--	16.3329	9.9810	4.5491	
Rot. str.	--	9.3583	-9.8626	7.7319	
Frequencies	--	1373.1374	1393.4380	1447.6094	
IR Inten	--	11.4159	55.6888	7.7561	
Rot. str.	--	8.8282	-34.4255	-1.5199	
Frequencies	--	1454.1281	1463.9012	1609.3403	
IR Inten	--	3.2993	2.0265	31.3987	
Rot. str.	--	-2.4682	-2.2119	-7.3072	
Frequencies	--	2877.7459	2895.8961	2971.9934	
IR Inten	--	40.5196	119.0647	24.1000	
Rot. str.	--	-41.3841	21.6587	4.2846	
Frequencies	--	3005.8735	3038.6768	3058.1743	
IR Inten	--	31.4759	25.4084	18.8688	
Rot. str.	--	-2.3430	0.3150	-4.1003	
Frequencies	--	3427.2081	3509.3891	3577.7168	
IR Inten	--	0.2700	1.6695	64.5007	
Rot. str.	--	-0.6406	-0.6794	0.4835	

Conformer tGg'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.749361	-0.727498	0.215360
2	1	0	-0.647599	-0.817626	1.313766
3	1	0	-0.776419	-1.744317	-0.199474
4	6	0	0.463283	0.038128	-0.348146
5	1	0	0.367215	0.042509	-1.445045
6	6	0	1.764322	-0.671484	0.033140
7	1	0	1.905001	-0.675610	1.124079
8	1	0	1.762650	-1.715452	-0.305861
9	8	0	-2.008367	-0.141519	-0.129310
10	1	0	-2.072510	0.707840	0.334864
11	7	0	0.533494	1.448301	0.061240
12	1	0	-0.265599	1.979548	-0.281395
13	1	0	0.566452	1.542629	1.077306
14	1	0	2.623822	-0.160353	-0.414565

Frequencies	--	131.8271	199.7751	210.5908
IR Inten	--	4.0735	102.8860	2.8119
Rot. str.	--	3.3426	10.9742	4.9806
Frequencies	--	248.9927	321.5514	370.0869
IR Inten	--	15.7955	50.8333	8.1616
Rot. str.	--	-6.5266	29.6488	-15.5011
Frequencies	--	432.8814	502.2222	768.9144
IR Inten	--	7.3245	8.6195	157.3313
Rot. str.	--	8.1724	2.3072	26.4191
Frequencies	--	803.8274	892.3069	904.3512
IR Inten	--	6.7971	6.4854	0.5443
Rot. str.	--	-19.1847	-26.3295	-0.5398
Frequencies	--	977.0607	1025.4884	1072.0407
IR Inten	--	18.6893	96.1794	2.3310
Rot. str.	--	-66.5434	65.6490	-10.0380
Frequencies	--	1132.6165	1152.2925	1236.5451
IR Inten	--	12.2443	19.7006	11.3248
Rot. str.	--	23.3740	45.4471	-43.8012
Frequencies	--	1274.7715	1334.5323	1350.2836
IR Inten	--	2.3449	3.3634	4.0964
Rot. str.	--	9.8927	22.0398	5.3356
Frequencies	--	1365.1501	1371.6278	1441.6744
IR Inten	--	28.1896	7.1485	0.1722
Rot. str.	--	-10.0375	10.3776	-0.1464
Frequencies	--	1449.1383	1455.0743	1606.2202
IR Inten	--	8.2483	3.9396	21.6219
Rot. str.	--	4.4957	3.8997	5.7325
Frequencies	--	2897.1122	2962.2070	2970.1601
IR Inten	--	50.1250	5.1886	41.4657
Rot. str.	--	14.4299	3.7375	-3.1197
Frequencies	--	3008.2977	3032.3052	3058.9011
IR Inten	--	22.9899	42.9746	18.1195
Rot. str.	--	7.8342	-4.4843	-1.6880
Frequencies	--	3409.2783	3503.2782	3705.9581
IR Inten	--	2.5494	0.3703	10.7260
Rot. str.	--	0.6826	0.7751	2.9212

Conformer g'G't

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.946747	-0.068701	0.673777
2	1	0	1.169108	-0.988158	1.242480
3	1	0	1.301462	0.800038	1.250184
4	6	0	-0.563426	0.058680	0.474436
5	1	0	-0.996489	0.095918	1.487689
6	6	0	-1.154955	-1.157660	-0.260501
7	1	0	-0.723311	-1.254769	-1.264090
8	1	0	-0.961594	-2.091950	0.286153
9	8	0	1.580694	-0.110325	-0.617360
10	1	0	2.530227	0.027309	-0.493230
11	7	0	-0.841563	1.357212	-0.160097
12	1	0	-0.362831	1.397382	-1.060736
13	1	0	-1.838375	1.452512	-0.351844
14	1	0	-2.243003	-1.050085	-0.363323

Frequencies	--	132.6786	187.8202	228.3538
IR Inten	--	2.6892	102.4869	6.5637
Rot. str.	--	4.0255	53.5730	-15.8469
Frequencies	--	245.4284	283.3538	365.0464
IR Inten	--	20.2051	20.1149	0.6729
Rot. str.	--	-3.8861	5.6298	-2.8942
Frequencies	--	398.8308	602.7253	776.6581
IR Inten	--	10.8685	14.8707	11.1560
Rot. str.	--	7.0775	-7.3300	1.3050
Frequencies	--	847.5782	907.4145	919.8252
IR Inten	--	138.8561	0.9585	10.6066
Rot. str.	--	7.8100	6.8023	23.2151
Frequencies	--	962.5933	1014.4750	1084.4832
IR Inten	--	52.0625	22.8574	17.4020
Rot. str.	--	-67.3507	41.4075	-29.3685
Frequencies	--	1136.4267	1161.4475	1216.4374
IR Inten	--	14.3206	20.2068	16.2100
Rot. str.	--	-25.8444	58.2015	9.8292
Frequencies	--	1259.4018	1319.2509	1352.0385
IR Inten	--	11.3974	7.2778	5.8333
Rot. str.	--	-38.6228	-0.0814	14.2382
Frequencies	--	1360.8003	1395.1111	1445.6729
IR Inten	--	6.0487	2.6976	6.4240
Rot. str.	--	-23.6125	-6.4302	7.2940
Frequencies	--	1456.3076	1460.5867	1606.2171
IR Inten	--	5.1078	3.9977	30.8018
Rot. str.	--	-1.2553	0.2563	-11.2467
Frequencies	--	2921.5410	2949.7057	2961.5105
IR Inten	--	45.2520	41.3778	34.3234
Rot. str.	--	-5.8242	-10.7783	11.4168
Frequencies	--	2973.2848	3026.8420	3049.9610
IR Inten	--	42.8217	38.3958	21.9832
Rot. str.	--	-2.9188	3.0737	-6.9333
Frequencies	--	3416.5776	3496.1987	3754.4751
IR Inten	--	3.3995	1.7443	28.7237
Rot. str.	--	3.0183	-3.3050	2.5308