

Supporting Information

Exploring the Conformational Space of Cysteine by Matrix Isolation Spectroscopy Combined with Near-Infrared Laser Induced Conformational Change

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Table S1. B3LYP/6-31++G** Cartesian coordinates (in Angstroms) and SQM wavenumbers (in cm⁻¹) and IR (*I* in km mol⁻¹) and Raman intensities of Cysteine conformers.

Conformer 1

CONVERGED GEOMETRY						
Coordinates (Angstroms)						
	X	Y	Z			
n	0.49993997179621	-1.37176359093702	-0.52233946530023			
h	-0.00869077874302	-2.12371152401399	-0.97572233946465			
c	-0.24228368853941	-0.10594564679038	-0.53929687909106			
h	-0.81090747130733	-0.06490990714297	-1.47889646496349			
c	-1.24092757229729	0.10974540829534	0.60929591832697			
c	0.76009931400567	1.06921273358888	-0.63474821289523			
h	-1.71002637920946	1.09013279232432	0.51489022958209			
s	-0.50344234922868	-0.05037860793560	2.28998961650119			
o	0.45235602026060	2.21752196428848	-0.40124906877442			
h	0.18121688651780	1.11123458946316	2.26556105472991			
h	0.70283039098813	-1.65105209353528	0.43741959898165			
o	1.98500229683120	0.70508383639008	-1.03299611454888			
h	1.95600304252228	-0.27991196783465	-1.09954543019318			
h	-2.02116968359668	-0.65525798616040	0.56763755710936			

Calculated	Experimental	Weight	Difference	percent	IR	Raman
68.14	0.00	0.0000	68.14	inf	2.7180	-14.4352
88.25	0.00	0.0000	88.25	inf	4.3893	-4.7091
196.84	0.00	0.0000	196.84	inf	1.6853	-5.2037
265.15	0.00	0.0000	265.15	inf	25.5005	30.5566
297.06	0.00	0.0000	297.06	inf	21.9622	27.4820
353.26	0.00	0.0000	353.26	inf	1.6888	-18.9002
363.81	0.00	0.0000	363.81	inf	12.1277	35.3536
494.31	0.00	0.0000	494.31	inf	6.5578	1.4501
525.71	0.00	0.0000	525.71	inf	2.2223	-12.0396
561.72	0.00	0.0000	561.72	inf	2.5925	-1.3871
673.67	0.00	0.0000	673.67	inf	0.9782	-5.8212
743.72	0.00	0.0000	743.72	inf	6.5687	33.1442
772.64	0.00	0.0000	772.64	inf	0.6939	11.1629
822.61	0.00	0.0000	822.61	inf	19.2943	-11.4083
842.10	0.00	0.0000	842.10	inf	144.0380	-175.8124
887.83	0.00	0.0000	887.83	inf	69.8064	109.4844
948.13	0.00	0.0000	948.13	inf	37.4429	0.5632
1026.33	0.00	0.0000	1026.33	inf	33.6322	26.4710
1082.56	0.00	0.0000	1082.56	inf	18.0092	6.2925
1140.99	0.00	0.0000	1140.99	inf	8.9909	-24.0507
1184.99	0.00	0.0000	1184.99	inf	11.5840	-4.9361
1218.23	0.00	0.0000	1218.23	inf	1.5359	2.0705
1261.48	0.00	0.0000	1261.48	inf	7.1720	25.1987
1302.86	0.00	0.0000	1302.86	inf	34.0261	-44.6637
1366.71	0.00	0.0000	1366.71	inf	9.5490	-43.4774
1386.25	0.00	0.0000	1386.25	inf	405.0196	119.4319
1422.65	0.00	0.0000	1422.65	inf	16.8769	0.9108
1615.12	0.00	0.0000	1615.12	inf	38.5370	-62.6116
1779.05	0.00	0.0000	1779.05	inf	292.5353	-105.5304
2596.80	0.00	0.0000	2596.80	inf	0.5455	0.3856
2912.74	0.00	0.0000	2912.74	inf	9.3393	5.9101
2959.72	0.00	0.0000	2959.72	inf	14.8122	-8.2922
3023.34	0.00	0.0000	3023.34	inf	0.9499	3.9097
3288.47	0.00	0.0000	3288.47	inf	251.9140	-17.0424
3319.05	0.00	0.0000	3319.05	inf	22.9214	16.1999
3428.06	0.00	0.0000	3428.06	inf	18.5167	-20.3380

Conformer 2

CONVERGED GEOMETRY			
Coordinates (Angstroms)			
	X	Y	Z
n	0.75352824753950	-1.19368207533490	-0.36454822182744
h	1.01548482096493	-1.50297433887319	-1.29693801281760
c	0.03575177665551	0.08571644184322	-0.40617414484527
h	-0.54615467348119	0.22891524417332	-1.32586617655519
c	-0.90901127939224	0.23743206107020	0.80084227448001
c	1.05129519559504	1.24877796727075	-0.34372310901528
h	-0.34523265502468	0.13768072097218	1.73404096017955
s	-2.22163103123240	-1.04760709455410	0.91422953067674
o	0.75419287707992	2.38956785284075	-0.61640687316996
h	-2.89547121902248	-0.68561774257171	-0.19731167196829
h	0.16574777800322	-1.92116363424577	0.03852512863813
o	2.27238716103385	0.88554153475899	0.07720792942302
h	2.22937528151571	-0.09292733592667	0.20103227665359
h	-1.36026228023468	1.23034039857693	0.78509011014799

Calculated	Experimental	Weight	Difference	percent	IR	Raman
75.22	0.00	0.0000	75.22	inf	2.7353	-7.6548
108.51	0.00	0.0000	108.51	inf	7.2691	35.3809
169.52	0.00	0.0000	169.52	inf	10.5623	-11.6567
248.11	0.00	0.0000	248.11	inf	4.5270	-16.7857
267.02	0.00	0.0000	267.02	inf	12.4697	5.2090
322.62	0.00	0.0000	322.62	inf	30.9106	-52.4691
345.96	0.00	0.0000	345.96	inf	12.4727	21.8077
403.81	0.00	0.0000	403.81	inf	4.9019	-15.1376
542.73	0.00	0.0000	542.73	inf	2.2267	2.6296
647.57	0.00	0.0000	647.57	inf	7.2407	-62.9506
660.48	0.00	0.0000	660.48	inf	11.4212	53.9592
761.98	0.00	0.0000	761.98	inf	16.2144	16.0502
792.44	0.00	0.0000	792.44	inf	2.0958	12.1167
839.29	0.00	0.0000	839.29	inf	18.0227	62.2671
855.92	0.00	0.0000	855.92	inf	74.1370	55.1159
881.82	0.00	0.0000	881.82	inf	44.1070	-41.0914
934.21	0.00	0.0000	934.21	inf	82.0602	-19.3464
1005.14	0.00	0.0000	1005.14	inf	56.2428	97.9458
1075.65	0.00	0.0000	1075.65	inf	16.4359	-9.2014
1152.96	0.00	0.0000	1152.96	inf	14.7798	44.1562
1184.74	0.00	0.0000	1184.74	inf	9.7706	15.5022
1252.07	0.00	0.0000	1252.07	inf	9.9779	19.5263
1274.11	0.00	0.0000	1274.11	inf	7.7154	33.8647
1314.17	0.00	0.0000	1314.17	inf	7.9928	9.1943
1345.99	0.00	0.0000	1345.99	inf	36.4107	-28.8368
1378.85	0.00	0.0000	1378.85	inf	411.8528	-106.3589
1436.16	0.00	0.0000	1436.16	inf	7.4710	-1.1247
1629.49	0.00	0.0000	1629.49	inf	40.9941	-44.1025
1783.58	0.00	0.0000	1783.58	inf	345.4311	-76.6705
2588.65	0.00	0.0000	2588.65	inf	6.7193	2.8573
2915.78	0.00	0.0000	2915.78	inf	15.8686	8.2339
2953.51	0.00	0.0000	2953.51	inf	6.5218	3.9905
3022.83	0.00	0.0000	3022.83	inf	0.6789	-5.6285
3297.00	0.00	0.0000	3297.00	inf	246.1437	-27.7580
3332.16	0.00	0.0000	3332.16	inf	7.1947	16.6768
3410.60	0.00	0.0000	3410.60	inf	24.0820	-23.4892

Conformer 3

CONVERGED GEOMETRY			
Coordinates (Angstroms)			
	X	Y	Z
n	0.60568616625734	-1.44847921264876	-0.24500627726756
h	1.39344504984715	-1.38938544850276	0.39743495435129
c	-0.03834305844539	-0.14933803238222	-0.36718685514828
h	-0.63324176571210	-0.12994741998882	-1.28570005799157
c	-0.99482000442336	0.09414892317756	0.82256299937180
c	0.96362864267362	1.00919838003400	-0.42789008677432
h	-0.43510193520449	0.04633116884032	1.76245935757089
s	-2.38881946255902	-1.09776502476759	0.87015752035757
o	2.11752125287229	0.95313274681748	-0.05762986174047
h	-1.60598178652131	-2.18973128001374	0.74655530419936
h	0.97562181048640	-1.75917237256194	-1.13824019346537
o	0.40606310595822	2.13977105907295	-0.92317547588107
h	1.08440982151252	2.83689807352222	-0.90077213408080
h	-1.45006783674186	1.08433843940130	0.74643080649850

Calculated	Experimental	Weight	Difference	percent	IR	Raman
47.43	0.00	0.0000	47.43	inf	1.9986	-0.0658
98.09	0.00	0.0000	98.09	inf	3.3387	-0.1308
167.71	0.00	0.0000	167.71	inf	0.8837	0.0813
211.17	0.00	0.0000	211.17	inf	12.8240	-0.0964
235.54	0.00	0.0000	235.54	inf	6.7718	0.0412
297.93	0.00	0.0000	297.93	inf	10.2535	0.0991
321.33	0.00	0.0000	321.33	inf	35.7349	0.1064
380.58	0.00	0.0000	380.58	inf	19.9808	0.0848
504.62	0.00	0.0000	504.62	inf	12.7152	-0.0010
584.84	0.00	0.0000	584.84	inf	93.4582	-0.0630
642.13	0.00	0.0000	642.13	inf	12.3863	-0.0021
688.63	0.00	0.0000	688.63	inf	39.1942	-0.2461
756.26	0.00	0.0000	756.26	inf	15.5164	0.2095
785.99	0.00	0.0000	785.99	inf	29.8117	-0.0290
834.52	0.00	0.0000	834.52	inf	116.3711	0.1069
897.54	0.00	0.0000	897.54	inf	35.1436	0.0901
918.37	0.00	0.0000	918.37	inf	5.4827	-0.0049
991.64	0.00	0.0000	991.64	inf	27.8423	-0.0078
1097.93	0.00	0.0000	1097.93	inf	157.2932	0.1190
1122.06	0.00	0.0000	1122.06	inf	53.4854	0.0026
1139.89	0.00	0.0000	1139.89	inf	75.2130	0.0379
1224.98	0.00	0.0000	1224.98	inf	7.3598	0.3062
1276.61	0.00	0.0000	1276.61	inf	0.5518	-0.0969
1296.07	0.00	0.0000	1296.07	inf	10.7882	0.2117
1320.20	0.00	0.0000	1320.20	inf	52.2512	0.0046
1394.11	0.00	0.0000	1394.11	inf	6.5264	-0.1297
1442.75	0.00	0.0000	1442.75	inf	5.7221	0.0799
1633.37	0.00	0.0000	1633.37	inf	35.9199	-0.0667
1752.23	0.00	0.0000	1752.23	inf	316.2230	-0.1634
2588.36	0.00	0.0000	2588.36	inf	4.7313	-0.1149
2937.69	0.00	0.0000	2937.69	inf	13.1124	-0.0260
2963.31	0.00	0.0000	2963.31	inf	5.7583	0.0381
3006.19	0.00	0.0000	3006.19	inf	4.2289	0.4973
3339.76	0.00	0.0000	3339.76	inf	4.4445	0.0361
3424.44	0.00	0.0000	3424.44	inf	10.3121	-0.0833
3565.90	0.00	0.0000	3565.90	inf	65.5785	-0.0177

Conformer 4

CONVERGED GEOMETRY			
Coordinates (Angstroms)			
	X	Y	Z
n	0.75749943712780	-1.21441908440477	-0.42334427425422
h	0.17043561288524	-1.92997869630575	-0.84079086296665
c	0.04298710709853	0.06444991493296	-0.31698422917908
h	-0.55175059621384	0.17798680140251	-1.23268047802569
c	-0.88801106855479	0.21953073391911	0.89491175575122
c	1.06595603479284	1.22604711322966	-0.36561414500962
h	-0.33066499844566	0.04207571925432	1.82104933550125
s	-2.27538369770840	-0.99005715186080	0.93083694336939
o	0.79438243532024	2.36017002886860	-0.04168740528148
h	-3.02495585161687	-0.40070357010928	-0.02343156004371
h	1.03322316348688	-1.55907309039949	0.49467621976725
o	2.26876430261335	0.86892380198993	-0.83929643511467
h	2.21334170977898	-0.10256968949336	-1.00066412067719
h	-1.27582359056432	1.23761716897635	0.94301925616321

Calculated	Experimental	Weight	Difference	percent	IR	Raman
66.65	0.00	0.0000	66.65	inf	1.8823	-16.8812
91.59	0.00	0.0000	91.59	inf	7.6960	11.0142
172.19	0.00	0.0000	172.19	inf	18.1286	-37.3238
214.15	0.00	0.0000	214.15	inf	17.8380	56.8674
260.40	0.00	0.0000	260.40	inf	7.4717	4.6197
304.63	0.00	0.0000	304.63	inf	20.5977	72.9484
343.33	0.00	0.0000	343.33	inf	11.8870	5.1615
419.80	0.00	0.0000	419.80	inf	3.6542	-7.0870
516.08	0.00	0.0000	516.08	inf	1.1165	1.1301
587.36	0.00	0.0000	587.36	inf	8.1807	-68.7555
686.96	0.00	0.0000	686.96	inf	10.1783	40.8402
753.72	0.00	0.0000	753.72	inf	4.8589	-2.6472
784.69	0.00	0.0000	784.69	inf	1.8160	16.4941
836.69	0.00	0.0000	836.69	inf	32.6294	2.3937
844.44	0.00	0.0000	844.44	inf	111.8089	-100.5317
880.26	0.00	0.0000	880.26	inf	83.1005	53.1995
944.41	0.00	0.0000	944.41	inf	62.4277	61.8152
1032.05	0.00	0.0000	1032.05	inf	57.7374	-97.6253
1093.29	0.00	0.0000	1093.29	inf	8.7279	9.5689
1129.23	0.00	0.0000	1129.23	inf	10.4946	17.8861
1180.58	0.00	0.0000	1180.58	inf	13.1626	-72.0260
1229.90	0.00	0.0000	1229.90	inf	5.7924	37.4336
1253.46	0.00	0.0000	1253.46	inf	4.2838	-3.1605
1310.43	0.00	0.0000	1310.43	inf	4.2430	-31.4429
1369.64	0.00	0.0000	1369.64	inf	5.2187	-49.5266
1378.26	0.00	0.0000	1378.26	inf	464.9286	97.2802
1438.54	0.00	0.0000	1438.54	inf	7.1642	-4.5450
1630.93	0.00	0.0000	1630.93	inf	37.3618	-14.4460
1780.52	0.00	0.0000	1780.52	inf	321.0137	-11.6032
2589.21	0.00	0.0000	2589.21	inf	7.4485	3.2031
2923.72	0.00	0.0000	2923.72	inf	4.2400	6.1053
2948.83	0.00	0.0000	2948.83	inf	10.1119	3.2362
3024.05	0.00	0.0000	3024.05	inf	0.8474	-1.1074
3310.32	0.00	0.0000	3310.32	inf	251.5196	-14.9278
3337.91	0.00	0.0000	3337.91	inf	3.1138	7.7539
3426.64	0.00	0.0000	3426.64	inf	11.1427	-2.1106

Conformer 5

CONVERGED GEOMETRY			
Coordinates (Angstroms)			
	X	Y	Z
n	0.34043660091985	-1.66410861352863	-0.69022341341014
h	0.92323843735737	-1.84855379784340	0.12428733163077
c	-0.26556527084261	-0.35282580032913	-0.57047479388302
h	-0.94446398303167	-0.20648677533729	-1.42477130019366
c	-1.14761221667450	-0.26693975038218	0.68836277955904
c	0.73820446033913	0.80719788917835	-0.65836542365274
h	-1.70168085229405	0.67170517150617	0.71365594234907
s	-0.24872460167290	-0.48510803410812	2.28325253963562
o	1.91521456348905	0.69727226161430	-0.92170713463614
h	0.32084162400602	0.73710971534656	2.31765800696421
h	0.94993987957644	-1.70352578339296	-1.50233010300690
o	0.14806739589265	2.01347393146338	-0.44785557644514
h	0.83181425001899	2.69513521589435	-0.56707514022973
h	-1.85971028708372	-1.09434563008142	0.65558628531874

Calculated	Experimental	Weight	Difference	percent	IR	Raman
40.61	0.00	0.0000	40.61	inf	1.6752	-1.6265
85.62	0.00	0.0000	85.62	inf	1.3527	-5.1940
184.09	0.00	0.0000	184.09	inf	0.4279	-4.3531
227.39	0.00	0.0000	227.39	inf	21.6555	-31.1242
243.15	0.00	0.0000	243.15	inf	21.0457	-4.9050
291.56	0.00	0.0000	291.56	inf	32.9290	-11.0989
340.56	0.00	0.0000	340.56	inf	27.0096	9.4433
448.36	0.00	0.0000	448.36	inf	11.3894	-39.8911
489.10	0.00	0.0000	489.10	inf	10.0413	21.0552
571.23	0.00	0.0000	571.23	inf	24.6083	-66.4972
626.36	0.00	0.0000	626.36	inf	101.8046	62.0999
673.98	0.00	0.0000	673.98	inf	2.2055	-1.6634
721.83	0.00	0.0000	721.83	inf	23.8639	23.6680
772.02	0.00	0.0000	772.02	inf	4.9273	12.5509
832.20	0.00	0.0000	832.20	inf	39.5898	-27.1489
888.01	0.00	0.0000	888.01	inf	120.4772	5.4296
924.59	0.00	0.0000	924.59	inf	4.8011	-3.3056
1025.84	0.00	0.0000	1025.84	inf	71.2103	-3.7582
1100.53	0.00	0.0000	1100.53	inf	201.1191	-87.0232
1121.58	0.00	0.0000	1121.58	inf	21.1699	10.1531
1159.78	0.00	0.0000	1159.78	inf	15.5800	20.7254
1237.95	0.00	0.0000	1237.95	inf	1.2171	-9.4198
1272.10	0.00	0.0000	1272.10	inf	7.9977	22.5798
1296.79	0.00	0.0000	1296.79	inf	16.8565	0.1530
1337.02	0.00	0.0000	1337.02	inf	12.9978	-49.4860
1364.68	0.00	0.0000	1364.68	inf	1.6452	-3.0964
1425.20	0.00	0.0000	1425.20	inf	9.2573	2.5074
1629.56	0.00	0.0000	1629.56	inf	42.3166	30.2493
1760.35	0.00	0.0000	1760.35	inf	296.1791	40.4165
2591.53	0.00	0.0000	2591.53	inf	7.3732	-0.7952
2888.79	0.00	0.0000	2888.79	inf	13.2534	9.4460
2972.74	0.00	0.0000	2972.74	inf	9.3106	-0.7447
3032.20	0.00	0.0000	3032.20	inf	1.9064	5.4410
3334.95	0.00	0.0000	3334.95	inf	3.3238	-2.4470
3417.86	0.00	0.0000	3417.86	inf	12.2155	3.8964
3566.77	0.00	0.0000	3566.77	inf	61.0229	2.8765

Conformer 6

CONVERGED GEOMETRY			
Coordinates (Angstroms)			
	X	Y	Z
n	0.72707583643800	-1.09459439191057	-0.43973893066053
h	0.22364558003769	-1.84850599361865	-0.89548952385954
c	-0.05513744130478	0.14890394191214	-0.40315477893987
h	-0.65613693066828	0.18047928847009	-1.32006507744905
c	-0.99819714162488	0.32015582943260	0.79506032009337
c	0.90553624627310	1.36050374191530	-0.50373623953588
h	-0.44376741204805	0.26907878521681	1.73792785744849
s	-2.39473221790219	-0.87407219563546	0.83471973578548
o	0.56460445127112	2.49396889362844	-0.25211366797091
h	-1.68044805454416	-1.96633510697081	1.17571203340986
h	0.99094902231890	-1.40850306456177	0.49174295349002
o	2.13668427653237	1.04513660043346	-0.93207775007409
h	2.13814848710325	0.06471431447279	-1.03622984737037
h	-1.45822470188207	1.30906935721561	0.74744291563299

Calculated	Experimental	Weight	Difference	percent	IR	Raman
70.60	0.00	0.0000	70.60	inf	2.3562	-10.3428
90.62	0.00	0.0000	90.62	inf	6.9248	26.3405
175.36	0.00	0.0000	175.36	inf	6.1382	-23.1175
207.10	0.00	0.0000	207.10	inf	32.6705	-36.8740
261.54	0.00	0.0000	261.54	inf	5.5429	1.8000
330.97	0.00	0.0000	330.97	inf	9.6307	54.3372
347.24	0.00	0.0000	347.24	inf	20.1615	32.3066
407.94	0.00	0.0000	407.94	inf	2.9366	2.4176
516.75	0.00	0.0000	516.75	inf	0.9476	1.2050
587.84	0.00	0.0000	587.84	inf	9.4842	-71.8752
695.79	0.00	0.0000	695.79	inf	11.0283	60.2222
731.25	0.00	0.0000	731.25	inf	8.6898	41.1442
778.10	0.00	0.0000	778.10	inf	0.5128	1.6412
830.52	0.00	0.0000	830.52	inf	148.1652	-132.8629
852.06	0.00	0.0000	852.06	inf	51.3562	31.4248
874.21	0.00	0.0000	874.21	inf	41.4779	23.3069
932.28	0.00	0.0000	932.28	inf	63.8123	65.8981
1025.15	0.00	0.0000	1025.15	inf	24.7275	-63.6911
1097.41	0.00	0.0000	1097.41	inf	9.0948	5.5174
1122.96	0.00	0.0000	1122.96	inf	24.0709	-29.0556
1178.26	0.00	0.0000	1178.26	inf	14.7035	-60.4122
1213.25	0.00	0.0000	1213.25	inf	9.3510	56.8719
1259.53	0.00	0.0000	1259.53	inf	0.9964	4.0501
1305.73	0.00	0.0000	1305.73	inf	5.1643	-24.2479
1372.26	0.00	0.0000	1372.26	inf	9.5608	-61.9158
1376.63	0.00	0.0000	1376.63	inf	463.5360	98.5836
1435.45	0.00	0.0000	1435.45	inf	6.5359	-7.8445
1623.56	0.00	0.0000	1623.56	inf	32.7602	-11.3665
1782.00	0.00	0.0000	1782.00	inf	321.1711	-18.9155
2587.95	0.00	0.0000	2587.95	inf	13.3394	3.7944
2934.87	0.00	0.0000	2934.87	inf	3.8274	7.2418
2947.90	0.00	0.0000	2947.90	inf	10.4737	-2.9553
3017.63	0.00	0.0000	3017.63	inf	1.7708	2.8688
3316.88	0.00	0.0000	3316.88	inf	244.1057	-8.8141
3343.74	0.00	0.0000	3343.74	inf	4.4847	6.8422
3437.74	0.00	0.0000	3437.74	inf	11.6493	-4.0383

Conformer 7

CONVERGED GEOMETRY			
Coordinates (Angstroms)			
	X	Y	Z
n	0.45232948764329	-1.52669598161572	-0.51309525015126
h	1.24076125606722	-1.50164925923856	0.13019042887402
c	-0.21081048266875	-0.23341738692164	-0.52996613604981
h	-0.85123448468990	-0.18927026425015	-1.42232703513490
c	-1.15688006313069	-0.07359394550330	0.67562681433458
c	0.76352109209501	0.94694382027147	-0.65402695642425
h	-1.66640506769361	0.89068359051847	0.63057351414715
s	-0.32833602050755	-0.10627401886044	2.31938497921591
o	1.96635124124919	0.85164725231966	-0.75873258889217
h	-0.06142389896280	-1.42785645984150	2.33038352248817
h	0.84339144252887	-1.73756168735637	-1.42671262383914
o	0.11877989401112	2.14037796359848	-0.66743042439112
h	0.79467433204285	2.83444572160859	-0.75344102410080
h	-1.90471872798429	-0.86777934472896	0.63957277992360

Calculated	Experimental	Weight	Difference	percent	IR	Raman
52.31	0.00	0.0000	52.31	inf	6.1845	3.8454
73.12	0.00	0.0000	73.12	inf	0.3343	-3.8418
154.64	0.00	0.0000	154.64	inf	47.9573	-14.0626
175.52	0.00	0.0000	175.52	inf	4.8292	4.0719
252.57	0.00	0.0000	252.57	inf	8.1110	11.1968
299.02	0.00	0.0000	299.02	inf	9.5859	11.0649
346.38	0.00	0.0000	346.38	inf	21.2939	-4.4882
440.48	0.00	0.0000	440.48	inf	15.2950	-45.4304
492.68	0.00	0.0000	492.68	inf	9.2085	18.4807
577.41	0.00	0.0000	577.41	inf	34.5470	-85.9264
617.96	0.00	0.0000	617.96	inf	94.7620	48.8564
683.34	0.00	0.0000	683.34	inf	2.5731	-12.8292
728.42	0.00	0.0000	728.42	inf	26.4049	24.1260
741.45	0.00	0.0000	741.45	inf	3.1813	-8.3395
847.93	0.00	0.0000	847.93	inf	57.8985	-0.4425
886.49	0.00	0.0000	886.49	inf	101.3184	27.3054
917.65	0.00	0.0000	917.65	inf	2.4535	8.0515
1022.13	0.00	0.0000	1022.13	inf	45.9306	34.2710
1104.06	0.00	0.0000	1104.06	inf	177.6739	-27.4992
1120.39	0.00	0.0000	1120.39	inf	78.0305	-12.1949
1178.01	0.00	0.0000	1178.01	inf	14.1531	-67.4092
1216.96	0.00	0.0000	1216.96	inf	1.0615	11.4908
1265.22	0.00	0.0000	1265.22	inf	5.3988	32.3065
1295.94	0.00	0.0000	1295.94	inf	15.9911	-21.1839
1328.90	0.00	0.0000	1328.90	inf	20.1606	-49.6447
1380.01	0.00	0.0000	1380.01	inf	3.3658	2.4770
1427.18	0.00	0.0000	1427.18	inf	8.1147	11.2458
1632.62	0.00	0.0000	1632.62	inf	38.5993	17.8013
1761.13	0.00	0.0000	1761.13	inf	294.7399	57.8691
2595.61	0.00	0.0000	2595.61	inf	4.4487	-2.7818
2909.16	0.00	0.0000	2909.16	inf	10.7693	10.7153
2969.75	0.00	0.0000	2969.75	inf	12.3993	9.6849
3027.60	0.00	0.0000	3027.60	inf	2.3980	-3.6670
3343.18	0.00	0.0000	3343.18	inf	2.4919	0.2629
3419.60	0.00	0.0000	3419.60	inf	8.1701	7.6529
3571.05	0.00	0.0000	3571.05	inf	64.3346	3.5599

Conformer 8

CONVERGED GEOMETRY			
Coordinates (Angstroms)			
	X	Y	Z
n	0.51832870490018	-1.15715407825365	-0.67851725069379
h	-0.04309389300976	-1.87186748617393	-1.12993321018503
c	-0.20047216626155	0.11187296089529	-0.52605890201712
h	-0.82532387666925	0.24466033965300	-1.42037271902229
c	-1.12736955273321	0.24329328045276	0.69441011260013
c	0.81030699078854	1.28390099208398	-0.58780734442024
h	-1.47098156991900	1.27677745285831	0.76340632162972
s	-0.30760022218660	-0.12976982018992	2.30693504217569
o	0.53049513243718	2.41085662062401	-0.24700125973016
h	-0.66757265451597	-1.42708923920810	2.38060954788200
h	0.82665202163878	-1.50716014953391	0.22757891621332
o	1.99984331549907	0.94915532698666	-1.10558591596469
h	1.95671754516574	-0.02273747952578	-1.26424911453414
h	-1.99992977513413	-0.40473872066873	0.58658577606659

Calculated	Experimental	Weight	Difference	percent	IR	Raman
70.68	0.00	0.0000	70.68	inf	2.9118	-8.9878
76.23	0.00	0.0000	76.23	inf	0.8697	-14.0020
171.01	0.00	0.0000	171.01	inf	18.7925	37.5760
205.78	0.00	0.0000	205.78	inf	5.6059	-12.3191
277.16	0.00	0.0000	277.16	inf	19.7307	8.6955
349.38	0.00	0.0000	349.38	inf	5.5107	43.2331
351.50	0.00	0.0000	351.50	inf	17.0239	50.2906
493.48	0.00	0.0000	493.48	inf	8.6836	-9.7320
524.04	0.00	0.0000	524.04	inf	1.5865	-10.4837
562.76	0.00	0.0000	562.76	inf	2.8962	9.1490
686.08	0.00	0.0000	686.08	inf	0.8471	-9.6540
738.76	0.00	0.0000	738.76	inf	9.4954	-2.7447
750.43	0.00	0.0000	750.43	inf	11.0208	-46.5826
826.81	0.00	0.0000	826.81	inf	140.9199	-138.8514
840.15	0.00	0.0000	840.15	inf	26.0201	38.3952
875.21	0.00	0.0000	875.21	inf	65.1898	68.9830
935.93	0.00	0.0000	935.93	inf	40.3477	10.2459
1033.90	0.00	0.0000	1033.90	inf	27.5402	10.4576
1075.29	0.00	0.0000	1075.29	inf	13.4850	5.0299
1140.96	0.00	0.0000	1140.96	inf	14.3952	8.3498
1182.06	0.00	0.0000	1182.06	inf	11.3909	11.2478
1206.02	0.00	0.0000	1206.02	inf	7.6187	-3.8356
1264.62	0.00	0.0000	1264.62	inf	10.9881	7.0501
1300.55	0.00	0.0000	1300.55	inf	34.4457	-54.3835
1367.01	0.00	0.0000	1367.01	inf	20.1656	-79.2807
1381.54	0.00	0.0000	1381.54	inf	399.0549	157.0688
1423.60	0.00	0.0000	1423.60	inf	14.5792	2.5910
1610.85	0.00	0.0000	1610.85	inf	30.8407	-53.7932
1784.51	0.00	0.0000	1784.51	inf	298.3588	-77.5038
2591.59	0.00	0.0000	2591.59	inf	10.1029	-4.4998
2912.68	0.00	0.0000	2912.68	inf	8.7884	7.8461
2965.66	0.00	0.0000	2965.66	inf	15.3465	-6.7035
3026.13	0.00	0.0000	3026.13	inf	0.6056	1.3629
3315.69	0.00	0.0000	3315.69	inf	151.0649	9.6066
3329.72	0.00	0.0000	3329.72	inf	103.3047	-0.8126
3430.02	0.00	0.0000	3430.02	inf	16.7578	-19.7597

Conformer 9

CONVERGED GEOMETRY			
Coordinates (Angstroms)			
	X	Y	Z
n	0.25589011815263	-1.55913632235563	-0.60157753440365
h	0.77991309941181	-1.76222719009407	0.24710026713733
c	-0.34967880455599	-0.23739347503247	-0.51062640426989
h	-0.95961069818431	-0.09208512364175	-1.41658988962721
c	-1.30985085371201	-0.15506167954140	0.68246997744561
c	0.62494356321074	0.95138299783442	-0.51254873373420
h	-1.82780139723365	0.80432892790291	0.69666142594395
s	-0.52110031495574	-0.42963642094320	2.32682945882460
o	0.46630011836596	1.99681792911429	0.08421550789792
h	0.05548700092979	0.78529915349897	2.41768482170344
h	0.89496288852904	-1.61774679812620	-1.38810110226928
o	1.69617854821886	0.73228993087992	-1.31376079515969
h	2.24095479471808	1.53767329355234	-1.29425029652040
h	-2.04658806289517	-0.95450522304816	0.58249329703144

Calculated	Experimental	Weight	Difference	percent	IR	Raman
29.22	0.00	0.0000	29.22	Infinity	1.4766	-4.4322
94.70	0.00	0.0000	94.70	Infinity	0.9320	-2.1107
186.36	0.00	0.0000	186.36	Infinity	0.4180	-5.4622
252.78	0.00	0.0000	252.78	Infinity	5.1566	-4.5964
273.79	0.00	0.0000	273.79	Infinity	23.1244	-28.3893
318.53	0.00	0.0000	318.53	Infinity	28.8629	8.4466
345.95	0.00	0.0000	345.95	Infinity	40.2830	-50.9769
417.06	0.00	0.0000	417.06	Infinity	3.0283	17.2108
528.28	0.00	0.0000	528.28	Infinity	14.7664	20.4637
549.28	0.00	0.0000	549.28	Infinity	46.9442	3.4346
628.30	0.00	0.0000	628.30	Infinity	105.5983	-38.5060
675.62	0.00	0.0000	675.62	Infinity	7.3469	24.0238
721.12	0.00	0.0000	721.12	Infinity	23.6344	49.8217
763.91	0.00	0.0000	763.91	Infinity	9.7332	23.1311
832.15	0.00	0.0000	832.15	Infinity	63.0191	-35.1346
870.37	0.00	0.0000	870.37	Infinity	94.6439	-28.6210
922.38	0.00	0.0000	922.38	Infinity	1.7745	-9.6733
1022.63	0.00	0.0000	1022.63	Infinity	35.1711	-16.6413
1103.40	0.00	0.0000	1103.40	Infinity	77.4629	-58.5226
1129.27	0.00	0.0000	1129.27	Infinity	162.9595	-40.1777
1148.31	0.00	0.0000	1148.31	Infinity	54.6976	179.9899
1239.77	0.00	0.0000	1239.77	Infinity	3.0568	3.7138
1283.25	0.00	0.0000	1283.25	Infinity	15.8960	16.2442
1297.69	0.00	0.0000	1297.69	Infinity	22.3650	-20.3416
1341.62	0.00	0.0000	1341.62	Infinity	26.0836	20.6289
1361.27	0.00	0.0000	1361.27	Infinity	1.5224	-19.7595
1421.10	0.00	0.0000	1421.10	Infinity	13.3796	-2.2098
1620.92	0.00	0.0000	1620.92	Infinity	52.1814	37.4062
1745.96	0.00	0.0000	1745.96	Infinity	261.9611	-90.3101
2601.48	0.00	0.0000	2601.48	Infinity	1.4556	1.0734
2879.33	0.00	0.0000	2879.33	Infinity	14.5205	0.8243
2975.13	0.00	0.0000	2975.13	Infinity	9.9778	-1.1638
3033.58	0.00	0.0000	3033.58	Infinity	1.7682	4.8091
3338.18	0.00	0.0000	3338.18	Infinity	3.1249	-2.7972
3432.21	0.00	0.0000	3432.21	Infinity	13.7469	4.7600
3573.90	0.00	0.0000	3573.90	Infinity	73.6346	-5.1606

Conformer 10

CONVERGED GEOMETRY			
Coordinates (Angstroms)			
	X	Y	Z
n	0.41009514526775	-1.43945153723292	-0.38375379505190
h	1.03104763023374	-1.41265834001060	0.42124366170675
c	-0.26072760287977	-0.15946508791312	-0.54871660279782
h	-0.78561325699910	-0.18073003528230	-1.51476396047542
c	-1.34879120068585	0.04508970035909	0.51930090749306
c	0.63083867819321	1.09220067529578	-0.62568589475410
h	-1.81542697786767	1.02243184301059	0.38601839974323
s	-0.72639461472791	0.03237510006037	2.25433120346114
o	0.20596469335907	2.22768378915254	-0.67189180610671
h	-0.59633242832605	-1.30532782247027	2.36321184750397
h	0.98707492168099	-1.65377743686141	-1.19140160758647
o	1.95304298749693	0.80643506360041	-0.67873511108062
h	2.42411897280101	1.65534772114623	-0.74013782756892
h	-2.10889694754634	-0.73015363285441	0.41098058551383

Calculated	Experimental	Weight	Difference	percent	IR	Raman
38.31	0.00	0.0000	38.31	Infinity	1.2997	-2.3264
79.80	0.00	0.0000	79.80	Infinity	0.2258	0.4157
180.13	0.00	0.0000	180.13	Infinity	3.1291	-2.9414
209.80	0.00	0.0000	209.80	Infinity	52.5539	-18.8230
254.16	0.00	0.0000	254.16	Infinity	3.5029	20.2467
318.83	0.00	0.0000	318.83	Infinity	8.7717	23.6490
344.20	0.00	0.0000	344.20	Infinity	24.0905	-52.5177
456.75	0.00	0.0000	456.75	Infinity	4.6339	4.8402
507.04	0.00	0.0000	507.04	Infinity	7.9051	1.4735
549.05	0.00	0.0000	549.05	Infinity	48.4600	31.0181
642.18	0.00	0.0000	642.18	Infinity	114.9824	-39.4136
684.67	0.00	0.0000	684.67	Infinity	5.7813	-11.4092
726.42	0.00	0.0000	726.42	Infinity	25.6039	64.6544
745.17	0.00	0.0000	745.17	Infinity	7.8781	-20.1975
835.94	0.00	0.0000	835.94	Infinity	79.9692	11.1949
878.99	0.00	0.0000	878.99	Infinity	74.2067	6.4282
912.37	0.00	0.0000	912.37	Infinity	2.7688	5.5383
1019.91	0.00	0.0000	1019.91	Infinity	47.3420	-10.3130
1104.96	0.00	0.0000	1104.96	Infinity	61.4686	16.4687
1138.36	0.00	0.0000	1138.36	Infinity	157.4293	-34.4575
1173.56	0.00	0.0000	1173.56	Infinity	38.9393	85.3113
1219.56	0.00	0.0000	1219.56	Infinity	6.6836	3.4838
1278.20	0.00	0.0000	1278.20	Infinity	9.8103	24.2705
1302.25	0.00	0.0000	1302.25	Infinity	17.4423	-38.9141
1328.26	0.00	0.0000	1328.26	Infinity	38.0875	3.8086
1367.02	0.00	0.0000	1367.02	Infinity	6.7693	-11.5095
1421.39	0.00	0.0000	1421.39	Infinity	12.3081	4.0037
1627.86	0.00	0.0000	1627.86	Infinity	54.0501	25.1992
1751.21	0.00	0.0000	1751.21	Infinity	266.6237	-95.7935
2594.10	0.00	0.0000	2594.10	Infinity	5.6960	-3.1949
2905.30	0.00	0.0000	2905.30	Infinity	10.6508	8.2392
2974.34	0.00	0.0000	2974.34	Infinity	10.3639	2.2390
3033.98	0.00	0.0000	3033.98	Infinity	1.3231	-1.0599
3348.56	0.00	0.0000	3348.56	Infinity	2.1755	0.5457
3428.60	0.00	0.0000	3428.60	Infinity	8.4619	3.8412
3570.94	0.00	0.0000	3570.94	Infinity	70.6978	-4.4099

Conformer 11

CONVERGED GEOMETRY			
Coordinates (Angstroms)			
	X	Y	Z
n	0.52240900257269	-1.72603486596456	-0.12253759109207
h	1.11521253549758	-1.70715300710159	0.70406576517372
c	-0.16620587212057	-0.44322449310977	-0.32015957014758
h	-0.68752829210006	-0.49054457782752	-1.28031529148993
c	-1.18454444550852	-0.24179054729479	0.80387045335538
c	0.83918239333535	0.70916977485710	-0.38136590304707
h	-1.85222567143298	-1.10579766091907	0.81473370259413
s	-2.26583334720115	1.23062743666931	0.59742505103668
o	1.19511855652713	1.38881133819869	0.56091045113987
h	-1.34971984723756	2.14815244959957	0.96516534948221
h	1.09803406711391	-1.96898153376515	-0.92374613956997
o	1.37317687746950	0.84563017703169	-1.61954672761596
h	2.04669384410694	1.54613118896995	-1.57212738522021
h	-0.68376980102227	-0.18499567934391	1.77362783540083

Calculated	Experimental	Weight	Difference	percent	IR	Raman
40.64	0.00	0.0000	40.64	Infinity	2.0496	8.7383
94.82	0.00	0.0000	94.82	Infinity	0.6186	-0.3739
170.73	0.00	0.0000	170.73	Infinity	0.5514	7.6822
250.10	0.00	0.0000	250.10	Infinity	4.7701	-17.6868
261.27	0.00	0.0000	261.27	Infinity	16.7628	2.6953
280.92	0.00	0.0000	280.92	Infinity	0.6675	-15.3786
294.29	0.00	0.0000	294.29	Infinity	53.0566	12.6462
382.41	0.00	0.0000	382.41	Infinity	5.4334	-19.1072
479.77	0.00	0.0000	479.77	Infinity	34.7653	0.2510
589.13	0.00	0.0000	589.13	Infinity	32.2998	28.9709
618.74	0.00	0.0000	618.74	Infinity	89.2132	-24.0108
712.04	0.00	0.0000	712.04	Infinity	10.6273	-53.7946
762.37	0.00	0.0000	762.37	Infinity	54.1093	33.9346
780.36	0.00	0.0000	780.36	Infinity	43.3170	6.8462
811.40	0.00	0.0000	811.40	Infinity	90.4022	-9.4490
848.24	0.00	0.0000	848.24	Infinity	36.0060	-4.7101
969.49	0.00	0.0000	969.49	Infinity	13.6792	36.5232
1017.71	0.00	0.0000	1017.71	Infinity	20.3326	10.2673
1069.03	0.00	0.0000	1069.03	Infinity	54.8576	-107.1600
1123.41	0.00	0.0000	1123.41	Infinity	239.9466	3.0249
1135.91	0.00	0.0000	1135.91	Infinity	7.2669	23.3694
1222.67	0.00	0.0000	1222.67	Infinity	9.3514	55.3595
1267.19	0.00	0.0000	1267.19	Infinity	7.1757	27.8122
1292.74	0.00	0.0000	1292.74	Infinity	19.0144	-1.5321
1368.16	0.00	0.0000	1368.16	Infinity	4.0482	-20.9118
1374.42	0.00	0.0000	1374.42	Infinity	27.2900	21.2171
1430.20	0.00	0.0000	1430.20	Infinity	11.2862	11.5014
1618.96	0.00	0.0000	1618.96	Infinity	35.5306	17.2549
1746.65	0.00	0.0000	1746.65	Infinity	269.8822	83.7278
2601.67	0.00	0.0000	2601.67	Infinity	1.8974	-1.5442
2959.48	0.00	0.0000	2959.48	Infinity	6.7024	2.3983
2971.00	0.00	0.0000	2971.00	Infinity	7.5182	-7.4408
3019.11	0.00	0.0000	3019.11	Infinity	2.7625	-4.2819
3337.46	0.00	0.0000	3337.46	Infinity	1.7869	0.9435
3430.23	0.00	0.0000	3430.23	Infinity	6.5579	1.8900
3566.50	0.00	0.0000	3566.50	Infinity	65.7439	0.7856

Conformer 12

CONVERGED GEOMETRY			
Coordinates (Angstroms)			
	X	Y	Z
n	0.49623513998190	-1.37276023952101	-0.28662556469092
h	1.22608198186300	-1.32472678824887	0.41962072747643
c	-0.15853238345041	-0.07990542234450	-0.45859749695003
h	-0.76246144776382	-0.11333132283220	-1.36894244932364
c	-1.09673722536556	0.20736842319627	0.73355396668706
c	0.78551155035236	1.11497620612532	-0.62657176060152
h	-0.52569349182713	0.20775158756618	1.66737211999164
s	-2.48618569084490	-0.98638996163225	0.85115395934948
o	0.59454549942543	2.05359014708312	-1.36950871445387
h	-1.70527234800662	-2.08128219059732	0.74303977786560
h	0.91971425396951	-1.69475169975073	-1.15134825562236
o	1.87251167781632	1.03669656962626	0.18573509147432
h	2.39936383440825	1.84153743048495	0.04329075478543
h	-1.55908135055828	1.19122726084480	0.61782784401240

Calculated	Experimental	Weight	Difference	percent	IR	Raman
27.08	0.00	0.0000	27.08	Infinity	0.9414	-8.4828
101.73	0.00	0.0000	101.73	Infinity	1.1988	-4.9651
163.27	0.00	0.0000	163.27	Infinity	0.3107	2.0875
230.28	0.00	0.0000	230.28	Infinity	4.8292	7.7425
249.15	0.00	0.0000	249.15	Infinity	8.8546	-8.5696
288.41	0.00	0.0000	288.41	Infinity	0.7279	1.9625
318.23	0.00	0.0000	318.23	Infinity	46.3175	12.5527
373.25	0.00	0.0000	373.25	Infinity	14.9448	-43.6970
532.00	0.00	0.0000	532.00	Infinity	4.0578	5.6012
585.17	0.00	0.0000	585.17	Infinity	101.9927	-5.6459
618.78	0.00	0.0000	618.78	Infinity	53.5403	10.3786
696.27	0.00	0.0000	696.27	Infinity	26.6047	21.9447
765.92	0.00	0.0000	765.92	Infinity	22.3239	24.6683
780.29	0.00	0.0000	780.29	Infinity	48.8952	27.3821
820.21	0.00	0.0000	820.21	Infinity	75.6922	-20.5513
874.17	0.00	0.0000	874.17	Infinity	64.4334	112.4314
919.65	0.00	0.0000	919.65	Infinity	5.0249	4.2845
979.70	0.00	0.0000	979.70	Infinity	21.3826	-52.9798
1098.01	0.00	0.0000	1098.01	Infinity	16.4557	-1.6991
1121.18	0.00	0.0000	1121.18	Infinity	113.7565	-108.1060
1139.57	0.00	0.0000	1139.57	Infinity	112.6658	26.6423
1243.68	0.00	0.0000	1243.68	Infinity	17.4587	37.4932
1275.06	0.00	0.0000	1275.06	Infinity	10.0887	-3.9781
1305.02	0.00	0.0000	1305.02	Infinity	32.3320	-14.8355
1320.73	0.00	0.0000	1320.73	Infinity	21.4415	-8.4839
1379.98	0.00	0.0000	1379.98	Infinity	9.5775	-33.9870
1443.41	0.00	0.0000	1443.41	Infinity	6.0684	-5.6548
1628.32	0.00	0.0000	1628.32	Infinity	40.5680	22.1747
1755.71	0.00	0.0000	1755.71	Infinity	333.4372	-38.3037
2589.02	0.00	0.0000	2589.02	Infinity	4.5362	2.0222
2940.34	0.00	0.0000	2940.34	Infinity	13.6851	-9.7041
2980.85	0.00	0.0000	2980.85	Infinity	2.5124	-1.3538
3001.70	0.00	0.0000	3001.70	Infinity	5.3991	12.7611
3349.75	0.00	0.0000	3349.75	Infinity	3.5471	0.6676
3436.12	0.00	0.0000	3436.12	Infinity	9.5907	4.4496
3574.51	0.00	0.0000	3574.51	Infinity	76.2455	-1.0488

Conformer 13

CONVERGED GEOMETRY			
Coordinates (Angstroms)			
	X	Y	Z
n	-0.06937844559088	-1.06200208806228	1.45980996108134
h	-0.37467142264346	-0.33110528201106	2.09825227920680
c	0.03731929095309	-0.56303075133286	0.08187455189001
h	0.48010806461334	-1.35751127442274	-0.52540677710565
c	-1.36205838367065	-0.23871359486247	-0.44473929178819
c	0.96077268895272	0.65569457499055	0.01513503509592
h	-1.97833691525347	-1.13434745885482	-0.34245740964785
s	-1.42001301057133	0.21422196347891	-2.22551502531937
o	0.60750326282537	1.81670561107090	0.07559685555168
h	-0.94021596512376	1.46545855935916	-2.08224097949937
h	0.81706380258689	-1.42908224423468	1.79412226987802
o	2.26610491062147	0.29416120878205	-0.03668655276002
h	2.79673741858024	1.10917036989748	-0.01066210678416
h	-1.82093529627958	0.56038040620185	0.14291719020083

Calculated	Experimental	Weight	Difference	percent	IR	Raman
40.38	0.00	0.0000	40.38	Infinity	2.0323	9.0701
94.36	0.00	0.0000	94.36	Infinity	0.6341	-0.3814
170.65	0.00	0.0000	170.65	Infinity	0.5818	7.8572
249.03	0.00	0.0000	249.03	Infinity	5.9612	-14.9810
261.69	0.00	0.0000	261.69	Infinity	14.9808	1.2102
279.22	0.00	0.0000	279.22	Infinity	0.3957	-0.1439
295.33	0.00	0.0000	295.33	Infinity	53.4829	-3.9181
382.74	0.00	0.0000	382.74	Infinity	5.7919	-20.8995
479.84	0.00	0.0000	479.84	Infinity	35.0363	0.8240
588.00	0.00	0.0000	588.00	Infinity	32.9365	29.3488
617.65	0.00	0.0000	617.65	Infinity	88.5969	-24.1427
711.27	0.00	0.0000	711.27	Infinity	10.9873	-54.6742
761.43	0.00	0.0000	761.43	Infinity	50.8590	31.4802
780.54	0.00	0.0000	780.54	Infinity	41.4316	9.0857
812.86	0.00	0.0000	812.86	Infinity	91.6956	-6.9501
848.45	0.00	0.0000	848.45	Infinity	38.8618	-5.8400
969.24	0.00	0.0000	969.24	Infinity	13.6885	37.1638
1017.60	0.00	0.0000	1017.60	Infinity	20.3003	10.1643
1069.11	0.00	0.0000	1069.11	Infinity	56.7976	-109.2777
1123.12	0.00	0.0000	1123.12	Infinity	239.0357	7.4942
1136.35	0.00	0.0000	1136.35	Infinity	6.5750	21.0452
1221.84	0.00	0.0000	1221.84	Infinity	9.1590	54.6346
1266.86	0.00	0.0000	1266.86	Infinity	7.3574	28.1088
1293.22	0.00	0.0000	1293.22	Infinity	19.2675	-1.5415
1368.18	0.00	0.0000	1368.18	Infinity	3.3448	-16.8850
1374.16	0.00	0.0000	1374.16	Infinity	27.6859	17.9670
1430.02	0.00	0.0000	1430.02	Infinity	11.1994	11.5187
1619.61	0.00	0.0000	1619.61	Infinity	35.5067	17.2627
1747.14	0.00	0.0000	1747.14	Infinity	270.2115	84.1978
2602.04	0.00	0.0000	2602.04	Infinity	1.8488	-1.6135
2959.36	0.00	0.0000	2959.36	Infinity	6.5527	2.2177
2970.44	0.00	0.0000	2970.44	Infinity	7.7002	-7.3664
3019.05	0.00	0.0000	3019.05	Infinity	2.7555	-4.3167
3337.51	0.00	0.0000	3337.51	Infinity	1.7898	0.9696
3430.26	0.00	0.0000	3430.26	Infinity	6.5724	1.8198
3567.16	0.00	0.0000	3567.16	Infinity	65.9900	0.7632

Conformer 14

CONVERGED GEOMETRY			
Coordinates (Angstroms)			
	X	Y	Z
n	0.74500700631241	-1.33644192862881	-0.37299733136882
h	1.58869834326948	-1.25717679703520	0.19279522534488
c	0.02435821429090	-0.07315617456873	-0.34838003287928
h	-0.67633544662535	-0.06241906049337	-1.19281892068434
c	-0.79427847997160	0.04046812450076	0.95846264352635
c	0.95827497867913	1.15131164153327	-0.44657693490614
h	-0.12108057596783	-0.05483178138228	1.81598563461494
s	-2.13565522500044	-1.20671623976783	1.07120551899564
o	2.11922831708916	1.13029493227976	-0.11712213086133
h	-1.33638066223643	-2.25273319856919	0.77536863028253
h	1.04517309941286	-1.56737204822194	-1.31563874999318
o	0.39644089470191	2.30650314993281	-0.89339949074812
h	-0.52465219322497	2.16893418366133	-1.16064608361561
h	-1.28879827072926	1.01333519675941	1.03376202229249

Calculated	Experimental	Weight	Difference	percent	IR	Raman
52.39	0.00	0.0000	52.39	Infinity	7.8261	7.7523
94.87	0.00	0.0000	94.87	Infinity	6.1383	-11.1110
170.40	0.00	0.0000	170.40	Infinity	7.5124	12.5766
223.48	0.00	0.0000	223.48	Infinity	10.9220	25.5135
235.70	0.00	0.0000	235.70	Infinity	14.4674	-28.3125
302.58	0.00	0.0000	302.58	Infinity	27.2686	-10.8835
327.74	0.00	0.0000	327.74	Infinity	28.1391	-0.3516
378.01	0.00	0.0000	378.01	Infinity	24.6063	4.5746
473.12	0.00	0.0000	473.12	Infinity	92.9646	-7.6851
508.59	0.00	0.0000	508.59	Infinity	3.1039	-9.8797
659.48	0.00	0.0000	659.48	Infinity	16.9222	26.7491
670.11	0.00	0.0000	670.11	Infinity	3.1305	-14.6981
751.31	0.00	0.0000	751.31	Infinity	7.4799	14.6798
791.49	0.00	0.0000	791.49	Infinity	2.8825	14.0602
839.18	0.00	0.0000	839.18	Infinity	68.0497	-9.1334
895.87	0.00	0.0000	895.87	Infinity	75.1541	48.0454
918.13	0.00	0.0000	918.13	Infinity	6.6271	21.8078
990.44	0.00	0.0000	990.44	Infinity	42.5544	-92.0491
1093.48	0.00	0.0000	1093.48	Infinity	24.5862	47.4117
1118.39	0.00	0.0000	1118.39	Infinity	7.0828	-32.4238
1133.97	0.00	0.0000	1133.97	Infinity	13.4106	-34.3366
1224.57	0.00	0.0000	1224.57	Infinity	86.6611	85.5332
1266.58	0.00	0.0000	1266.58	Infinity	225.3767	-17.7507
1285.02	0.00	0.0000	1285.02	Infinity	86.7473	-62.9130
1304.03	0.00	0.0000	1304.03	Infinity	38.4110	-48.9094
1396.35	0.00	0.0000	1396.35	Infinity	2.3088	24.2830
1442.99	0.00	0.0000	1442.99	Infinity	6.3012	-5.9830
1633.44	0.00	0.0000	1633.44	Infinity	39.4018	21.3126
1784.31	0.00	0.0000	1784.31	Infinity	262.8771	-12.0656
2588.69	0.00	0.0000	2588.69	Infinity	4.5207	1.5154
2923.74	0.00	0.0000	2923.74	Infinity	12.2386	11.7489
2942.85	0.00	0.0000	2942.85	Infinity	14.2791	-22.4243
2994.12	0.00	0.0000	2994.12	Infinity	7.1873	17.7890
3334.28	0.00	0.0000	3334.28	Infinity	6.6276	-6.4214
3419.49	0.00	0.0000	3419.49	Infinity	11.1595	11.5445
3612.13	0.00	0.0000	3612.13	Infinity	42.2517	2.8492

Conformer 15 (differs only in the CCSH conformation from conformer 14)

$$\Delta G^{\circ}_{0\text{K}}(\text{B3LYP}) = 38.1 \text{ kJ mol}^{-1}$$

CONVERGED GEOMETRY			
Coordinates (Angstroms)			
	X	Y	Z
n	0.79256410286923	-1.43797635420607	-0.53485548895416
h	1.59829884435350	-1.45647863304359	0.08735476280483
c	0.10931963216791	-0.16236311521624	-0.42552039670327
h	-0.62471508824629	-0.10344866087076	-1.23990211084857
c	-0.64908577908280	-0.08685534423369	0.91340845988663
c	1.05892352711834	1.05395242986386	-0.50981486951036
h	0.06562144401143	-0.16983979985434	1.73775683927144
s	-1.88284439872768	-1.45948081289602	1.01521465528293
o	2.21820994944593	1.01647896107680	-0.17781587198149
h	-2.76096804048416	-0.78379371035858	1.78506411610033
h	1.13949757749370	-1.59051762812506	-1.47736262888763
o	0.51281569718599	2.21962529068294	-0.95268761579141
h	-0.40692163844963	2.09189199638689	-1.22903800820002
h	-1.17071582965546	0.86880538079382	1.00819815753075

Calculated	Experimental	Weight	Difference	percent	IR	Raman
41.88	0.00	0.0000	41.88	Infinity	5.4995	3.7895
83.14	0.00	0.0000	83.14	Infinity	2.2020	-11.8462
164.99	0.00	0.0000	164.99	Infinity	6.8992	6.0259
173.72	0.00	0.0000	173.72	Infinity	58.1755	17.8579
227.36	0.00	0.0000	227.36	Infinity	13.2418	-22.9925
244.71	0.00	0.0000	244.71	Infinity	9.3227	24.8266
302.37	0.00	0.0000	302.37	Infinity	13.9190	-17.1198
367.15	0.00	0.0000	367.15	Infinity	19.5215	-16.0285
473.72	0.00	0.0000	473.72	Infinity	91.2295	-11.0578
507.01	0.00	0.0000	507.01	Infinity	3.3045	-9.4700
657.13	0.00	0.0000	657.13	Infinity	19.8037	1.4155
678.01	0.00	0.0000	678.01	Infinity	0.8260	17.2044
781.05	0.00	0.0000	781.05	Infinity	5.2650	12.4405
799.20	0.00	0.0000	799.20	Infinity	1.9684	-5.5671
833.63	0.00	0.0000	833.63	Infinity	95.5208	-14.9775
891.15	0.00	0.0000	891.15	Infinity	59.1811	51.2162
951.87	0.00	0.0000	951.87	Infinity	12.6273	-16.8854
972.14	0.00	0.0000	972.14	Infinity	36.3744	-15.4981
1090.57	0.00	0.0000	1090.57	Infinity	32.7679	55.1642
1104.71	0.00	0.0000	1104.71	Infinity	3.6538	-10.8607
1130.65	0.00	0.0000	1130.65	Infinity	11.1886	-47.2995
1228.32	0.00	0.0000	1228.32	Infinity	121.7346	107.9356
1262.24	0.00	0.0000	1262.24	Infinity	182.1305	-62.9811
1287.16	0.00	0.0000	1287.16	Infinity	76.3581	-40.6530
1308.48	0.00	0.0000	1308.48	Infinity	54.5653	-70.6851
1395.26	0.00	0.0000	1395.26	Infinity	1.9084	17.7958
1449.96	0.00	0.0000	1449.96	Infinity	6.0878	-4.8840
1635.22	0.00	0.0000	1635.22	Infinity	38.7946	17.2278
1786.74	0.00	0.0000	1786.74	Infinity	257.5002	0.6669
2586.89	0.00	0.0000	2586.89	Infinity	17.6983	-4.0354
2916.87	0.00	0.0000	2916.87	Infinity	15.6312	10.0597
2943.14	0.00	0.0000	2943.14	Infinity	15.0861	-14.8849
2997.72	0.00	0.0000	2997.72	Infinity	7.5790	17.5837
3339.18	0.00	0.0000	3339.18	Infinity	5.3000	-4.7078
3423.68	0.00	0.0000	3423.68	Infinity	9.1491	9.5881
3612.69	0.00	0.0000	3612.69	Infinity	40.4964	3.5807

Conformer 16 (differs only in the CCSH conformation from conformer 14)

$$\Delta G^{\circ}_{0\text{K}}(\text{B3LYP}) = 37.7 \text{ kJ mol}^{-1}$$

CONVERGED GEOMETRY			
Coordinates (Angstroms)			
	X	Y	Z
n	0.91856032462270	-1.40673124623805	-0.40154984888526
h	1.60060804812202	-1.41517005919805	0.35437465168868
c	0.19056153482496	-0.15151713506040	-0.40045777468704
h	-0.38269175236353	-0.09466495517025	-1.33510042053301
c	-0.80272688009318	-0.12187918665636	0.77713870242648
c	1.10394489689200	1.09002581623773	-0.28944318629504
h	-0.24936852895448	-0.20519463775821	1.71738179202544
s	-1.99674224430161	-1.52486946244266	0.62891998237350
o	2.18324556531463	1.07524740730522	0.24945843790118
h	-3.01921703537652	-0.88559825708269	1.23404088350046
h	1.43216789042437	-1.53421410037394	-1.26864265128138
o	0.61466496875634	2.25048190636964	-0.80641245940093
h	-0.23449156170665	2.10504280486843	-1.24956667883047
h	-1.35851522616108	0.81904110519956	0.78985856999735

Calculated	Experimental	Weight	Difference	percent	IR	Raman
42.42	0.00	0.0000	42.42	Infinity	5.2825	3.9862
82.17	0.00	0.0000	82.17	Infinity	2.2588	-11.6544
164.73	0.00	0.0000	164.73	Infinity	6.1001	2.4491
173.48	0.00	0.0000	173.48	Infinity	58.6209	22.3908
227.47	0.00	0.0000	227.47	Infinity	12.9114	-21.7316
243.63	0.00	0.0000	243.63	Infinity	9.6512	21.9427
301.26	0.00	0.0000	301.26	Infinity	13.8962	-16.3959
366.80	0.00	0.0000	366.80	Infinity	19.4009	-16.6077
476.50	0.00	0.0000	476.50	Infinity	91.2136	-7.7106
505.80	0.00	0.0000	505.80	Infinity	3.9678	-11.7862
656.96	0.00	0.0000	656.96	Infinity	19.9197	0.3362
677.81	0.00	0.0000	677.81	Infinity	0.8551	17.4333
780.95	0.00	0.0000	780.95	Infinity	5.5098	12.8861
798.78	0.00	0.0000	798.78	Infinity	1.8459	-5.6275
832.76	0.00	0.0000	832.76	Infinity	95.7175	-15.8450
890.45	0.00	0.0000	890.45	Infinity	59.1080	51.9329
951.44	0.00	0.0000	951.44	Infinity	11.9719	-16.1180
972.09	0.00	0.0000	972.09	Infinity	36.9213	-15.9869
1089.97	0.00	0.0000	1089.97	Infinity	32.6041	55.1609
1103.96	0.00	0.0000	1103.96	Infinity	3.8621	-10.3044
1130.27	0.00	0.0000	1130.27	Infinity	11.3069	-47.7419
1227.20	0.00	0.0000	1227.20	Infinity	112.5436	105.6524
1261.02	0.00	0.0000	1261.02	Infinity	184.5831	-58.2377
1286.63	0.00	0.0000	1286.63	Infinity	83.0559	-45.0627
1307.07	0.00	0.0000	1307.07	Infinity	54.3284	-69.6277
1394.42	0.00	0.0000	1394.42	Infinity	1.9344	18.0111
1448.49	0.00	0.0000	1448.49	Infinity	6.0716	-4.9055
1634.84	0.00	0.0000	1634.84	Infinity	38.7693	17.4059
1786.53	0.00	0.0000	1786.53	Infinity	257.4459	0.7747
2587.23	0.00	0.0000	2587.23	Infinity	17.6123	-4.0665
2916.98	0.00	0.0000	2916.98	Infinity	15.5652	10.1356
2943.31	0.00	0.0000	2943.31	Infinity	15.0577	-14.8717
2997.93	0.00	0.0000	2997.93	Infinity	7.5676	17.6839
3339.35	0.00	0.0000	3339.35	Infinity	5.3549	-4.8128
3423.88	0.00	0.0000	3423.88	Infinity	9.2340	9.7063
3612.52	0.00	0.0000	3612.52	Infinity	40.5362	3.5928

Table S2. Alternative assignments of bands that decrease more intensively during 6953 cm^{-1} and less intensively during 6938 cm^{-1} laser NIR irradiation. (Wavenumbers are in cm^{-1} .)

$\bar{\nu}$ exp. (Ar-matrix)	$\bar{\nu}$ comp. (SQM B3LYP/6-311++G**) – $\bar{\nu}$ exp. Conf. 3.	Conf. 5	Conf. 7
679.8	8.8	–53.4	–61.8
788.6	–2.6	–16.6	–60.2
819.6	14.9	12.6	28.3
897.9	–0.4	–9.9	–11.4
996.7	–5.1	29.1	25.4
1107.6	–9.7	–7.1	–3.5
1121.2	0.9	0.4	–0.8
1147.5	–7.6	12.3	30.5
1235.4	–10.4	36.7	29.8
1335.1	–14.9	1.9	–6.2
1769.0	–16.8	–8.6	–7.9
2583.3	5.1	8.2	12.3
2915.4	22.3	–26.6	–6.2
2955.8	7.5	16.9	14.0
3405.3	19.1	12.6	14.3
3562.5	3.4	4.3	8.6
RMS error	11.3	21.1	26.9

Table S3. Alternative assignments of bands that decrease more intensively during 6938 cm^{-1} and less intensively during 6953 cm^{-1} laser NIR irradiation. (Wavenumbers are in cm^{-1} .)

$\bar{\nu}$ exp. (Ar-matrix)	$\bar{\nu}$ comp. (SQM B3LYP/6-311++G**) – $\bar{\nu}$ exp. Conf. 3.	Conf. 5	Conf. 7
618.1	–33.3	8.3	–0.1
733.4	–44.8	–11.6	–5.0
769.5	16.5	2.5	–28.0
832.1	2.4	0.1	15.8
876.0	21.5	12.0	10.5
1023.1	–31.5	2.7	–1.0
1107.3	–9.4	–6.8	–3.2
1137.5	–15.4	–15.9	–17.1
1148.8	–8.9	11.0	29.2
1344.0	–23.8	–7.0	–15.1
1766.1	–13.9	–5.7	–5.0
2612.3	–23.9	–20.8	–16.7
2894.4	43.3	–5.6	14.8
3420.4	4.0	–2.5	–0.8
3555.3	10.6	11.5	15.8
RMS error	23.9	9.9	14.9

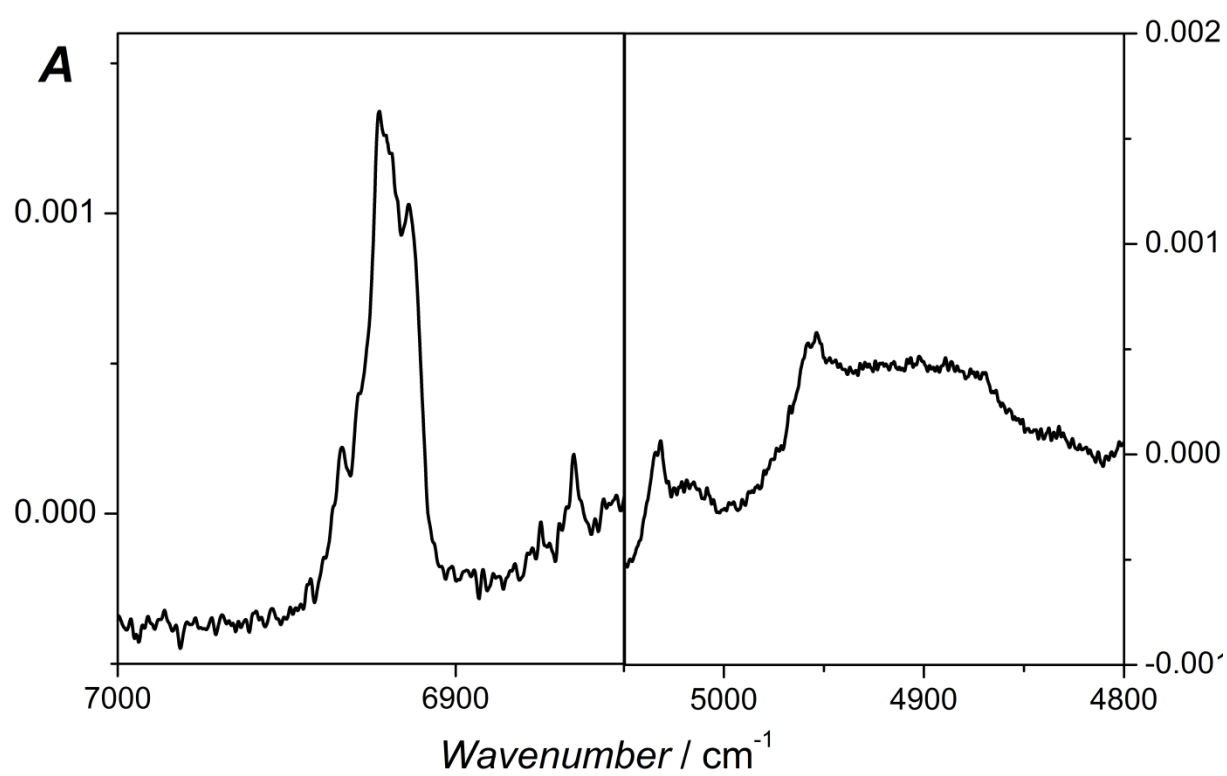


Figure S1. NIR spectrum of cysteine in Kr matrix.

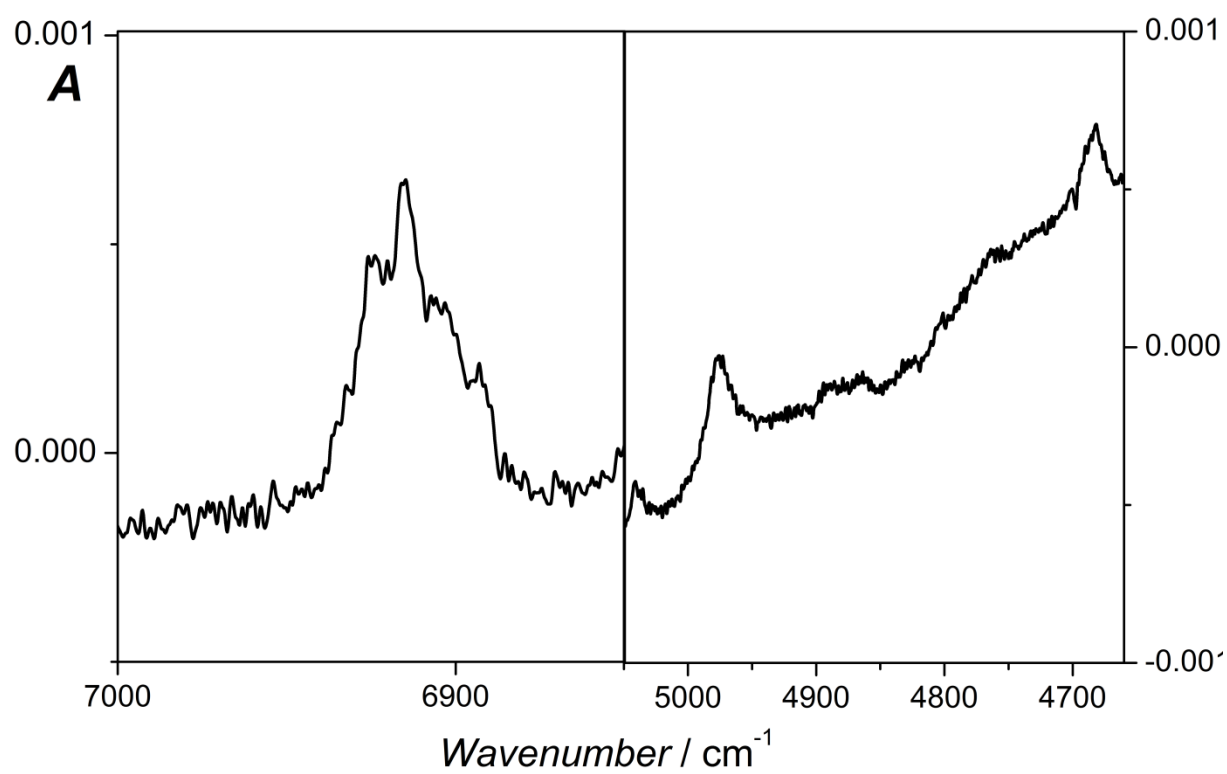


Figure S2. NIR spectrum of cysteine in N₂ matrix.

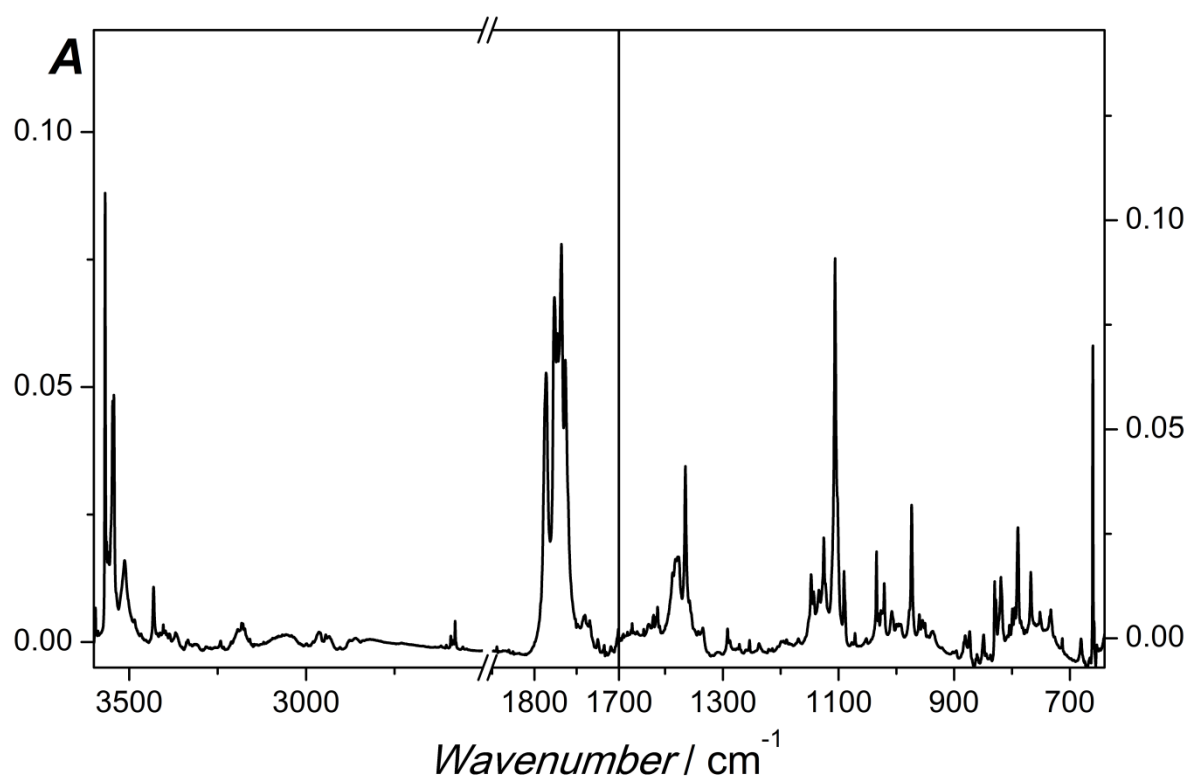


Figure S3. MIR spectrum of cysteine in Kr matrix.

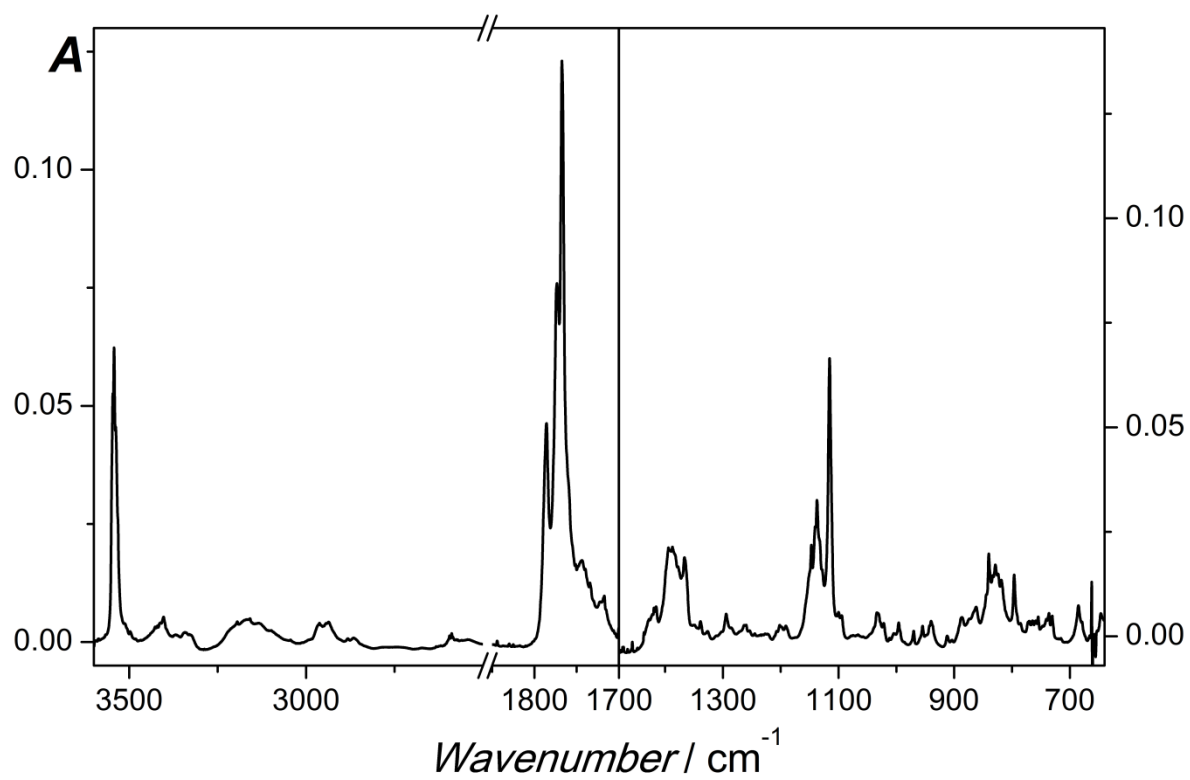


Figure S4. MIR spectrum of cysteine in N₂ matrix.

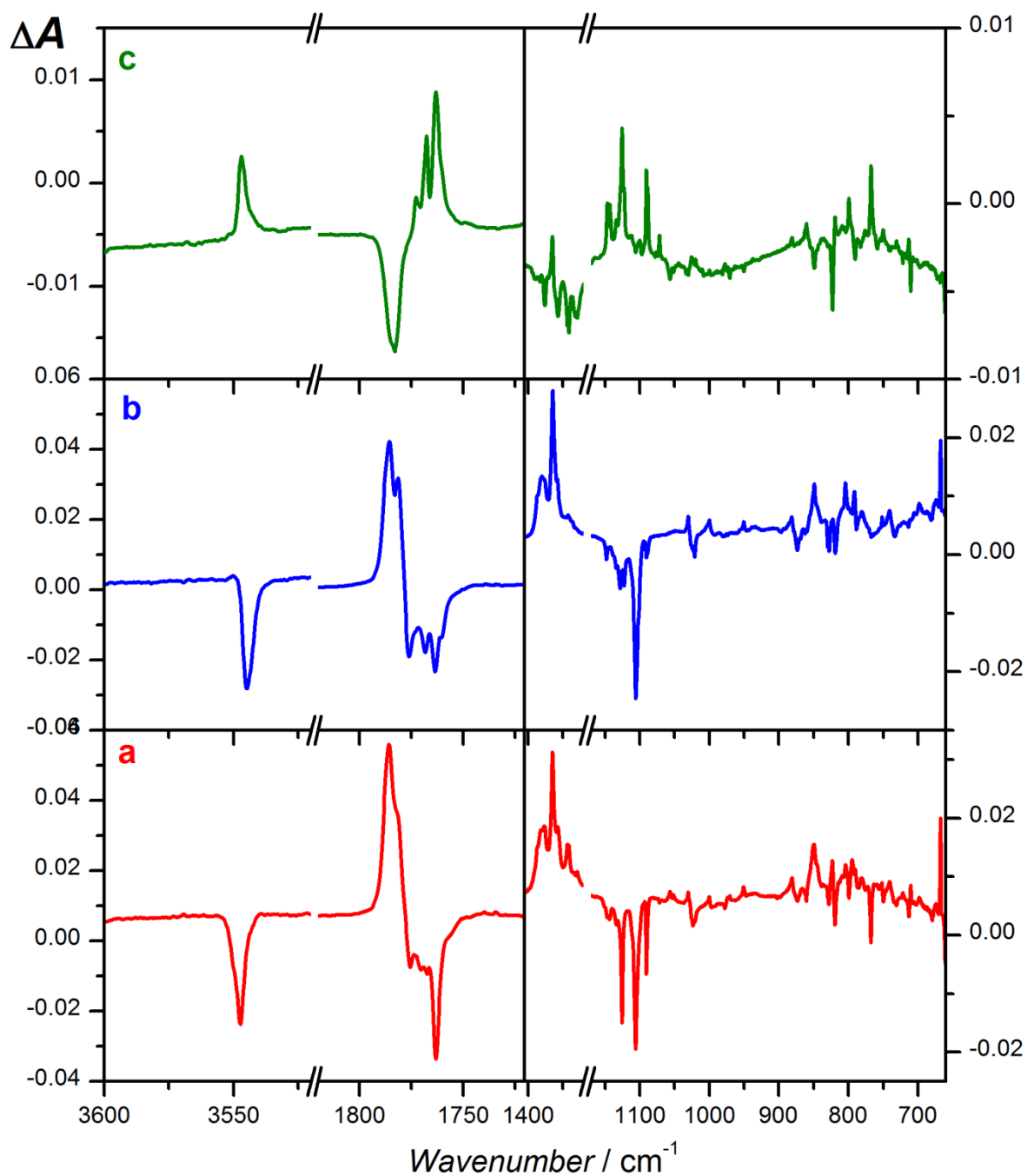


Figure S5. Difference MI-MIR spectra of cysteine in Kr matrix as obtained by subtracting the spectrum recorded before irradiation from the spectrum recorded after irradiation at 6925 cm^{-1} (a), at 6916 cm^{-1} (b), and at 6892 cm^{-1} (c).

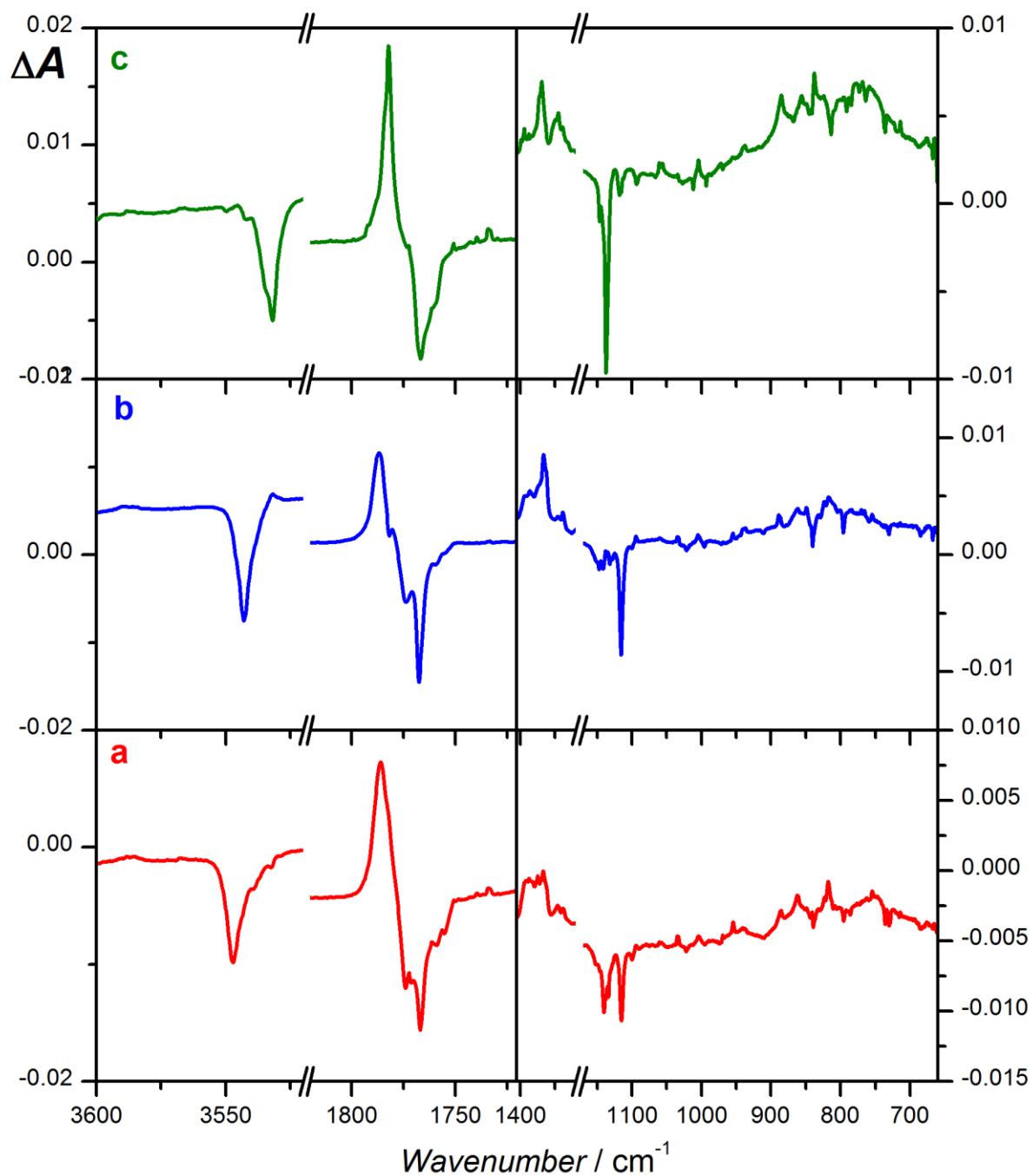


Figure S6. Difference MI-MIR spectra of cysteine in N₂ matrix as obtained by subtracting the spectrum recorded before irradiation from the spectrum recorded after irradiation at 6923 cm⁻¹ (a), at 6914 cm⁻¹ (b), and at 6588 cm⁻¹ (c).