

Jet-cooled rovibrational spectroscopy of methoxyphenols using two complementary FTIR and QCL based spectrometers

P. Asselin,¹ J. Bruckhuisen,¹ A. Roucou,^{2, a)} M. Goubet,³ M. A. Martin-Drumel,⁴
A. Jabri,^{2, b)} Y. Belkhodja,¹ P. Soulard,¹ R. Georges,⁵ and A. Cuisset^{2, c)}

¹⁾*Laboratoire MONARIS, UMR-CNRS 8233, Sciences Sorbonne université, Paris, Université Pierre et Marie Curie, 75252, Paris, France.*

²⁾*Laboratoire de Physico-Chimie de l'Atmosphère, EA-4493, Université du Littoral Côte d'Opale, 59140 Dunkerque, France.*

³⁾*Université Lille, CNRS, UMR8523 PhLAM Physique des Lasers Atomes et Molécules, F-59000 Lille, France*

⁴⁾*Institut des Sciences Moléculaires d'Orsay (ISMO), CNRS, Univ. Paris-Sud, Université Paris-Saclay, F-91405 Orsay, France*

⁵⁾*Univ Rennes, CNRS, IPR (Institut de Physique de Rennes) - UMR 6251, F-35000 Rennes, France.*

(Dated: 8 November 2019)

^{a)}Present address: Faculté des sciences, Institute of Condensed Matter and Nanosciences, Louvain la Neuve, Belgium

^{b)}Present address: Grupo de Espectroscopia Molecular, Universidad de Valladolid, Spain

^{c)}Electronic mail: arnaud.cuisset@univ-littoral.fr

I. SUPPLEMENTARY FIGURES

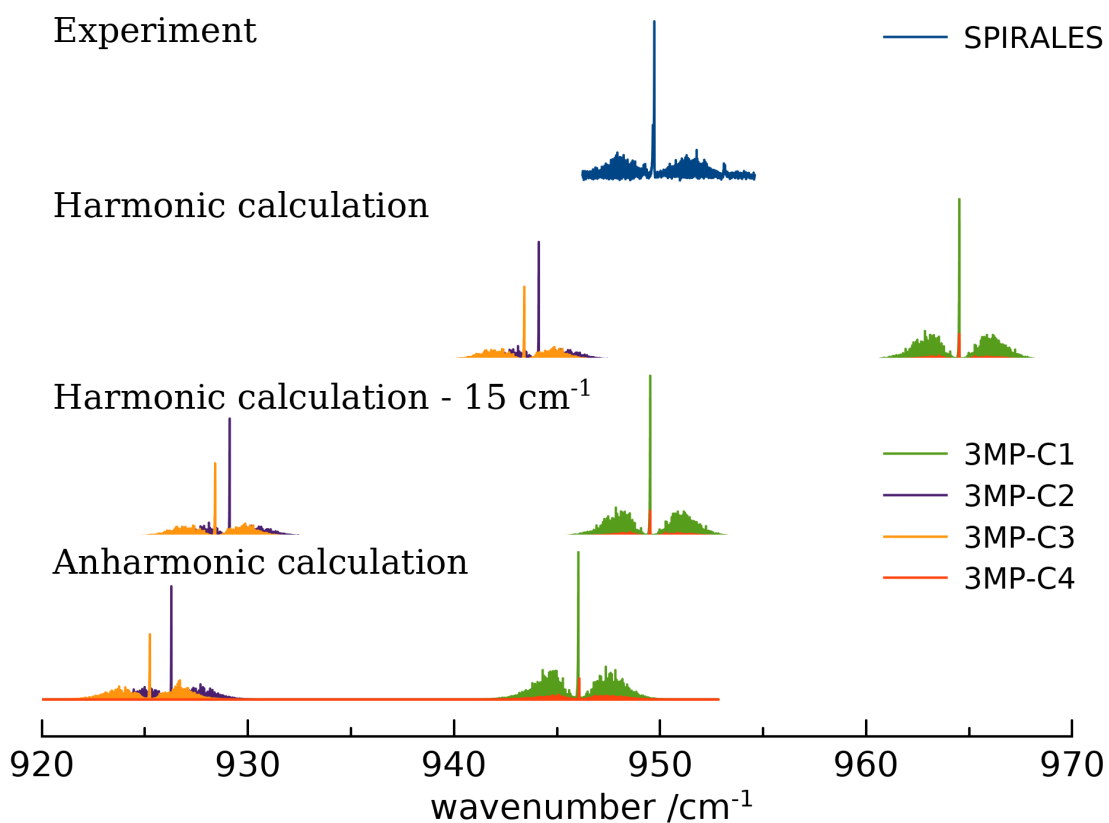


FIG. S1: SPIRALES spectrum of 3MP in the ν_{18} band region and comparison with simulations from the harmonic, shifted harmonic, and anharmonic calculations. The relative abundances are taken into account and the predicted (harmonic) intensities of 3MP-C1 is used for all conformers.

The shifted harmonic simulation (rather than a conventional scaling) serves as visual aid to identify experimental spacing between conformers and compare it in the experiment and calculation.

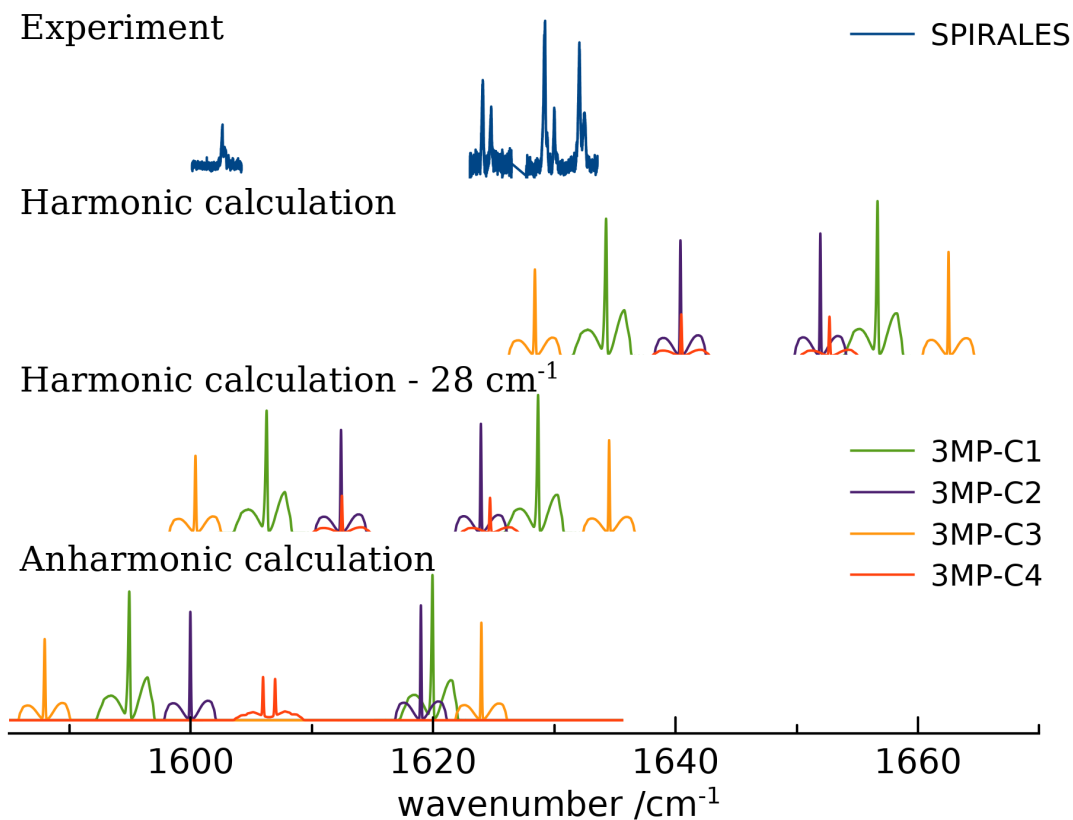


FIG. S2: SPIRALES spectrum of 3MP in the ν_{36} and ν_{37} bands region and comparison with simulations from the harmonic, shifted harmonic, and anharmonic calculations. The relative abundances are taken into account and the predicted (harmonic) intensities of 3MP-C1 is used for all conformers. The shifted harmonic simulation (rather than a conventional scaling) serves as visual aid to identify experimental spacing between conformers and compare it in the experiment and calculation.

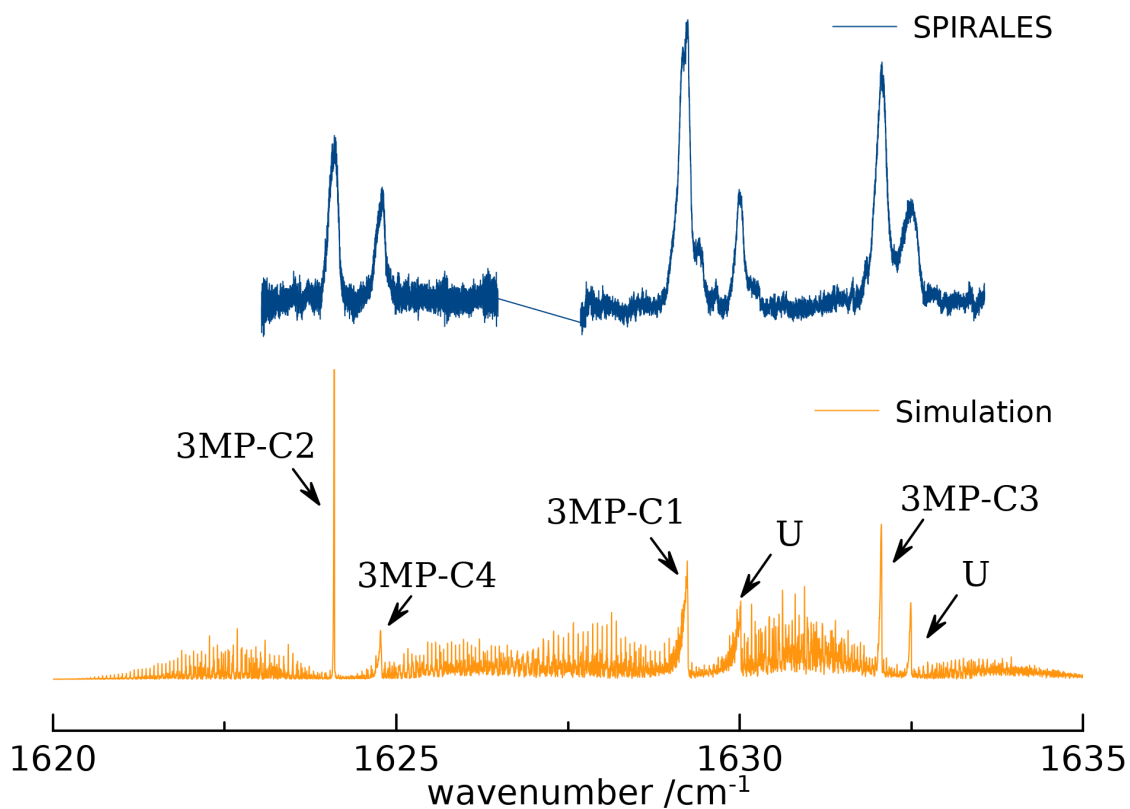


FIG. S3: SPIRALES spectrum of 3MP in the ν_{37} bands region and comparison with a simulation of the expected spectrum at high resolution using the parameters optimized for the ν_{18} band (30 K temperature and 0.004 cm^{-1} FWHM). Experimental ground state constants and scaled upper state constants of 3MP-C1 to 3MP-C4 have been used. Band centers of the four conformers were taken from the attribution of this work while their relative intensities is a function of their abundances. To reflect the high density of modes, the two bands non assigned in this work (indicated by a U), presumably hot bands, are also simulated using the spectroscopic parameters of the closest band in frequency. Despite the high density of lines, the rotational structure should have been resolved.

II. SUPPLEMENTARY TABLES

TABLE S1: B3LYP/cc-pVTZ calculations on 2MP-C1: Harmonic and anharmonic frequencies in cm^{-1} and intensities in km/mol , symmetry, excited state rotational constants in cm^{-1} . The designation of the mode is obtained with the GAUSSVIEW6 software.

mode	ν_{harm}	I_{harm}	ν_{anharm}	I_{anharm}	symmetry	designation	A	B	C
1	77	3.43	76.19	3.03	A''	-OCH ₃ out-of-plane bending	0.086884	0.051414	0.032571
2	178.62	0.29	105.84	0.00	A''	-OCH ₃ torsion	0.086842	0.051378	0.032534
3	224.26	1.14	216.68	1.00	A'	-OCH ₃ in-plane bending	0.087142	0.051409	0.032494
4	236.68	0.36	265.25	0.27	A''	-OCH ₃ torsion	0.087028	0.051304	0.032506
5	309.29	0.23	319.11	0.57	A''	-CH/-CO out-of-plane bending	0.086914	0.051396	0.032536
6	343.67	4.84	336.6	4.16	A'	intramolecular stretching	0.086921	0.051441	0.032509
7	446.89	73.16	312.98	65.75	A''	-OH out-of-plane bending	0.086781	0.051442	0.032526
8	472.21	19.33	573.59	7.59	A''	-OH out-of-plane bending	0.08686	0.051436	0.032534
9	510.27	0.98	503.84	0.73	A'	intramolecular stretching	0.086965	0.051426	0.032509
10	537.71	9.51	528.72	8.35	A'	-OH in-plane bending	0.086945	0.051429	0.032506
11	579.81	0.39	574.25	0.33	A''	-CH out-of-plane bending	0.086894	0.05142	0.032534
12	597.61	3.30	588.25	3.33	A'	ring deformation	0.086949	0.051426	0.032535
13	733.66	0.01	747.52	0.02	A''	-CH/-CO out-of-plane bending	0.086893	0.051415	0.03253
14	756.18	73.10	745.99	67.33	A''	-CH out-of-plane bending	0.086906	0.051421	0.032533
15	771.44	25.49	756.72	20.72	A'	ring deformation	0.086898	0.051395	0.032497
16	849.54	6.49	831.77	4.75	A'	ring deformation	0.086919	0.051418	0.032509
17	856.93	0.08	847.42	0.19	A''	-CH out-of-plane bending	0.086895	0.051421	0.03253
18	931.81	5.73	921.79	4.74	A''	-CH out-of-plane bending	0.086905	0.051407	0.032529
19	970.47	0.08	982.62	0.08	A''	-CH out-of-plane bending	0.086865	0.051409	0.032527
20	1051.86	33.24	1027.24	22.62	A'	ring deformation	0.086901	0.051399	0.032501
21	1068.12	42.24	1045.25	18.11	A'	ring deformation	0.086898	0.05138	0.032489
22	1133.89	31.94	1113.44	23.39	A'	-CH in-plane bending	0.086941	0.051398	0.032512
23	1176.79	0.90	1150.74	0.14	A''	-CH ₃ wagging	0.086831	0.051381	0.03251
24	1183.41	1.80	1168.39	1.71	A'	-CH in-plane bending	0.086941	0.051398	0.032512
25	1199.01	15.52	1170.21	12.44	A'	-OH/OCH in-plane bending	0.086962	0.051411	0.032505
26	1230.99	55.98	1209.08	57.10	A'	-OH/OCH in-plane bending	0.086896	0.051417	0.032509
27	1252.11	181.45	1219.11	127.01	A'	C-O stretching	0.086818	0.051374	0.032471
28	1288.58	201.60	1256.81	141.24	A'	C-O stretching	0.086799	0.051393	0.032486
29	1335.02	6.78	1306.99	8.58	A'	-CH in-plane bending	0.086862	0.051404	0.032511
30	1401.38	48.73	1367.13	27.80	A'	-OH in-plane bending	0.086828	0.051395	0.032501
31	1481.71	16.17	1444.29	27.60	A'	-CH ₃ scissoring	0.08691	0.051412	0.032464
32	1492.87	7.55	1448.45	6.34	A''	-CH ₃ scissoring	0.086949	0.051415	0.032526
33	1503.55	5.98	1464.23	9.48	A'	-CH in-plane bending	0.086902	0.051406	0.032527
34	1511.09	33.66	1475.23	16.21	A'	-CH ₃ scissoring	0.086904	0.05142	0.032526
35	1539.1	169.69	1501.19	109.38	A'	-CH in-plane bending	0.08687	0.051388	0.032528
36	1637.38	27.97	1597.7	13.64	A'	C-C stretching	0.086807	0.051383	0.032488
37	1653.01	9.93	1609.73	7.94	A'	C-C stretching	0.086965	0.051426	0.032509
38	3008.71	49.82	2819.48	17.56	A'	-CH ₃ stretching	0.086919	0.051431	0.032529
39	3065.41	34.29	2930.84	33.53	A''	-CH ₃ stretching	0.086927	0.051437	0.032531
40	3129.52	19.54	2990.96	22.97	A'	-CH ₃ stretching	0.086939	0.051414	0.032523
41	3171.78	0.57	3018.8	1.05	A'	C-H stretching	0.086907	0.051419	0.03252
42	3184.59	13.82	3039.68	6.80	A'	C-H stretching	0.086905	0.051415	0.032518
43	3194.78	14.69	3057.61	10.63	A'	C-H stretching	0.086904	0.051413	0.032517
44	3204.15	5.82	3107.01	6.42	A'	C-H stretching	0.086943	0.05138	0.03251
45	3767.16	90.80	3581.45	79.89	A'	O-H stretching	0.087	0.051412	0.03253

TABLE S2: B3LYP/cc-pVTZ calculations on 3MP-C1: Harmonic and anharmonic frequencies in cm^{-1} and intensities in km/mol , symmetry, excited state rotational constants in cm^{-1} . The designation of the mode is obtained with the GAUSSVIEW6 software.

mode	ν_{harm}	I_{harm}	ν_{anharm}	I_{anharm}	symmetry	designation	A	B	C
1	95.93	6.3033	87.34	5.6519	A''	-OCH ₃ out-of-plane bending	0.094866	0.042901	0.02976
2	199.18	0.4844	114.79	0.4732	A''	-CH ₃ torsion	0.094721	0.042894	0.029732
3	220.59	4.3329	216.26	3.9184	A'	-OCH ₃ in-plane bending	0.09488	0.04291	0.029749
4	238.21	0.9637	236.02	0.1359	A''	-COH out-of-plane bending	0.094917	0.042857	0.029715
5	269.39	0.5992	302.15	39.7591	A''	-CH ₃ torsion	0.094757	0.042915	0.029729
6	354.82	94.9	377.3	51.731	A''	-OH out-of-plane bending	0.094875	0.04293	0.029747
7	402.2	4.119	400.34	3.2704	A'	-OCH ₃ /OH in-plane bending	0.095005	0.042919	0.029717
8	468.2	1.3948	463.48	1.4711	A''	-CH out-of-plane bending	0.094875	0.04293	0.029747
9	477.61	0.0635	473.32	0.0595	A'	-OH in-plane bending	0.094892	0.042941	0.029723
10	538.79	1.9675	533.58	1.9226	A'	ring deformation	0.094882	0.042934	0.029729
11	562.12	9.8807	559.14	7.7813	A'	-OCH ₃ in-plane bending	0.094926	0.04292	0.029733
12	633.65	1.1426	623.32	0.8832	A''	-CH out-of-plane bending	0.09489	0.042939	0.029744
13	701	22.2057	689.96	32.7224	A''	-CH out-of-plane bending	0.094802	0.042932	0.02974
14	742.78	0.7363	734.11	1.7311	A'	ring deformation	0.094885	0.042932	0.029726
15	770.73	38.3029	769.25	12.3118	A''	-CH out-of-plane bending	0.094853	0.042937	0.029742
16	859.25	9.2833	847.86	39.629	A''	-CH out-of-plane bending	0.09484	0.042935	0.029743
17	863.4	25.8496	857.24	3.5615	A''	-CH out-of-plane bending	0.094837	0.042933	0.029743
18	964.53	72.7129	946.04	59.6605	A'	ring deformation	0.094864	0.042886	0.029698
19	970.99	0.0563	977.72	0.6348	A''	-CH out-of-plane bending	0.094818	0.042923	0.029738
20	1012.36	0.0099	997.2	0.0441	A'	ring deformation	0.094868	0.042925	0.029721
21	1065.91	45.6977	1040.36	46.1394	A'	ring deformation	0.094743	0.042913	0.029702
22	1103.91	4.8646	1084.9	3.5667	A'	-CH in-plane bending	0.094827	0.042948	0.029736
23	1174.38	1.0323	1149.06	0.6155	A''	-CH ₃ rocking	0.094809	0.042906	0.029725
24	1174.95	155.9033	1146.86	156.9668	A'	-CH in-plane bending	0.094866	0.042919	0.029717
25	1183.26	41.9703	1156.56	110.8015	A'	-CH in-plane bending	0.094841	0.042936	0.029726
26	1206.41	47.9688	1177.81	40.0247	A'	-CH ₃ wagging OH in-plane bending	0.094849	0.04294	0.029724
27	1236.72	73.767	1220.71	36.8771	A'	-CH ₃ wagging CH in-plane bending	0.09482	0.042908	0.029712
28	1317.43	109.2954	1288.39	88.821	A'	C-O sym stretching	0.094762	0.042894	0.029665
29	1337.45	47.0274	1311.48	12.5323	A'	-CH in-plane bending	0.094861	0.042931	0.029746
30	1365.73	43.4207	1332.13	39.8203	A'	C-C stretching	0.094732	0.042888	0.029711
31	1474.17	26.4995	1434.55	8.0811	A'	-CH ₃ wagging	0.094441	0.042909	0.029693
32	1495.01	7.0917	1453.5	5.9472	A''	-CH ₃ twisting	0.095247	0.042943	0.029736
33	1505.03	25.4955	1464.73	12.2775	A'	-CH ₃ scissoring	0.094865	0.042929	0.029768
34	1517.76	23.1105	1484.62	6.2097	A'	C-C stretching	0.09492	0.042901	0.029718
35	1529.66	98.1127	1501.36	64.2865	A'	C-C stretching	0.094804	0.042924	0.029717
36	1634.33	138.0243	1595	86.4605	A'	C-C stretching	0.094733	0.042903	0.02963
37	1656.71	139.1321	1619.77	63.2536	A'	C-C stretching	0.094797	0.042881	0.029772
38	3005.24	48.5241	2820.01	17.5962	A'	C-H stretching	0.094887	0.042934	0.029739
39	3060.76	36.8785	2927.47	34.7226	A''	C-H stretching	0.094905	0.042935	0.02974
40	3127.96	22.0128	2991.85	24.7011	A'	C-H stretching	0.094898	0.042923	0.029733
41	3158.35	11.481	3017.44	7.2387	A''	C-H stretching	0.094864	0.042928	0.029732
42	3178.16	13.9603	3044.77	3.5555	A'	C-H stretching	0.094847	0.042932	0.029732
43	3202.11	4.6043	3077.93	11.0676	A'	C-H stretching	0.094846	0.04293	0.029731
44	3218.98	1.4948	3088.28	0.0423	A'	C-H stretching	0.094905	0.042878	0.029711
45	3818.3	60.0147	3640.17	48.6092	A'	O-H stretching	0.094857	0.042935	0.029734

TABLE S3: B3LYP/cc-pVTZ calculations on 3MP-C2: Harmonic and anharmonic frequencies in cm^{-1} and intensities in km/mol , symmetry, excited state rotational constants in cm^{-1} . The designation of the mode is obtained with the GAUSSVIEW6 software.

mode	ν_{harm}	I_{harm}	ν_{anharm}	I_{anharm}	symmetry	designation	A	B	C
1	87.32	3.2096	80.23	3.1356 A''	-OCH ₃ out-of-plane bending	0.120293	0.037381	0.028727	
2	205.08	0.8076	111.55	0.307 A''	-CH ₃ torsion	0.120579	0.037327	0.028688	
3	235.62	0.2269	230.88	0.2333 A'	-OCH ₃ in-plane bending	0.120504	0.037368	0.028714	
4	236.64	2.7613	230.32	2.5528 A''	-COH out-of-plane bending	0.120962	0.037362	0.028674	
5	268.69	1.6595	309.92	41.4309 A''	-CH ₃ torsion	0.120612	0.037326	0.028682	
6	360.77	98.0436	359.32	52.6936 A''	-OH out-of-plane bending	0.120639	0.037334	0.028689	
7	367.64	2.0736	363.02	1.43 A'	-OCH ₃ /-OH in-plane bending	0.12081	0.037354	0.02868	
8	467.65	7.302	460.9	6.8503 A''	-CH out-of-plane bending	0.120713	0.037353	0.028705	
9	477.39	12.3462	473.82	11.059 A'	-OH in-plane bending	0.120847	0.03735	0.028687	
10	532.68	6.1279	527.9	6.014 A'	ring deformation	0.120706	0.037358	0.028687	
11	589.6	8.7477	583	8.4175 A'	-OCH ₃ in-plane bending	0.120779	0.037347	0.028689	
12	635.33	0.0115	622.95	0.0046 A''	-CH out-of-plane bending	0.120718	0.037358	0.028701	
13	700.96	20.0964	688.82	25.8631 A''	-CH out-of-plane bending	0.120639	0.037351	0.028698	
14	749.1	5.4641	740.34	2.4894 A'	ring deformation	0.120699	0.037348	0.028683	
15	775.53	25.5884	759.42	8.9632 A''	-CH out-of-plane bending	0.120712	0.037354	0.0287	
16	851.72	43.4325	845.51	44.2859 A''	-CH out-of-plane bending	0.1207	0.037349	0.0287	
17	869.01	0.5254	852.08	8.5067 A''	-CH out-of-plane bending	0.120598	0.03736	0.028701	
18	944.12	8.3226	926.59	5.703 A'	ring deformation	0.120699	0.037316	0.028662	
19	976.74	0.1548	972.3	0.34 A''	-CH out-of-plane bending	0.120622	0.037347	0.028695	
20	1013.39	3.3159	999.32	2.8936 A'	ring deformation	0.12072	0.037348	0.028679	
21	1075.76	30.7264	1050.41	30.4626 A'	ring deformation	0.120738	0.037312	0.028656	
22	1104.99	8.4433	1085.63	2.972 A'	-CH in-plane bending	0.120722	0.037342	0.028691	
23	1174.79	1.1257	1149.91	0.7822 A''	-CH ₃ rocking	0.120591	0.037326	0.028681	
24	1178.67	215.3121	1145.68	42.297 A'	-CH in-plane bending	0.120693	0.037344	0.028678	
25	1192.64	27.2715	1166.12	17.4084 A'	-CH in-plane bending	0.120723	0.037341	0.028678	
26	1198.4	53.7219	1178.06	20.3408 A'	-CH ₃ wagging -OH in-plane bending	0.120834	0.037341	0.028678	
27	1227.94	205.9629	1203.08	162.0983 A'	-CH ₃ wagging -CH in-plane bending	0.12068	0.037332	0.028673	
28	1320.09	67.2024	1287.3	44.8956 A'	C-O sym stretching	0.120641	0.037314	0.02864	
29	1350.04	11.82	1319.83	11.316 A'	-CH in-plane bending	0.120706	0.03734	0.028691	
30	1361.42	25.0208	1333.9	10.3887 A'	C-C stretching	0.120545	0.037311	0.028665	
31	1477.83	8.1618	1437.12	20.2445 A'	-CH ₃ wagging	0.120729	0.037342	0.028664	
32	1494.4	7.1668	1452.75	4.6704 A''	-CH ₃ twisting	0.120703	0.037321	0.02866	
33	1496.69	22.5403	1463.8	16.958 A'	-CH ₃ scissoring	0.120691	0.037349	0.028701	
34	1510.36	37.602	1474.19	15.0231 A'	C-C stretching	0.120592	0.037345	0.0287	
35	1540.79	80.2116	1506.33	52.1388 A'	C-C stretching	0.120494	0.037334	0.028666	
36	1640.43	63.3713	1600.24	35.5921 A'	C-C stretching	0.120633	0.037302	0.028655	
37	1651.95	227.5899	1618.74	56.1102 A'	C-C stretching	0.120687	0.03736	0.028697	
38	3005.63	51.0912	2821.1	16.1496 A'	C-H stretching	0.120704	0.037353	0.028693	
39	3061.17	37.6442	2897.73	18.8125 A''	C-H stretching	0.120667	0.037348	0.028687	
40	3127.37	22.0133	2989.24	26.7031 A'	C-H stretching	0.120704	0.037353	0.028693	
41	3168.91	9.4284	3031.95	4.9862 A''	C-H stretching	0.120667	0.037348	0.028687	
42	3172.07	6.9805	3041.32	6.2321 A'	C-H stretching	0.120677	0.037351	0.02869	
43	3202.08	6.1895	3080.13	4.485 A'	C-H stretching	0.120671	0.03735	0.028689	
44	3217.05	5.1735	3094.67	7.5933 A'	C-H stretching	0.120624	0.037335	0.028678	
45	3816.42	55.6427	3637.29	45.0379 A'	O-H stretching	0.120695	0.037351	0.028691	

TABLE S4: B3LYP/cc-pVTZ calculations on 3MP-C3: Harmonic and anharmonic frequencies in cm^{-1} and intensities in km/mol , symmetry, excited state rotational constants in cm^{-1} . The designation of the mode is obtained with the GAUSSVIEW6 software.

mode	ν_{harm}	I_{harm}	ν_{anharm}	I_{anharm}	symmetry	designation	A	B	C
1	86.59	5.8053	82.94	5.4611	A''	-OCH ₃ out-of-plane bending	0.12019	0.037456	0.028766
2	204.53	0.1684	121.13	0.0025	A''	-CH ₃ torsion	0.120477	0.037403	0.028727
3	235.66	0.4823	233.25	0.6487	A'	-OCH ₃ in-plane bending	0.120396	0.037443	0.028753
4	237.68	2.364	233.27	2.21	A''	-COH out-of-plane bending	0.120855	0.037437	0.028713
5	268.39	0.0128	314.56	38.051	A''	-CH ₃ torsion	0.120512	0.0374	0.028721
6	349.3	94.7212	344.97	54.216	A''	-OH out-of-plane bending	0.120609	0.037428	0.028744
7	368.64	7.7856	363.73	7.0759	A'	-OCH ₃ /OH in-plane bending	0.120611	0.037435	0.02874
8	469.27	2.0781	463.79	2.5547	A''	-CH out-of-plane bending	0.1207	0.037432	0.028719
9	474.58	2.0344	472.36	1.4825	A'	-OH in-plane bending	0.120733	0.037426	0.028726
10	533.69	1.1676	528.39	1.2736	A'	ring deformation	0.120595	0.037434	0.028726
11	588.58	7.6265	582.08	7.1506	A'	-OCH ₃ in-plane bending	0.120661	0.037423	0.028729
12	636.46	1.0893	625.84	0.9852	A''	-CH out-of-plane bending	0.120534	0.037426	0.028734
13	699.63	21.8067	685.9	38.7644	A''	-CH out-of-plane bending	0.120528	0.037427	0.028737
14	746.99	4.4234	736.62	5.5753	A'	ring deformation	0.120643	0.037423	0.028722
15	763.3	43.855	765.53	17.5124	A''	-CH out-of-plane bending	0.120567	0.037429	0.028738
16	847.62	0.0003	838.42	0.5027	A''	-CH out-of-plane bending	0.120519	0.037435	0.028741
17	875.53	31.094	871.94	34.1125	A''	-CH out-of-plane bending	0.1207	0.037432	0.028719
18	943.42	22.8896	925.23	12.7002	A'	ring deformation	0.120584	0.03739	0.028702
19	963.83	0.0056	968.37	0.4905	A''	-CH out-of-plane bending	0.120534	0.037426	0.028734
20	1012.28	5.1029	997.36	5.5723	A'	ring deformation	0.120618	0.037422	0.028718
21	1071.19	55.4092	1046.2	59.9793	A'	ring deformation	0.120629	0.037391	0.028699
22	1114.41	7.5264	1095.76	2.6073	A'	-CH in-plane bending	0.120585	0.037418	0.028726
23	1169.09	333.4427	1133.44	226.588	A''	-CH ₃ rocking	0.120577	0.03741	0.028709
24	1174.57	1.0877	1149.64	0.5161	A'	-CH in-plane bending	0.120503	0.037402	0.02872
25	1190.04	4.5981	1167.04	2.6711	A'	-CH in-plane bending	0.12056	0.037437	0.028727
26	1204.16	3.8276	1181.31	36.7003	A'	-CH ₃ wagging OH in-plane bending	0.120744	0.037415	0.02872
27	1244.13	47.2773	1231.14	17.408	A'	-CH ₃ wagging CH in-plane bending	0.120574	0.037408	0.028712
28	1317.38	64.6862	1283.45	47.1156	A'	C-O sym stretching	0.120501	0.037384	0.028686
29	1335.53	78.3258	1307.39	43.4766	A'	-CH in-plane bending	0.120574	0.037426	0.028717
30	1361.88	35.404	1333.28	49.6265	A'	C-C stretching	0.120438	0.037388	0.028709
31	1476.97	23.2197	1439.54	5.5664	A'	-CH ₃ wagging	0.120622	0.037418	0.028691
32	1494.77	7.0437	1452.62	5.9768	A''	-CH ₃ twisting	0.120598	0.037423	0.028733
33	1505.88	31.5209	1464.64	27.6396	A'	-CH ₃ scissoring	0.120588	0.037424	0.028763
34	1518.43	17.5926	1486.22	29.7678	A'	C-C stretching	0.120577	0.037408	0.028715
35	1529.11	136.2752	1499.3	74.2931	A'	C-C stretching	0.120512	0.037415	0.028713
36	1628.44	82.8536	1588.39	68.0933	A'	C-C stretching	0.12038	0.037409	0.02866
37	1662.54	175.2786	1623.65	101.8866	A'	C-C stretching	0.120537	0.037378	0.028739
38	3004.57	51.7713	2819.02	16.7192	A'	C-H stretching	0.120582	0.037435	0.028736
39	3059.78	38.4355	2891.62	18.9811	A''	C-H stretching	0.120582	0.03744	0.028738
40	3127.22	22.2552	2989.53	25.9117	A'	C-H stretching	0.120599	0.037428	0.028731
41	3157.26	10.2193	3016.38	6.6607	A''	C-H stretching	0.120601	0.037424	0.028729
42	3178	15.6673	3048.14	19.7206	A'	C-H stretching	0.120576	0.037425	0.028728
43	3205.46	0.3918	3074.27	0.5741	A'	C-H stretching	0.120588	0.037417	0.028724
44	3217.36	5.3639	3094.26	6.3858	A'	C-H stretching	0.120517	0.03741	0.028716
45	3819.3	61.4344	3640.46	49.828	A'	O-H stretching	0.120593	0.037428	0.028731

TABLE S5: B3LYP/cc-pVTZ calculations on 3MP-C4: Harmonic and anharmonic frequencies in cm^{-1} and intensities in km/mol , symmetry, excited state rotational constants in cm^{-1} . The designation of the mode is obtained with the GAUSSVIEW6 software.

mode	ν_{harm}	I_{harm}	ν_{anharm}	I_{anharm}	symmetry	designation	A	B	C
1	92.76	2.3131	91.22	1.9976	A''	-OCH ₃ out-of-plane bending	0.095097	0.04272	0.029697
2	200.3	0.0839	119.21	0.7597	A''	-CH ₃ torsion	0.094928	0.042719	0.02967
3	221.34	0.5775	216.61	0.5228	A'	-OCH ₃ in-plane bending	0.095423	0.042737	0.029646
4	237.28	2.5213	202.47	31.3234	A''	-COH out-of-plane bending	0.095097	0.042732	0.029686
5	271.73	1.5294	357.27	21.662	A''	-CH ₃ torsion	0.095139	0.042674	0.02965
6	332.24	91.242	299.37	34.7161	A''	-OH out-of-plane bending	0.094985	0.042743	0.02967
7	402.63	9.2757	400.65	6.7972	A'	-OCH ₃ /OH in-plane bending	0.095228	0.042734	0.029652
8	465.48	8.7669	465.75	5.5641	A''	-CH out-of-plane bending	0.095095	0.042751	0.029683
9	477.32	8.7755	472.52	7.5212	A'	-OH in-plane bending	0.095113	0.042761	0.029659
10	538.2	2.8455	531.43	3.806	A'	ring deformation	0.095106	0.042752	0.029666
11	562.51	3.6791	553.95	1.4576	A'	-OCH ₃ in-plane bending	0.095146	0.04274	0.029668
12	631.16	0.0128	625.13	0.126	A''	-CH out-of-plane bending	0.09511	0.042757	0.02968
13	699.51	20.8835	702.82	35.1324	A''	-CH out-of-plane bending	0.095029	0.042755	0.029678
14	745.3	1.5181	735.97	0.8364	A'	ring deformation	0.095088	0.042749	0.029661
15	780.24	13.3416	772.67	2.2336	A''	-CH out-of-plane bending	0.095083	0.04276	0.029679
16	831.08	55.7138	840.39	44.2675	A''	-CH out-of-plane bending	0.095064	0.042755	0.02968
17	880.88	0.0017	872.07	0.1021	A''	-CH out-of-plane bending	0.095014	0.042762	0.029679
18	964.54	34.9309	946.09	18.6427	A'	ring deformation	0.09509	0.0427	0.029632
19	980.71	0.2917	990.96	0.9004	A''	-CH out-of-plane bending	0.095026	0.042744	0.029674
20	1013.34	0.1253	996.97	0.2613	A'	ring deformation	0.095088	0.042749	0.029661
21	1068.54	44.6284	1043.01	53.7662	A'	ring deformation	0.094971	0.042732	0.029637
22	1098.2	24.3853	1078.72	5.9438	A'	-CH in-plane bending	0.095058	0.042763	0.029672
23	1172.3	111.3497	1150.76	66.9947	A''	-CH ₃ rocking	0.095091	0.042758	0.029664
24	1174.14	1.0378	1145.96	0.5427	A'	-CH in-plane bending	0.095002	0.042727	0.029661
25	1195.88	125.9884	1182.69	112.4075	A'	-CH in-plane bending	0.095095	0.042733	0.029653
26	1197.02	31.1653	1171.98	18.6656	A'	-CH ₃ wagging OH in-plane bending	0.095095	0.042744	0.029654
27	1230.09	100.7523	1203.15	66.5893	A'	-CH ₃ wagging CH in-plane bending	0.095038	0.042738	0.02965
28	1315.21	127.3523	1285.04	75.0599	A'	C-O sym stretching	0.09498	0.0427	0.029608
29	1348.08	14.0833	1318.6	8.2036	A'	-CH in-plane bending	0.095101	0.042751	0.02967
30	1366.71	30.9466	1332.88	19.5023	A'	C-C stretching	0.094965	0.042704	0.029649
31	1473.37	4.9253	1429	1.9005	A'	-CH ₃ wagging	0.094736	0.042732	0.029629
32	1493.91	55.5939	1467.28	13.6806	A''	-CH ₃ twisting	0.095077	0.04272	0.029654
33	1495.45	6.9543	1450.67	5.5223	A'	-CH ₃ scissoring	0.095463	0.042759	0.029672
34	1509.55	31.1572	1463.83	21.8446	A'	C-C stretching	0.095095	0.042747	0.029679
35	1540.83	67.4102	1499.02	74.02	A'	C-C stretching	0.095016	0.042741	0.029676
36	1640.5	188.3268	1606.14	80.7514	A'	C-C stretching	0.095011	0.042705	0.029636
37	1652.73	81.0096	1607.3	49.1566	A'	C-C stretching	0.094957	0.042722	0.02964
38	3000.42	49.5051	2811.39	17.7499	A'	C-H stretching	0.095103	0.042757	0.029676
39	3054.56	39.8731	2887.78	19.0398	A''	C-H stretching	0.095122	0.042758	0.029676
40	3127.34	20.961	2992.33	25.1367	A'	C-H stretching	0.095117	0.042744	0.029669
41	3172.71	10.9588	3032.18	14.5677	A''	C-H stretching	0.095064	0.042754	0.029668
42	3183.18	6.7943	3049.91	0.3364	A'	C-H stretching	0.095112	0.042705	0.02965
43	3199.59	6.4197	3072.42	9.8126	A'	C-H stretching	0.095064	0.042751	0.029667
44	3204.46	3.4751	3093.31	4.3602	A'	C-H stretching	0.09506	0.042752	0.029667
45	3819.42	49.3325	3637.93	38.3587	A'	O-H stretching	0.095075	0.042754	0.02967

TABLE S6: B3LYP/cc-pVTZ calculations on 4MP-C1: Harmonic and anharmonic frequencies in cm^{-1} and intensities in km/mol , symmetry, excited state rotational constants in cm^{-1} . The designation of the mode is obtained with the GAUSSVIEW6 software.

mode	ν_{harm}	I_{harm}	ν_{anharm}	I_{anharm}	symmetry	designation	A	B	C
1	80.99	2.1399	66.52	2.481	A''	-OCH ₃ out-of-plane bending	0.163013	0.032706	0.027438
2	156.24	0.43	127.48	0.0589	A''	-CO out-of-plane bending	0.163204	0.032691	0.027417
3	232.08	0.6347	238.94	0.5247	A'	-OCH ₃ in-plane bending	0.164323	0.032676	0.027381
4	245.87	0.1202	275.71	1.7763	A''	-CH ₃ torsion	0.163709	0.032632	0.02737
5	309.8	100.0475	370.52	88.2042	A''	-OH out-of-plane bending	0.163504	0.032678	0.027403
6	377.38	0.0732	371.73	1.5906	A''	-CO out-of-plane bending	0.162755	0.032707	0.027419
7	381.13	9.8743	378.57	7.7217	A'	-OCH ₃ /-OH in-plane bending	0.163907	0.032689	0.027393
8	433.6	0.744	425.06	0.2768	A''	ring out-of-plane bending	0.163425	0.032702	0.027416
9	437.93	4.9878	438.13	4.1291	A'	-OH in-plane bending	0.164177	0.032697	0.027399
10	527.27	17.1376	528.09	11.8213	A''	-CH out-of-plane bending	0.163577	0.032694	0.027413
11	533.75	0.3239	530.85	0.2439	A'	-OCH ₃ in-plane bending	0.163863	0.032692	0.027396
12	657.29	0.4424	649.28	0.0639	A'	ring deformation	0.163533	0.032698	0.027397
13	725.64	0.0628	726.63	0.6525	A''	ring out-of-plane bending	0.163552	0.032692	0.027409
14	743.19	46.5481	730.85	43.8567	A'	ring deformation	0.163562	0.032675	0.027387
15	803.51	13.1505	796.44	3.0188	A''	-CH out-of-plane bending	0.163384	0.032697	0.02741
16	850.87	53.1886	845.47	50.5446	A''	-CH out-of-plane bending	0.163382	0.032694	0.027409
17	855.76	3.0399	836.39	0.6899	A'	ring deformation	0.163639	0.032681	0.027393
18	920.03	0.1434	905.27	0.4619	A''	-CH out-of-plane bending	0.163382	0.032694	0.027409
19	969.06	0.0036	967.43	3.5727	A''	-CH out-of-plane bending	0.16344	0.032695	0.02741
20	1026.25	0.1841	1008.94	0.8086	A'	ring deformation	0.163547	0.032702	0.027387
21	1068.46	74.8964	1041.4	71.8985	A'	O-CH ₃ stretching	0.1633	0.032664	0.027373
22	1124.88	24.3517	1104.69	13.2811	A'	-CH in-plane bending	0.163624	0.032693	0.027402
23	1175.07	1.1837	1153.45	0.6904	A''	-CH ₃ twisting	0.163345	0.032678	0.027394
24	1186.68	102.6508	1150.05	1.1449	A'	-OH/-CH in-plane bending	0.163525	0.03269	0.027392
25	1191.86	43.1632	1198.29	40.2106	A'	-CH in-plane bending	0.163566	0.032695	0.027396
26	1207.07	3.104	1178.22	68.0942	A'	-CH ₃ wagging OH in-plane bending	0.163634	0.032691	0.027393
27	1264.8	328.7952	1228.98	247.5314	A'	-CH ₃ wagging CH in-plane bending	0.163458	0.032665	0.027363
28	1290.23	4.0624	1256.89	1.3154	A'	C-O sym stretching	0.163492	0.03265	0.027366
29	1335.23	24.8298	1306.01	4.7522	A'	-CH in-plane bending	0.163425	0.032684	0.027395
30	1367.68	17.3815	1341.87	7.3433	A'	-CH in-plane bending	0.163393	0.032674	0.027387
31	1475.74	44.2574	1434.12	39.6826	A'	-CH ₃ wagging -CH in-plane bending	0.163568	0.032673	0.027377
32	1478.46	1.161	1453.42	6.7494	A'	-CH ₃ wagging	0.163525	0.032688	0.027369
33	1493.69	6.8953	1458.03	5.2889	A''	-CH ₃ twisting	0.163623	0.032692	0.027405
34	1509.06	23.9503	1476.44	12.6943	A'	-CH ₃ scissoring	0.163527	0.032695	0.027431
35	1549.43	235.0333	1510.95	188.6113	A'	-CH in-plane bending	0.16336	0.032686	0.0274
36	1638.95	11.5333	1598.52	7.6151	A'	C-C stretching	0.163315	0.032669	0.027317
37	1662.64	0.6969	1618.64	0.1981	A'	C-C stretching	0.163326	0.032663	0.027431
38	2995.73	55.6232	2815.36	24.0864	A'	C-H stretching	0.163542	0.032701	0.027409
39	3047.49	43.5801	2891.72	28.0437	A''	C-H stretching	0.163573	0.032704	0.027411
40	3124.11	23.8239	2987.58	24.9058	A'	C-H stretching	0.163592	0.032692	0.027403
41	3150.81	19.0646	3014.21	5.3292	A'	C-H stretching	0.16349	0.032693	0.0274
42	3183.48	4.9279	3053.58	0.4336	A'	C-H stretching	0.163495	0.032691	0.027399
43	3198.16	5.1003	3068.83	1.8251	A'	C-H stretching	0.16349	0.03269	0.027399
44	3206.95	5.8802	3082.71	4.4006	A'	C-H stretching	0.163598	0.032667	0.027385
45	3822.1	55.9552	3652.75	49.0246	A'	O-H stretching	0.163519	0.032693	0.027402

TABLE S7: B3LYP/cc-pVTZ calculations on 4MP-C2: Harmonic and anharmonic frequencies in cm^{-1} and intensities in km/mol , symmetry, excited state rotational constants in cm^{-1} . The designation of the mode is obtained with the GAUSSVIEW6 software.

mode	ν_{harm}	I_{harm}	ν_{anharm}	I_{anharm}	symmetry	designation	A	B	C
1	79.75	4.4514	75.72	4.7148	A''	-OCH ₃ out-of-plane bending	0.162796	0.032723	0.027444
2	155.32	0.9791	120.3	0.4524	A''	-CO out-of-plane bending	0.16297	0.03271	0.027424
3	232.07	4.5364	225.29	1.9454	A'	-OCH ₃ in-plane bending	0.164094	0.032692	0.027387
4	245.26	0.0004	259.6	26.4948	A''	-CH ₃ torsion	0.16348	0.032649	0.027376
5	302.78	99.2441	301.22	67.437	A''	-OH out-of-plane bending	0.163297	0.032694	0.027409
6	376.96	0.3095	371.52	0.1205	A''	-CO out-of-plane bending	0.162525	0.032724	0.027424
7	382.24	1.9036	376.37	1.0896	A'	-OCH ₃ /-OH in-plane bending	0.16368	0.032705	0.027399
8	433.62	0.9415	425.76	0.2284	A''	ring out-of-plane bending	0.163202	0.032719	0.027422
9	436.59	3.7683	434.32	3.7884	A'	-OH in-plane bending	0.163933	0.032714	0.027405
10	526.63	18.0636	525.71	14.0093	A''	-CH out-of-plane bending	0.163351	0.032711	0.02742
11	534.34	3.9522	531.47	1.8575	A'	-OCH ₃ in-plane bending	0.163641	0.032709	0.027401
12	657.42	0.6418	648.08	0.3502	A'	ring deformation	0.163305	0.032714	0.027403
13	726.04	0.024	720.1	0.2443	A''	ring out-of-plane bending	0.163325	0.032709	0.027415
14	742.03	53.6366	729.86	50.6264	A'	ring deformation	0.163331	0.032691	0.027392
15	809.97	1.4749	800.69	0.1266	A''	-CH out-of-plane bending	0.163123	0.032712	0.027414
16	843.76	63.7781	834.83	53.4561	A''	-CH out-of-plane bending	0.163152	0.032712	0.027415
17	855.49	3.7193	836.55	2.1779	A'	ring deformation	0.163453	0.032697	0.027399
18	939.46	0.1625	921.73	0.4925	A''	-CH out-of-plane bending	0.163196	0.032711	0.027415
19	955.09	0.3146	946.58	0.4209	A''	-CH out-of-plane bending	0.163202	0.032707	0.027414
20	1026.29	0.034	1007.02	0.1152	A'	ring deformation	0.16332	0.032719	0.027393
21	1068.69	66.1306	1042.17	67.096	A'	O-CH ₃ stretching	0.163068	0.032681	0.027378
22	1126.11	15.3409	1103.34	8.5271	A'	-CH in-plane bending	0.163399	0.032707	0.027406
23	1174.96	1.1661	1150.84	0.9803	A''	-CH ₃ twisting	0.163132	0.032695	0.0274
24	1187.65	39.4982	1150.42	6.8422	A'	-OH/-CH in-plane bending	0.163293	0.032717	0.027405
25	1191.51	116.6097	1204.39	193.0422	A'	-CH in-plane bending	0.163284	0.032708	0.027398
26	1207.29	42.1321	1170.68	19.7427	A'	-CH ₃ wagging -OH in-plane bending	0.163401	0.032708	0.027398
27	1268.74	281.615	1237.92	180.1286	A'	-CH ₃ wagging -CH in-plane bending	0.163259	0.032686	0.027373
28	1286.38	1.4136	1250.5	2.5274	A'	C-O sym stretching	0.163206	0.032659	0.027364
29	1332.53	11.0813	1301.65	4.6037	A'	-CH in-plane bending	0.163184	0.032699	0.027402
30	1370.2	58.0641	1340.17	33.5831	A'	-CH in-plane bending	0.163181	0.032694	0.027394
31	1472.42	34.2109	1432.14	19.0919	A'	-CH ₃ wagging -CH in-plane bending	0.163064	0.032691	0.02738
32	1480.15	0.7255	1450.44	1.1299	A'	-CH ₃ wagging	0.163317	0.0327	0.027377
33	1493.93	6.8658	1455.41	5.8702	A''	-CH ₃ twisting	0.163642	0.032713	0.027411
34	1508.75	42.3967	1477.18	33.8326	A'	-CH ₃ scissoring	0.1633	0.032712	0.027437
35	1549.27	230.5365	1509.75	188.42	A'	-CH in-plane bending	0.163138	0.032701	0.027404
36	1636.49	0.1017	1596.54	0.9126	A'	C-C stretching	0.16308	0.032686	0.027336
37	1666.3	0.3473	1620.89	0.4225	A'	C-C stretching	0.163112	0.032679	0.027424
38	2996.82	56.2891	2815.51	23.072	A'	C-H stretching	0.163317	0.032717	0.027415
39	3048.99	42.8436	2890.71	27.2552	A''	C-H stretching	0.163349	0.03272	0.027416
40	3123.97	23.5963	2988.67	28.692	A'	C-H stretching	0.163366	0.032708	0.027409
41	3151.05	18.0206	3020.11	13.1596	A'	C-H stretching	0.163283	0.032709	0.027406
42	3186.95	7.9006	3036.1	5.5621	A'	C-H stretching	0.163292	0.032703	0.027403
43	3192.47	3.3751	3064.02	1.0339	A'	C-H stretching	0.163265	0.032707	0.027404
44	3208.33	5.7409	3072.69	7.0518	A'	C-H stretching	0.163361	0.032686	0.027392
45	3823.44	60.0179	3644.06	49.0197	A'	O-H stretching	0.163291	0.03271	0.027407

TABLE S8: Scaling of the rotational constants of 3MP-C1 and 3MP-C4 and comparison with the experimental values. Each scaled constant is calculated as $B_{\text{US scaled}} = B_{\text{US calc}} \times B_{\text{GS exp}}/B_{\text{GS calc}}$ where US refers to the upper state ($\nu_{18} = 1$) and GS to the ground state ($\nu = 0$)

Conformer	Mode	type	A	B	C
3MP-C1	$\nu = 0$	Calc.	0.094877	0.043397	0.029994
		Exp.	0.094762	0.043481	0.029987
	$\nu_{18} = 1$	Calc.	0.094864	0.042886	0.029698
		Scaled	0.094749	0.042969	0.029691
		Exp.	0.094742	0.043390	0.029958
3MP-C4	$\nu = 0$	Calc.	0.095095	0.042760	0.029674
		Exp.	0.094968	0.043301	0.029923
	$\nu_{18} = 1$	Calc.	0.095090	0.042700	0.029632
		Scaled	0.094963	0.043240	0.029881
		Exp.	0.094920	0.043209	0.029890

TABLE S9: Assigned transitions in the ν_{18} band of 3MP-C1, experimental frequencies, uncertainties, and weight of each component (calculated at 30 K). $\nu' = 1$ refers to $\nu_{18} = 1$ and $\nu'' = 0$ to the vibrational ground state.

J'	K'_a	K'_c	ν'	J''	K''_a	K''_c	ν''	freq.	unc.	weight
38	6	33	1	39	5	34	0	946.988085	-0.0015	9.53E-04
38	6	33	1	39	6	34	0	946.988085	-0.0015	1.71E-03
39	4	35	1	40	4	36	0	946.988085	-0.0015	1.71E-03
39	5	35	1	40	4	36	0	946.988085	-0.0015	1.04E-03
39	5	35	1	40	5	36	0	946.988085	-0.0015	1.71E-03
40	3	37	1	41	3	38	0	946.988085	-0.0015	1.72E-03
40	4	37	1	41	3	38	0	946.988085	-0.0015	1.12E-03
40	4	37	1	41	4	38	0	946.988085	-0.0015	1.72E-03
41	2	39	1	42	2	40	0	946.988085	-0.0015	1.75E-03
41	3	39	1	42	2	40	0	946.988085	-0.0015	1.20E-03
41	3	39	1	42	3	40	0	946.988085	-0.0015	1.75E-03
42	1	41	1	43	1	42	0	946.988085	-0.0015	1.78E-03
42	2	41	1	43	1	42	0	946.988085	-0.0015	1.29E-03
42	2	41	1	43	2	42	0	946.988085	-0.0015	1.78E-03
43	1	43	1	44	0	44	0	946.988085	-0.0015	1.38E-03
43	1	43	1	44	1	44	0	946.988085	-0.0015	1.83E-03
37	6	32	1	38	5	33	0	947.050778	-0.0015	1.04E-03
37	6	32	1	38	6	33	0	947.050778	-0.0015	1.89E-03
38	4	34	1	39	4	35	0	947.050778	-0.0015	1.90E-03
38	5	34	1	39	4	35	0	947.050778	-0.0015	1.14E-03
38	5	34	1	39	5	35	0	947.050778	-0.0015	1.90E-03
39	3	36	1	40	3	37	0	947.050778	-0.0015	1.91E-03
39	4	36	1	40	3	37	0	947.050778	-0.0015	1.23E-03
39	4	36	1	40	4	37	0	947.050778	-0.0015	1.91E-03
40	2	38	1	41	2	39	0	947.050778	-0.0015	1.94E-03
40	3	38	1	41	2	39	0	947.050778	-0.0015	1.33E-03
40	3	38	1	41	3	39	0	947.050778	-0.0015	1.94E-03
41	1	40	1	42	1	41	0	947.050778	-0.0015	1.98E-03
41	2	40	1	42	1	41	0	947.050778	-0.0015	1.43E-03
41	2	40	1	42	2	41	0	947.050778	-0.0015	1.98E-03
42	1	42	1	43	0	43	0	947.050778	-0.0015	1.53E-03
42	1	42	1	43	1	43	0	947.050778	-0.0015	2.03E-03
36	6	31	1	37	5	32	0	947.114413	-0.0015	1.13E-03
36	6	31	1	37	6	32	0	947.114413	-0.0015	2.09E-03
37	4	33	1	38	4	34	0	947.114413	-0.0015	2.09E-03
37	5	33	1	38	4	34	0	947.114413	-0.0015	1.24E-03
37	5	33	1	38	5	34	0	947.114413	-0.0015	2.09E-03
38	3	35	1	39	3	36	0	947.114413	-0.0015	2.11E-03
38	4	35	1	39	3	36	0	947.114413	-0.0015	1.35E-03
38	4	35	1	39	4	36	0	947.114413	-0.0015	2.11E-03
39	2	37	1	40	2	38	0	947.114413	-0.0015	2.14E-03
39	3	37	1	40	2	38	0	947.114413	-0.0015	1.46E-03
39	3	37	1	40	3	38	0	947.114413	-0.0015	2.14E-03

Continued on next page

TABLE S9 – *Continued from previous page*

J'	K'_a	K'_c	v'	J''	K''_a	K''_c	v''	freq.	unc.	weigh
40	1	39	1	41	1	40	0	947.114413	-0.0015	2.18E-03
40	2	39	1	41	1	40	0	947.114413	-0.0015	1.57E-03
40	2	39	1	41	2	40	0	947.114413	-0.0015	2.18E-03
41	1	41	1	42	0	42	0	947.114413	-0.0015	1.69E-03
41	1	41	1	42	1	42	0	947.114413	-0.0015	2.24E-03
36	4	32	1	37	4	33	0	947.179631	-0.0015	2.30E-03
36	5	32	1	37	4	33	0	947.179631	-0.0015	1.35E-03
36	5	32	1	37	5	33	0	947.179631	-0.0015	2.30E-03
37	3	34	1	38	3	35	0	947.179631	-0.0015	2.32E-03
37	4	34	1	38	3	35	0	947.179631	-0.0015	1.48E-03
37	4	34	1	38	4	35	0	947.179631	-0.0015	2.32E-03
38	3	36	1	39	2	37	0	947.179631	-0.0015	1.60E-03
38	3	36	1	39	3	37	0	947.179631	-0.0015	2.36E-03
39	1	38	1	40	1	39	0	947.179631	-0.0015	2.41E-03
39	2	38	1	40	1	39	0	947.179631	-0.0015	1.73E-03
39	2	38	1	40	2	39	0	947.179631	-0.0015	2.41E-03
40	1	40	1	41	0	41	0	947.179631	-0.0015	1.87E-03
40	1	40	1	41	1	41	0	947.179631	-0.0015	2.48E-03
33	6	27	1	34	6	28	0	947.232773	-0.0015	2.52E-03
35	4	31	1	36	4	32	0	947.241516	-0.0015	2.52E-03
35	5	31	1	36	4	32	0	947.241516	-0.0015	1.47E-03
35	5	31	1	36	5	32	0	947.241516	-0.0015	2.52E-03
36	3	33	1	37	3	34	0	947.241516	-0.0015	2.54E-03
36	4	33	1	37	3	34	0	947.241516	-0.0015	1.61E-03
36	4	33	1	37	4	34	0	947.241516	-0.0015	2.54E-03
37	2	35	1	38	2	36	0	947.241516	-0.0015	2.58E-03
37	3	35	1	38	2	36	0	947.241516	-0.0015	1.75E-03
37	3	35	1	38	3	36	0	947.241516	-0.0015	2.58E-03
38	1	37	1	39	1	38	0	947.241516	-0.0015	2.64E-03
38	2	37	1	39	1	38	0	947.241516	-0.0015	1.90E-03
38	2	37	1	39	2	38	0	947.241516	-0.0015	2.64E-03
39	1	39	1	40	0	40	0	947.241516	-0.0015	2.05E-03
39	1	39	1	40	1	40	0	947.241516	-0.0015	2.72E-03
34	4	30	1	35	4	31	0	947.303088	-0.0015	2.74E-03
34	5	30	1	35	4	31	0	947.303088	-0.0015	1.59E-03
34	5	30	1	35	5	31	0	947.303088	-0.0015	2.74E-03
35	3	32	1	36	3	33	0	947.303088	-0.0015	2.78E-03
35	4	32	1	36	3	33	0	947.303088	-0.0015	1.75E-03
35	4	32	1	36	4	33	0	947.303088	-0.0015	2.78E-03
36	2	34	1	37	2	35	0	947.303088	-0.0015	2.83E-03
36	3	34	1	37	2	35	0	947.303088	-0.0015	1.91E-03
36	3	34	1	37	3	35	0	947.303088	-0.0015	2.83E-03
37	2	36	1	38	1	37	0	947.303088	-0.0015	2.07E-03
37	2	36	1	38	2	37	0	947.303088	-0.0015	2.89E-03
38	1	38	1	39	1	39	0	947.303088	-0.0015	2.98E-03
31	6	25	1	32	6	26	0	947.356773	-0.0015	2.97E-03
36	1	35	1	37	1	36	0	947.369589	-0.0015	3.15E-03
37	1	37	1	38	0	38	0	947.369589	-0.0015	2.45E-03

Continued on next page

TABLE S9 – *Continued from previous page*

J'	K'_a	K'_c	v'	J''	K''_a	K''_c	v''	freq.	unc.	weigh
37	1	37	1	38	1	38	0	947.369589	-0.0015	3.25E-03
30	6	24	1	31	6	25	0	947.418187	-0.0015	3.21E-03
35	1	34	1	36	1	35	0	947.432592	-0.0015	3.43E-03
36	1	36	1	37	0	37	0	947.432592	-0.0015	2.66E-03
36	1	36	1	37	1	37	0	947.432592	-0.0015	3.54E-03
29	6	23	1	30	6	24	0	947.47832	-0.0015	3.46E-03
29	6	24	1	30	6	25	0	947.550373	-0.0015	3.71E-03
33	1	32	1	34	1	33	0	947.558267	-0.0015	4.00E-03
34	1	34	1	35	0	35	0	947.558267	-0.0015	3.11E-03
34	1	34	1	35	1	35	0	947.558267	-0.0015	4.14E-03
28	6	23	1	29	6	24	0	947.610889	-0.0015	3.96E-03
30	4	27	1	31	3	28	0	947.620629	-0.0015	2.46E-03
32	1	31	1	33	1	32	0	947.620629	-0.0015	4.30E-03
33	1	33	1	34	0	34	0	947.620629	-0.0015	3.34E-03
33	1	33	1	34	1	34	0	947.620629	-0.0015	4.45E-03
27	6	22	1	28	6	23	0	947.673689	-0.0015	4.21E-03
29	4	26	1	30	3	27	0	947.681857	-0.0015	2.60E-03
31	1	30	1	32	1	31	0	947.681857	-0.0015	4.60E-03
31	2	30	1	32	1	31	0	947.681857	-0.0015	3.24E-03
31	2	30	1	32	2	31	0	947.681857	-0.0015	4.60E-03
32	1	32	1	33	0	33	0	947.681857	-0.0015	3.58E-03
32	1	32	1	33	1	33	0	947.681857	-0.0015	4.77E-03
28	4	25	1	29	3	26	0	947.74372	-0.0015	2.73E-03
30	1	29	1	31	1	30	0	947.74372	-0.0015	4.90E-03
30	2	29	1	31	1	30	0	947.74372	-0.0015	3.45E-03
30	2	29	1	31	2	30	0	947.74372	-0.0015	4.90E-03
31	1	31	1	32	0	32	0	947.74372	-0.0015	3.82E-03
31	1	31	1	32	1	32	0	947.74372	-0.0015	5.09E-03
25	5	20	1	26	5	21	0	947.791698	-0.0015	4.71E-03
27	4	24	1	28	3	25	0	947.806889	-0.0015	2.85E-03
29	1	28	1	30	1	29	0	947.806889	-0.0015	5.21E-03
29	2	28	1	30	1	29	0	947.806889	-0.0015	3.65E-03
29	2	28	1	30	2	29	0	947.806889	-0.0015	5.21E-03
30	1	30	1	31	0	31	0	947.806889	-0.0015	4.06E-03
30	1	30	1	31	1	31	0	947.806889	-0.0015	5.42E-03
24	5	19	1	25	5	20	0	947.851326	-0.0015	4.95E-03
26	4	23	1	27	3	24	0	947.867314	-0.0015	2.96E-03
26	4	23	1	27	4	24	0	947.867314	-0.0015	5.15E-03
27	2	25	1	28	2	26	0	947.867314	-0.0015	5.31E-03
27	3	25	1	28	2	26	0	947.867314	-0.0015	3.41E-03
27	3	25	1	28	3	26	0	947.867314	-0.0015	5.31E-03
28	1	27	1	29	1	28	0	947.867314	-0.0015	5.51E-03
28	2	27	1	29	1	28	0	947.867314	-0.0015	3.84E-03
28	2	27	1	29	2	28	0	947.867314	-0.0015	5.51E-03
29	1	29	1	30	0	30	0	947.867314	-0.0015	4.29E-03
29	1	29	1	30	1	30	0	947.867314	-0.0015	5.74E-03
23	5	18	1	24	5	19	0	947.908721	-0.0015	5.18E-03
25	4	22	1	26	3	23	0	947.929521	-0.0015	3.06E-03

Continued on next page

TABLE S9 – *Continued from previous page*

J'	K'_a	K'_c	v'	J''	K''_a	K''_c	v''	freq.	unc.	weigh
25	4	22	1	26	4	23	0	947.929521	-0.0015	5.41E-03
26	2	24	1	27	2	25	0	947.929521	-0.0015	5.58E-03
26	3	24	1	27	2	25	0	947.929521	-0.0015	3.55E-03
26	3	24	1	27	3	25	0	947.929521	-0.0015	5.58E-03
27	1	26	1	28	1	27	0	947.929521	-0.0015	5.80E-03
27	2	26	1	28	1	27	0	947.929521	-0.0015	4.03E-03
27	2	26	1	28	2	27	0	947.929521	-0.0015	5.80E-03
28	1	28	1	29	0	29	0	947.929521	-0.0015	4.52E-03
28	1	28	1	29	1	29	0	947.929521	-0.0015	6.05E-03
23	6	18	1	24	5	19	0	947.941326	-0.0015	1.93E-03
22	5	17	1	23	5	18	0	947.966589	-0.0015	5.40E-03
24	4	21	1	25	3	22	0	947.99091	-0.0015	3.15E-03
24	4	21	1	25	4	22	0	947.99091	-0.0015	5.65E-03
25	2	23	1	26	2	24	0	947.99091	-0.0015	5.84E-03
25	3	23	1	26	2	24	0	947.99091	-0.0015	3.68E-03
25	3	23	1	26	3	24	0	947.99091	-0.0015	5.84E-03
26	1	25	1	27	1	26	0	947.99091	-0.0015	6.08E-03
26	2	25	1	27	1	26	0	947.99091	-0.0015	4.21E-03
26	2	25	1	27	2	26	0	947.99091	-0.0015	6.08E-03
27	1	27	1	28	0	28	0	947.99091	-0.0015	4.75E-03
27	1	27	1	28	1	28	0	947.99091	-0.0015	6.36E-03
21	5	16	1	22	5	17	0	948.017448	-0.0015	5.61E-03
22	6	17	1	23	5	18	0	948.017448	-0.0015	1.86E-03
23	4	20	1	24	3	21	0	948.052748	-0.0015	3.21E-03
23	4	20	1	24	4	21	0	948.052748	-0.0015	5.87E-03
24	2	22	1	25	2	23	0	948.052748	-0.0015	6.09E-03
24	3	22	1	25	2	23	0	948.052748	-0.0015	3.80E-03
24	3	22	1	25	3	23	0	948.052748	-0.0015	6.09E-03
25	1	24	1	26	1	25	0	948.052748	-0.0015	6.35E-03
25	2	24	1	26	1	25	0	948.052748	-0.0015	4.38E-03
25	2	24	1	26	2	25	0	948.052748	-0.0015	6.35E-03
26	1	26	1	27	0	27	0	948.052748	-0.0015	4.96E-03
26	1	26	1	27	1	27	0	948.052748	-0.0015	6.66E-03
20	5	15	1	21	5	16	0	948.072141	-0.0015	5.81E-03
21	6	16	1	22	5	17	0	948.104104	-0.0015	1.75E-03
22	4	19	1	23	3	20	0	948.114343	-0.0015	3.25E-03
22	4	19	1	23	4	20	0	948.114343	-0.0015	6.08E-03
23	2	21	1	24	2	22	0	948.114343	-0.0015	6.32E-03
23	3	21	1	24	2	22	0	948.114343	-0.0015	3.90E-03
23	3	21	1	24	3	22	0	948.114343	-0.0015	6.32E-03
24	1	23	1	25	1	24	0	948.114343	-0.0015	6.60E-03
24	2	23	1	25	1	24	0	948.114343	-0.0015	4.53E-03
24	2	23	1	25	2	24	0	948.114343	-0.0015	6.60E-03
25	1	25	1	26	0	26	0	948.114343	-0.0015	5.16E-03
25	1	25	1	26	1	26	0	948.114343	-0.0015	6.94E-03
19	5	14	1	20	5	15	0	948.128087	-0.0015	6.01E-03
21	4	18	1	22	3	19	0	948.175318	-0.0015	3.27E-03
21	4	18	1	22	4	19	0	948.175318	-0.0015	6.26E-03

Continued on next page

TABLE S9 – Continued from previous page

J'	K'_a	K'_c	v'	J''	K''_a	K''_c	v''	freq.	unc.	weigh
22	2	20	1	23	2	21	0	948.175318	-0.0015	6.52E-03
22	3	20	1	23	2	21	0	948.175318	-0.0015	3.98E-03
22	3	20	1	23	3	21	0	948.175318	-0.0015	6.52E-03
23	1	22	1	24	1	23	0	948.175318	-0.0015	6.83E-03
23	2	22	1	24	1	23	0	948.175318	-0.0015	4.66E-03
23	2	22	1	24	2	23	0	948.175318	-0.0015	6.83E-03
24	1	24	1	25	0	25	0	948.175318	-0.0015	5.35E-03
24	1	24	1	25	1	25	0	948.175318	-0.0015	7.19E-03
18	5	13	1	19	5	14	0	948.191749	-0.0015	6.18E-03
20	6	15	1	21	5	16	0	948.202289	-0.0015	1.59E-03
20	4	17	1	21	3	18	0	948.237141	-0.0015	3.26E-03
20	4	17	1	21	4	18	0	948.237141	-0.0015	6.41E-03
21	2	19	1	22	2	20	0	948.237141	-0.0015	6.70E-03
21	3	19	1	22	2	20	0	948.237141	-0.0015	4.03E-03
21	3	19	1	22	3	20	0	948.237141	-0.0015	6.70E-03
22	1	21	1	23	1	22	0	948.237141	-0.0015	7.04E-03
22	2	21	1	23	1	22	0	948.237141	-0.0015	4.77E-03
22	2	21	1	23	2	22	0	948.237141	-0.0015	7.04E-03
23	1	23	1	24	0	24	0	948.237141	-0.0015	5.51E-03
23	1	23	1	24	1	24	0	948.237141	-0.0015	7.43E-03
19	4	16	1	20	3	17	0	948.299686	-0.0015	3.21E-03
19	4	16	1	20	4	17	0	948.299686	-0.0015	6.53E-03
20	2	18	1	21	2	19	0	948.299686	-0.0015	6.85E-03
20	3	18	1	21	2	19	0	948.299686	-0.0015	4.06E-03
20	3	18	1	21	3	19	0	948.299686	-0.0015	6.85E-03
21	1	20	1	22	1	21	0	948.299686	-0.0015	7.21E-03
21	2	20	1	22	1	21	0	948.299686	-0.0015	4.86E-03
21	2	20	1	22	2	21	0	948.299686	-0.0015	7.21E-03
22	1	22	1	23	0	23	0	948.299686	-0.0015	5.66E-03
22	1	22	1	23	1	23	0	948.299686	-0.0015	7.64E-03
19	6	14	1	20	5	15	0	948.316435	-0.0015	1.39E-03
16	5	11	1	17	5	12	0	948.339459	-0.0015	6.35E-03
17	6	12	1	18	6	13	0	948.339459	-0.0015	5.96E-03
18	4	15	1	19	4	16	0	948.361556	-0.0015	6.62E-03
19	2	17	1	20	2	18	0	948.361556	-0.0015	6.96E-03
19	3	17	1	20	2	18	0	948.361556	-0.0015	4.05E-03
19	3	17	1	20	3	18	0	948.361556	-0.0015	6.96E-03
20	1	19	1	21	1	20	0	948.361556	-0.0015	7.36E-03
20	2	19	1	21	1	20	0	948.361556	-0.0015	4.92E-03
20	2	19	1	21	2	20	0	948.361556	-0.0015	7.36E-03
21	1	21	1	22	0	22	0	948.361556	-0.0015	5.78E-03
21	1	21	1	22	1	22	0	948.361556	-0.0015	7.81E-03
17	5	13	1	18	5	14	0	948.367656	-0.0015	6.32E-03
16	6	11	1	17	6	12	0	948.415566	-0.0015	5.93E-03
17	3	14	1	18	3	15	0	948.415566	-0.0015	6.68E-03
15	5	10	1	16	5	11	0	948.423153	-0.0015	6.31E-03
17	4	14	1	18	4	15	0	948.423153	-0.0015	6.67E-03
18	2	16	1	19	2	17	0	948.423153	-0.0015	7.04E-03

Continued on next page

TABLE S9 – *Continued from previous page*

J'	K'_a	K'_c	v'	J''	K''_a	K''_c	v''	freq.	unc.	weigh
18	3	16	1	19	2	17	0	948.423153	-0.0015	4.02E-03
18	3	16	1	19	3	17	0	948.423153	-0.0015	7.04E-03
19	1	18	1	20	1	19	0	948.423153	-0.0015	7.47E-03
19	2	18	1	20	1	19	0	948.423153	-0.0015	4.95E-03
19	2	18	1	20	2	19	0	948.423153	-0.0015	7.47E-03
20	1	20	1	21	0	21	0	948.423153	-0.0015	5.87E-03
20	1	20	1	21	1	21	0	948.423153	-0.0015	7.95E-03
16	5	12	1	17	5	13	0	948.436657	-0.0015	6.32E-03
17	2	15	1	18	2	16	0	948.484505	-0.0015	7.08E-03
17	3	15	1	18	2	16	0	948.484505	-0.0015	3.95E-03
17	3	15	1	18	3	16	0	948.484505	-0.0015	7.08E-03
18	1	17	1	19	1	18	0	948.484505	-0.0015	7.53E-03
18	2	17	1	19	1	18	0	948.484505	-0.0015	4.95E-03
18	2	17	1	19	2	18	0	948.484505	-0.0015	7.53E-03
19	1	19	1	20	0	20	0	948.484505	-0.0015	5.93E-03
19	1	19	1	20	1	20	0	948.484505	-0.0015	8.05E-03
15	6	10	1	16	6	11	0	948.492936	-0.0015	5.84E-03
15	5	11	1	16	5	12	0	948.505917	-0.0015	6.27E-03
14	5	9	1	15	5	10	0	948.514691	-0.0015	6.19E-03
15	3	12	1	16	3	13	0	948.531004	-0.0015	6.67E-03
16	3	14	1	17	2	15	0	948.545874	-0.0015	3.84E-03
16	3	14	1	17	3	15	0	948.545874	-0.0015	7.07E-03
17	1	16	1	18	1	17	0	948.545874	-0.0015	7.56E-03
17	2	16	1	18	1	17	0	948.545874	-0.0015	4.91E-03
17	2	16	1	18	2	17	0	948.545874	-0.0015	7.56E-03
18	1	18	1	19	0	19	0	948.545874	-0.0015	5.95E-03
18	1	18	1	19	1	19	0	948.545874	-0.0015	8.11E-03
14	5	10	1	15	5	11	0	948.578317	-0.0015	6.16E-03
14	3	11	1	15	3	12	0	948.586831	-0.0015	6.61E-03
17	6	12	1	18	5	13	0	948.586831	-0.0015	9.80E-04
13	5	8	1	14	5	9	0	948.607252	-0.0015	5.98E-03
15	3	13	1	16	3	14	0	948.607252	-0.0015	7.01E-03
16	1	15	1	17	1	16	0	948.607252	-0.0015	7.53E-03
16	2	15	1	17	1	16	0	948.607252	-0.0015	4.84E-03
16	2	15	1	17	2	16	0	948.607252	-0.0015	7.53E-03
17	1	17	1	18	0	18	0	948.607252	-0.0015	5.94E-03
17	1	17	1	18	1	18	0	948.607252	-0.0015	8.12E-03
13	3	10	1	14	3	11	0	948.643565	-0.0015	6.52E-03
13	5	9	1	14	5	10	0	948.654611	-0.0015	5.97E-03
13	6	8	1	14	6	9	0	948.654611	-0.0015	5.44E-03
14	3	12	1	15	3	13	0	948.669001	-0.0015	6.91E-03
15	1	14	1	16	1	15	0	948.669001	-0.0015	7.46E-03
15	2	14	1	16	1	15	0	948.669001	-0.0015	4.72E-03
15	2	14	1	16	2	15	0	948.669001	-0.0015	7.46E-03
16	1	16	1	17	0	17	0	948.669001	-0.0015	5.90E-03
16	1	16	1	17	1	17	0	948.669001	-0.0015	8.09E-03
12	3	9	1	13	3	10	0	948.704324	-0.0015	6.40E-03
12	5	8	1	13	5	9	0	948.730398	-0.0015	5.71E-03

Continued on next page

TABLE S9 – *Continued from previous page*

J'	K'_a	K'_c	v'	J''	K''_a	K''_c	v''	freq.	unc.	weigh
13	3	11	1	14	3	12	0	948.730398	-0.0015	6.75E-03
14	1	13	1	15	1	14	0	948.730398	-0.0015	7.34E-03
14	2	13	1	15	1	14	0	948.730398	-0.0015	4.57E-03
14	2	13	1	15	2	14	0	948.730398	-0.0015	7.34E-03
15	1	15	1	16	0	16	0	948.730398	-0.0015	5.81E-03
15	1	15	1	16	1	16	0	948.730398	-0.0015	8.00E-03
11	3	8	1	12	3	9	0	948.769236	-0.0015	6.22E-03
13	1	12	1	14	1	13	0	948.791323	-0.0015	7.16E-03
13	2	12	1	14	1	13	0	948.791323	-0.0015	4.37E-03
13	2	12	1	14	2	13	0	948.791323	-0.0015	7.16E-03
14	1	14	1	15	0	15	0	948.791323	-0.0015	5.68E-03
14	1	14	1	15	1	15	0	948.791323	-0.0015	7.85E-03
11	5	7	1	12	5	8	0	948.810485	-0.0015	5.36E-03
11	6	6	1	12	6	7	0	948.815298	-0.0015	4.73E-03
11	4	8	1	12	4	9	0	948.820257	-0.0015	5.88E-03
12	1	11	1	13	1	12	0	948.851913	-0.0015	6.93E-03
12	2	11	1	13	1	12	0	948.851913	-0.0015	4.13E-03
12	2	11	1	13	2	12	0	948.851913	-0.0015	6.93E-03
13	1	13	1	14	0	14	0	948.851913	-0.0015	5.51E-03
13	1	13	1	14	1	14	0	948.851913	-0.0015	7.66E-03
10	5	6	1	11	5	7	0	948.890071	-0.0015	4.94E-03
10	4	7	1	11	4	8	0	948.893628	-0.0015	5.51E-03
10	6	5	1	11	6	6	0	948.893628	-0.0015	4.25E-03
11	1	10	1	12	1	11	0	948.912189	-0.0015	6.65E-03
11	2	10	1	12	2	11	0	948.912189	-0.0015	6.65E-03
12	1	12	1	13	0	13	0	948.912189	-0.0015	5.30E-03
12	1	12	1	13	1	13	0	948.912189	-0.0015	7.41E-03
10	3	8	1	11	3	9	0	948.922723	-0.0015	5.93E-03
9	4	6	1	10	4	7	0	948.967979	-0.0015	5.05E-03
9	5	5	1	10	5	6	0	948.967979	-0.0015	4.42E-03
10	2	9	1	11	2	10	0	948.974553	-0.0015	6.30E-03
9	6	4	1	10	6	5	0	948.974553	-0.0015	3.66E-03
9	3	7	1	10	3	8	0	948.990537	-0.0015	5.53E-03
10	1	10	1	11	0	11	0	949.032427	-0.0015	4.74E-03
10	1	10	1	11	1	11	0	949.032427	-0.0015	6.73E-03
8	5	4	1	9	5	5	0	949.046817	-0.0015	3.80E-03
8	6	3	1	9	6	4	0	949.052557	-0.0015	2.96E-03
8	3	6	1	9	3	7	0	949.057351	-0.0015	5.06E-03
9	1	9	1	10	0	10	0	949.093819	-0.0015	4.40E-03
9	1	9	1	10	1	10	0	949.093819	-0.0015	6.31E-03
7	3	5	1	8	3	6	0	949.1293	-0.0015	4.50E-03
7	6	2	1	8	6	3	0	949.1293	-0.0015	2.14E-03
8	1	8	1	9	0	9	0	949.155856	-0.0015	4.02E-03
8	1	8	1	9	1	9	0	949.155856	-0.0015	5.84E-03
6	6	1	1	7	6	2	0	949.207021	-0.0015	1.17E-03
6	1	6	1	7	1	7	0	949.277997	-0.0015	4.75E-03
4	3	2	1	3	3	1	0	950.025293	-0.0015	1.29E-03
5	3	3	1	4	3	2	0	950.100312	-0.0015	2.32E-03

Continued on next page

TABLE S9 – *Continued from previous page*

J'	K'_a	K'_c	v'	J''	K''_a	K''_c	v''	freq.	unc.	weigh
5	4	2	1	4	4	1	0	950.100312	-0.0015	1.28E-03
6	3	4	1	5	3	3	0	950.174018	-0.0015	3.20E-03
6	4	3	1	5	4	2	0	950.174018	-0.0015	2.33E-03
7	1	7	1	6	1	6	0	950.174018	-0.0015	4.86E-03
8	1	8	1	7	0	7	0	950.234761	-0.0015	3.69E-03
8	1	8	1	7	1	7	0	950.234761	-0.0015	5.46E-03
7	4	4	1	6	4	3	0	950.248515	-0.0015	3.22E-03
9	1	9	1	8	0	8	0	950.293766	-0.0015	4.13E-03
9	1	9	1	8	1	8	0	950.293766	-0.0015	6.01E-03
8	3	6	1	7	3	5	0	950.318078	-0.0015	4.64E-03
8	4	5	1	7	4	4	0	950.323324	-0.0015	4.00E-03
10	1	10	1	9	0	9	0	950.353727	-0.0015	4.54E-03
10	1	10	1	9	1	9	0	950.353727	-0.0015	6.52E-03
8	3	5	1	7	3	4	0	950.353727	-0.0015	4.69E-03
10	1	9	1	9	1	8	0	950.41354	-0.0015	6.14E-03
11	1	11	1	10	0	10	0	950.41354	-0.0015	4.91E-03
11	1	11	1	10	1	10	0	950.41354	-0.0015	6.97E-03
10	4	7	1	9	4	6	0	950.471392	-0.0015	5.25E-03
11	1	10	1	10	1	9	0	950.471392	-0.0015	6.56E-03
12	1	12	1	11	0	11	0	950.471392	-0.0015	5.23E-03
12	1	12	1	11	1	11	0	950.471392	-0.0015	7.37E-03
10	3	7	1	9	3	6	0	950.520025	-0.0015	5.83E-03
12	1	11	1	11	1	10	0	950.530076	-0.0015	6.93E-03
12	2	11	1	11	1	10	0	950.530076	-0.0015	4.01E-03
13	1	13	1	12	0	12	0	950.530076	-0.0015	5.52E-03
13	1	13	1	12	1	12	0	950.530076	-0.0015	7.71E-03
11	4	8	1	10	4	7	0	950.546222	-0.0015	5.74E-03
13	1	12	1	12	1	11	0	950.58862	-0.0015	7.24E-03
13	2	12	1	12	1	11	0	950.58862	-0.0015	4.31E-03
13	2	12	1	12	2	11	0	950.58862	-0.0015	7.24E-03
14	1	14	1	13	0	13	0	950.58862	-0.0015	5.76E-03
14	1	14	1	13	1	13	0	950.58862	-0.0015	8.00E-03
11	3	8	1	10	3	7	0	950.59483	-0.0015	6.23E-03
12	4	9	1	11	4	8	0	950.616574	-0.0015	6.15E-03
14	1	13	1	13	1	12	0	950.647389	-0.0015	7.51E-03
14	2	13	1	13	1	12	0	950.647389	-0.0015	4.58E-03
14	2	13	1	13	2	12	0	950.647389	-0.0015	7.50E-03
15	1	15	1	14	0	14	0	950.647389	-0.0015	5.95E-03
15	1	15	1	14	1	14	0	950.647389	-0.0015	8.23E-03
13	4	10	1	12	4	9	0	950.684045	-0.0015	6.48E-03
15	1	14	1	14	1	13	0	950.7058	-0.0015	7.71E-03
15	2	14	1	14	1	13	0	950.7058	-0.0015	4.80E-03
15	2	14	1	14	2	13	0	950.7058	-0.0015	7.71E-03
16	1	16	1	15	0	15	0	950.7058	-0.0015	6.10E-03
16	1	16	1	15	1	15	0	950.7058	-0.0015	8.40E-03
14	4	11	1	13	4	10	0	950.74999	-0.0015	6.73E-03
16	1	15	1	15	1	14	0	950.765124	-0.0015	7.87E-03
16	2	15	1	15	1	14	0	950.765124	-0.0015	4.98E-03

Continued on next page

TABLE S9 – *Continued from previous page*

J'	K'_a	K'_c	v'	J''	K''_a	K''_c	v''	freq.	unc.	weigh
16	2	15	1	15	2	14	0	950.765124	-0.0015	7.87E-03
17	1	17	1	16	0	16	0	950.765124	-0.0015	6.21E-03
17	1	17	1	16	1	16	0	950.765124	-0.0015	8.52E-03
14	3	11	1	13	3	10	0	950.784309	-0.0015	6.90E-03
15	4	12	1	14	4	11	0	950.815167	-0.0015	6.92E-03
16	2	14	1	15	2	13	0	950.823482	-0.0015	7.42E-03
16	3	14	1	15	3	13	0	950.823482	-0.0015	7.42E-03
17	1	16	1	16	1	15	0	950.823482	-0.0015	7.97E-03
17	2	16	1	16	1	15	0	950.823482	-0.0015	5.11E-03
17	2	16	1	16	2	15	0	950.823482	-0.0015	7.97E-03
18	1	18	1	17	0	17	0	950.823482	-0.0015	6.28E-03
18	1	18	1	17	1	17	0	950.823482	-0.0015	8.59E-03
15	3	12	1	14	3	11	0	950.837551	-0.0015	7.01E-03
16	4	13	1	15	4	12	0	950.875608	-0.0015	7.04E-03
17	2	15	1	16	2	14	0	950.882332	-0.0015	7.50E-03
17	3	15	1	16	2	14	0	950.882332	-0.0015	4.07E-03
17	3	15	1	16	3	14	0	950.882332	-0.0015	7.50E-03
18	1	17	1	17	1	16	0	950.882332	-0.0015	8.01E-03
18	2	17	1	17	1	16	0	950.882332	-0.0015	5.20E-03
18	2	17	1	17	2	16	0	950.882332	-0.0015	8.01E-03
19	1	19	1	18	0	18	0	950.882332	-0.0015	6.31E-03
19	1	19	1	18	1	18	0	950.882332	-0.0015	8.60E-03
18	2	16	1	17	2	15	0	950.940833	-0.0015	7.53E-03
18	3	16	1	17	2	15	0	950.940833	-0.0015	4.19E-03
18	3	16	1	17	3	15	0	950.940833	-0.0015	7.53E-03
19	1	18	1	18	1	17	0	950.940833	-0.0015	8.01E-03
19	2	18	1	18	1	17	0	950.940833	-0.0015	5.26E-03
19	2	18	1	18	2	17	0	950.940833	-0.0015	8.01E-03
20	1	20	1	19	0	19	0	950.940833	-0.0015	6.30E-03
20	1	20	1	19	1	19	0	950.940833	-0.0015	8.56E-03
19	2	17	1	18	2	16	0	950.997895	-0.0015	7.51E-03
19	3	17	1	18	2	16	0	950.997895	-0.0015	4.28E-03
19	3	17	1	18	3	16	0	950.997895	-0.0015	7.51E-03
20	1	19	1	19	1	18	0	950.997895	-0.0015	7.97E-03
20	2	19	1	19	1	18	0	950.997895	-0.0015	5.28E-03
20	2	19	1	19	2	18	0	950.997895	-0.0015	7.97E-03
21	1	21	1	20	0	20	0	950.997895	-0.0015	6.26E-03
21	1	21	1	20	1	20	0	950.997895	-0.0015	8.48E-03
18	5	14	1	17	5	13	0	951.048434	-0.0015	6.77E-03
19	3	16	1	18	3	15	0	951.057868	-0.0015	7.10E-03
19	4	16	1	18	4	15	0	951.057868	-0.0015	7.09E-03
20	2	18	1	19	2	17	0	951.057868	-0.0015	7.45E-03
20	3	18	1	19	2	17	0	951.057868	-0.0015	4.33E-03
20	3	18	1	19	3	17	0	951.057868	-0.0015	7.45E-03
21	1	20	1	20	1	19	0	951.057868	-0.0015	7.87E-03
21	2	20	1	20	1	19	0	951.057868	-0.0015	5.26E-03
21	2	20	1	20	2	19	0	951.057868	-0.0015	7.87E-03
22	1	22	1	21	0	21	0	951.057868	-0.0015	6.18E-03

Continued on next page

TABLE S9 – *Continued from previous page*

J'	K'_a	K'_c	v'	J''	K''_a	K''_c	v''	freq.	unc.	weigh
22	1	22	1	21	1	21	0	951.057868	-0.0015	8.36E-03
20	3	17	1	19	3	16	0	951.115115	-0.0015	7.02E-03
20	4	17	1	19	4	16	0	951.115115	-0.0015	7.02E-03
21	2	19	1	20	2	18	0	951.115115	-0.0015	7.35E-03
21	3	19	1	20	2	18	0	951.115115	-0.0015	4.35E-03
21	3	19	1	20	3	18	0	951.115115	-0.0015	7.35E-03
22	1	21	1	21	1	20	0	951.115115	-0.0015	7.74E-03
22	2	21	1	21	1	20	0	951.115115	-0.0015	5.21E-03
22	2	21	1	21	2	20	0	951.115115	-0.0015	7.74E-03
23	1	23	1	22	0	22	0	951.115115	-0.0015	6.07E-03
23	1	23	1	22	1	22	0	951.115115	-0.0015	8.20E-03
19	4	15	1	18	4	14	0	951.132707	-0.0015	6.79E-03
20	5	16	1	19	5	15	0	951.172502	-0.0015	6.66E-03
21	3	18	1	20	3	17	0	951.172502	-0.0015	6.91E-03
21	4	18	1	20	4	17	0	951.172502	-0.0015	6.91E-03
22	2	20	1	21	2	19	0	951.172502	-0.0015	7.21E-03
22	3	20	1	21	2	19	0	951.172502	-0.0015	4.34E-03
22	3	20	1	21	3	19	0	951.172502	-0.0015	7.21E-03
23	1	22	1	22	1	21	0	951.172502	-0.0015	7.58E-03
23	2	22	1	22	1	21	0	951.172502	-0.0015	5.14E-03
23	2	22	1	22	2	21	0	951.172502	-0.0015	7.58E-03
24	1	24	1	23	0	23	0	951.172502	-0.0015	5.93E-03
24	1	24	1	23	1	23	0	951.172502	-0.0015	8.00E-03
20	4	16	1	19	4	15	0	951.185307	-0.0015	6.69E-03
21	5	17	1	20	5	16	0	951.230763	-0.0015	6.54E-03
22	3	19	1	21	3	18	0	951.230763	-0.0015	6.76E-03
22	4	19	1	21	3	18	0	951.230763	-0.0015	3.53E-03
22	4	19	1	21	4	18	0	951.230763	-0.0015	6.76E-03
23	2	21	1	22	2	20	0	951.230763	-0.0015	7.04E-03
23	3	21	1	22	2	20	0	951.230763	-0.0015	4.29E-03
23	3	21	1	22	3	20	0	951.230763	-0.0015	7.04E-03
24	1	23	1	23	1	22	0	951.230763	-0.0015	7.38E-03
24	2	23	1	23	1	22	0	951.230763	-0.0015	5.03E-03
24	2	23	1	23	2	22	0	951.230763	-0.0015	7.38E-03
25	1	25	1	24	0	24	0	951.230763	-0.0015	5.77E-03
25	1	25	1	24	1	24	0	951.230763	-0.0015	7.77E-03
22	5	18	1	21	5	17	0	951.289287	-0.0015	6.38E-03
23	3	20	1	22	3	19	0	951.289287	-0.0015	6.58E-03
23	4	20	1	22	3	19	0	951.289287	-0.0015	3.52E-03
23	4	20	1	22	4	19	0	951.289287	-0.0015	6.58E-03
24	2	22	1	23	2	21	0	951.289287	-0.0015	6.84E-03
24	3	22	1	23	2	21	0	951.289287	-0.0015	4.22E-03
24	3	22	1	23	3	21	0	951.289287	-0.0015	6.84E-03
25	1	24	1	24	1	23	0	951.289287	-0.0015	7.15E-03
25	2	24	1	24	1	23	0	951.289287	-0.0015	4.90E-03
25	2	24	1	24	2	23	0	951.289287	-0.0015	7.15E-03
26	1	26	1	25	0	25	0	951.289287	-0.0015	5.59E-03
26	1	26	1	25	1	25	0	951.289287	-0.0015	7.51E-03

Continued on next page

TABLE S9 – *Continued from previous page*

J'	K'_a	K'_c	v'	J''	K''_a	K''_c	v''	freq.	unc.	weigh
23	4	19	1	22	4	18	0	951.350311	-0.0015	6.20E-03
23	5	19	1	22	4	18	0	951.350311	-0.0015	2.79E-03
24	4	20	1	23	4	19	0	951.405632	-0.0015	5.99E-03
24	5	20	1	23	4	19	0	951.405632	-0.0015	2.79E-03
24	5	20	1	23	5	19	0	951.405632	-0.0015	5.99E-03
25	4	22	1	24	3	21	0	951.405632	-0.0015	3.43E-03
26	2	24	1	25	2	23	0	951.405632	-0.0015	6.37E-03
26	3	24	1	25	2	23	0	951.405632	-0.0015	4.01E-03
26	3	24	1	25	3	23	0	951.405632	-0.0015	6.37E-03
27	1	26	1	26	1	25	0	951.405632	-0.0015	6.63E-03
27	2	26	1	26	1	25	0	951.405632	-0.0015	4.59E-03
27	2	26	1	26	2	25	0	951.405632	-0.0015	6.63E-03
28	1	28	1	27	0	27	0	951.405632	-0.0015	5.17E-03
28	1	28	1	27	1	27	0	951.405632	-0.0015	6.93E-03
25	4	21	1	24	4	20	0	951.462056	-0.0015	5.76E-03
25	5	21	1	24	4	20	0	951.462056	-0.0015	2.78E-03
25	5	21	1	24	5	20	0	951.462056	-0.0015	5.76E-03
26	3	23	1	25	3	22	0	951.462056	-0.0015	5.91E-03
26	4	23	1	25	3	22	0	951.462056	-0.0015	3.34E-03
26	4	23	1	25	4	22	0	951.462056	-0.0015	5.91E-03
27	2	25	1	26	2	24	0	951.462056	-0.0015	6.10E-03
27	3	25	1	26	2	24	0	951.462056	-0.0015	3.88E-03
27	3	25	1	26	3	24	0	951.462056	-0.0015	6.10E-03
28	1	27	1	27	1	26	0	951.462056	-0.0015	6.34E-03
28	2	27	1	27	1	26	0	951.462056	-0.0015	4.41E-03
28	2	27	1	27	2	26	0	951.462056	-0.0015	6.34E-03
29	1	29	1	28	0	28	0	951.462056	-0.0015	4.94E-03
29	1	29	1	28	1	28	0	951.462056	-0.0015	6.62E-03
26	4	22	1	25	4	21	0	951.520263	-0.0015	5.52E-03
26	5	22	1	25	4	21	0	951.520263	-0.0015	2.73E-03
26	5	22	1	25	5	21	0	951.520263	-0.0015	5.52E-03
27	3	24	1	26	3	23	0	951.520263	-0.0015	5.65E-03
27	4	24	1	26	3	23	0	951.520263	-0.0015	3.25E-03
27	4	24	1	26	4	23	0	951.520263	-0.0015	5.65E-03
28	2	26	1	27	2	25	0	951.520263	-0.0015	5.82E-03
28	3	26	1	27	2	25	0	951.520263	-0.0015	3.73E-03
28	3	26	1	27	3	25	0	951.520263	-0.0015	5.82E-03
29	1	28	1	28	1	27	0	951.520263	-0.0015	6.03E-03
29	2	28	1	28	1	27	0	951.520263	-0.0015	4.21E-03
29	2	28	1	28	2	27	0	951.520263	-0.0015	6.03E-03
30	1	30	1	29	0	29	0	951.520263	-0.0015	4.70E-03
30	1	30	1	29	1	29	0	951.520263	-0.0015	6.29E-03
27	4	23	1	26	4	22	0	951.576698	-0.0015	5.26E-03
27	5	23	1	26	4	22	0	951.576698	-0.0015	2.67E-03
27	5	23	1	26	5	22	0	951.576698	-0.0015	5.26E-03
28	3	25	1	27	3	24	0	951.576698	-0.0015	5.38E-03
28	4	25	1	27	3	24	0	951.576698	-0.0015	3.13E-03
28	4	25	1	27	4	24	0	951.576698	-0.0015	5.38E-03

Continued on next page

TABLE S9 – Continued from previous page

J'	K'_a	K'_c	v'	J''	K''_a	K''_c	v''	freq.	unc.	weigh
29	2	27	1	28	2	26	0	951.576698	-0.0015	5.53E-03
29	3	27	1	28	2	26	0	951.576698	-0.0015	3.57E-03
29	3	27	1	28	3	26	0	951.576698	-0.0015	5.53E-03
30	1	29	1	29	1	28	0	951.576698	-0.0015	5.72E-03
30	2	29	1	29	1	28	0	951.576698	-0.0015	4.01E-03
30	2	29	1	29	2	28	0	951.576698	-0.0015	5.72E-03
31	1	31	1	30	0	30	0	951.576698	-0.0015	4.46E-03
31	1	31	1	30	1	30	0	951.576698	-0.0015	5.95E-03
28	4	24	1	27	4	23	0	951.636028	-0.0015	4.99E-03
28	5	24	1	27	4	23	0	951.636028	-0.0015	2.59E-03
28	5	24	1	27	5	23	0	951.636028	-0.0015	4.99E-03
29	4	26	1	28	3	25	0	951.636028	-0.0015	3.01E-03
29	4	26	1	28	4	25	0	951.636028	-0.0015	5.09E-03
30	2	28	1	29	2	27	0	951.636028	-0.0015	5.23E-03
30	3	28	1	29	2	27	0	951.636028	-0.0015	3.40E-03
30	3	28	1	29	3	27	0	951.636028	-0.0015	5.23E-03
31	1	30	1	30	1	29	0	951.636028	-0.0015	5.41E-03
31	2	30	1	30	1	29	0	951.636028	-0.0015	3.80E-03
31	2	30	1	30	2	29	0	951.636028	-0.0015	5.41E-03
32	1	32	1	31	0	31	0	951.636028	-0.0015	4.21E-03
32	1	32	1	31	1	31	0	951.636028	-0.0015	5.62E-03
29	4	25	1	28	4	24	0	951.692303	-0.0015	4.72E-03
29	5	25	1	28	4	24	0	951.692303	-0.0015	2.50E-03
29	5	25	1	28	5	24	0	951.692303	-0.0015	4.72E-03
30	3	27	1	29	3	26	0	951.692303	-0.0015	4.81E-03
30	4	27	1	29	3	26	0	951.692303	-0.0015	2.87E-03
30	4	27	1	29	4	26	0	951.692303	-0.0015	4.81E-03
31	2	29	1	30	2	28	0	951.692303	-0.0015	4.93E-03
31	3	29	1	30	2	28	0	951.692303	-0.0015	3.23E-03
31	3	29	1	30	3	28	0	951.692303	-0.0015	4.93E-03
32	1	31	1	31	1	30	0	951.692303	-0.0015	5.09E-03
32	2	31	1	31	1	30	0	951.692303	-0.0015	3.59E-03
32	2	31	1	31	2	30	0	951.692303	-0.0015	5.09E-03
33	1	33	1	32	0	32	0	951.692303	-0.0015	3.96E-03
33	1	33	1	32	1	32	0	951.692303	-0.0015	5.28E-03
30	4	26	1	29	4	25	0	951.748263	-0.0015	4.44E-03
30	5	26	1	29	4	25	0	951.748263	-0.0015	2.39E-03
30	5	26	1	29	5	25	0	951.748263	-0.0015	4.44E-03
31	3	28	1	30	3	27	0	951.748263	-0.0015	4.52E-03
31	4	28	1	30	3	27	0	951.748263	-0.0015	2.73E-03
31	4	28	1	30	4	27	0	951.748263	-0.0015	4.52E-03
32	2	30	1	31	2	29	0	951.748263	-0.0015	4.63E-03
32	3	30	1	31	2	29	0	951.748263	-0.0015	3.05E-03
32	3	30	1	31	3	29	0	951.748263	-0.0015	4.63E-03
33	1	32	1	32	1	31	0	951.748263	-0.0015	4.77E-03
33	2	32	1	32	2	31	0	951.748263	-0.0015	4.77E-03
34	1	34	1	33	0	33	0	951.748263	-0.0015	3.71E-03
34	1	34	1	33	1	33	0	951.748263	-0.0015	4.94E-03

Continued on next page

TABLE S9 – Continued from previous page

J'	K'_a	K'_c	v'	J''	K''_a	K''_c	v''	freq.	unc.	weigh
33	2	32	1	32	1	31	0	951.751467	-0.0015	3.37E-03
31	4	27	1	30	4	26	0	951.806244	-0.0015	4.16E-03
31	5	27	1	30	4	26	0	951.806244	-0.0015	2.28E-03
31	5	27	1	30	5	26	0	951.806244	-0.0015	4.16E-03
32	3	29	1	31	3	28	0	951.806244	-0.0015	4.23E-03
32	4	29	1	31	3	28	0	951.806244	-0.0015	2.58E-03
32	4	29	1	31	4	28	0	951.806244	-0.0015	4.23E-03
33	2	31	1	32	2	30	0	951.806244	-0.0015	4.33E-03
33	3	31	1	32	2	30	0	951.806244	-0.0015	2.86E-03
33	3	31	1	32	3	30	0	951.806244	-0.0015	4.33E-03
34	1	33	1	33	1	32	0	951.806244	-0.0015	4.45E-03
34	2	33	1	33	1	32	0	951.806244	-0.0015	3.16E-03
34	2	33	1	33	2	32	0	951.806244	-0.0015	4.45E-03
35	1	35	1	34	0	34	0	951.806244	-0.0015	3.46E-03
35	1	35	1	34	1	34	0	951.806244	-0.0015	4.60E-03
32	4	28	1	31	4	27	0	951.862439	-0.0015	3.89E-03
32	5	28	1	31	4	27	0	951.862439	-0.0015	2.16E-03
32	5	28	1	31	5	27	0	951.862439	-0.0015	3.89E-03
33	3	30	1	32	3	29	0	951.862439	-0.0015	3.95E-03
33	4	30	1	32	3	29	0	951.862439	-0.0015	2.42E-03
33	4	30	1	32	4	29	0	951.862439	-0.0015	3.95E-03
34	2	32	1	33	2	31	0	951.862439	-0.0015	4.03E-03
34	3	32	1	33	2	31	0	951.862439	-0.0015	2.68E-03
34	3	32	1	33	3	31	0	951.862439	-0.0015	4.03E-03
35	1	34	1	34	1	33	0	951.862439	-0.0015	4.14E-03
35	2	34	1	34	1	33	0	951.862439	-0.0015	2.94E-03
35	2	34	1	34	2	33	0	951.862439	-0.0015	4.14E-03
36	1	36	1	35	0	35	0	951.862439	-0.0015	3.22E-03
36	1	36	1	35	1	35	0	951.862439	-0.0015	4.28E-03
33	4	29	1	32	4	28	0	951.92158	-0.0015	3.62E-03
33	5	29	1	32	4	28	0	951.92158	-0.0015	2.04E-03
33	5	29	1	32	5	28	0	951.92158	-0.0015	3.62E-03
34	3	31	1	33	3	30	0	951.92158	-0.0015	3.66E-03
34	4	31	1	33	3	30	0	951.92158	-0.0015	2.27E-03
34	4	31	1	33	4	30	0	951.92158	-0.0015	3.66E-03
35	2	33	1	34	2	32	0	951.92158	-0.0015	3.74E-03
35	3	33	1	34	2	32	0	951.92158	-0.0015	2.50E-03
35	3	33	1	34	3	32	0	951.92158	-0.0015	3.74E-03
36	1	35	1	35	1	34	0	951.92158	-0.0015	3.84E-03
36	2	35	1	35	1	34	0	951.92158	-0.0015	2.73E-03
36	2	35	1	35	2	34	0	951.92158	-0.0015	3.84E-03
37	1	37	1	36	0	36	0	951.92158	-0.0015	2.98E-03
37	1	37	1	36	1	36	0	951.92158	-0.0015	3.96E-03
34	4	30	1	33	4	29	0	951.976919	-0.0015	3.35E-03
34	5	30	1	33	4	29	0	951.976919	-0.0015	1.91E-03
34	5	30	1	33	5	29	0	951.976919	-0.0015	3.35E-03
35	3	32	1	34	3	31	0	951.976919	-0.0015	3.39E-03
35	4	32	1	34	3	31	0	951.976919	-0.0015	2.12E-03

Continued on next page

TABLE S9 – Continued from previous page

J'	K'_a	K'_c	v'	J''	K''_a	K''_c	v''	freq.	unc.	weigh
35	4	32	1	34	4	31	0	951.976919	-0.0015	3.39E-03
36	2	34	1	35	2	33	0	951.976919	-0.0015	3.45E-03
36	3	34	1	35	2	33	0	951.976919	-0.0015	2.32E-03
36	3	34	1	35	3	33	0	951.976919	-0.0015	3.45E-03
37	1	36	1	36	1	35	0	951.976919	-0.0015	3.54E-03
37	2	36	1	36	1	35	0	951.976919	-0.0015	2.53E-03
37	2	36	1	36	2	35	0	951.976919	-0.0015	3.54E-03
38	1	38	1	37	0	37	0	951.976919	-0.0015	2.75E-03
38	1	38	1	37	1	37	0	951.976919	-0.0015	3.65E-03
35	4	31	1	34	4	30	0	952.035111	-0.0015	3.09E-03
35	5	31	1	34	4	30	0	952.035111	-0.0015	1.78E-03
35	5	31	1	34	5	30	0	952.035111	-0.0015	3.09E-03
36	3	33	1	35	3	32	0	952.035111	-0.0015	3.13E-03
36	4	33	1	35	3	32	0	952.035111	-0.0015	1.97E-03
36	4	33	1	35	4	32	0	952.035111	-0.0015	3.13E-03
37	2	35	1	36	2	34	0	952.035111	-0.0015	3.18E-03
37	3	35	1	36	2	34	0	952.035111	-0.0015	2.15E-03
37	3	35	1	36	3	34	0	952.035111	-0.0015	3.18E-03
38	1	37	1	37	1	36	0	952.035111	-0.0015	3.26E-03
38	2	37	1	37	1	36	0	952.035111	-0.0015	2.33E-03
38	2	37	1	37	2	36	0	952.035111	-0.0015	3.26E-03
39	1	39	1	38	0	38	0	952.035111	-0.0015	2.53E-03
39	1	39	1	38	1	38	0	952.035111	-0.0015	3.36E-03
36	4	32	1	35	4	31	0	952.090741	-0.0015	2.84E-03
36	5	32	1	35	4	31	0	952.090741	-0.0015	1.66E-03
36	5	32	1	35	5	31	0	952.090741	-0.0015	2.84E-03
37	3	34	1	36	3	33	0	952.090741	-0.0015	2.87E-03
37	4	34	1	36	3	33	0	952.090741	-0.0015	1.82E-03
37	4	34	1	36	4	33	0	952.090741	-0.0015	2.87E-03
38	2	36	1	37	2	35	0	952.090741	-0.0015	2.92E-03
38	3	36	1	37	2	35	0	952.090741	-0.0015	1.98E-03
38	3	36	1	37	3	35	0	952.090741	-0.0015	2.92E-03
39	1	38	1	38	1	37	0	952.090741	-0.0015	2.99E-03
39	2	38	1	38	1	37	0	952.090741	-0.0015	2.14E-03
39	2	38	1	38	2	37	0	952.090741	-0.0015	2.99E-03
40	1	40	1	39	0	39	0	952.090741	-0.0015	2.32E-03
40	1	40	1	39	1	39	0	952.090741	-0.0015	3.07E-03
37	4	33	1	36	4	32	0	952.147202	-0.0015	2.60E-03
37	5	33	1	36	4	32	0	952.147202	-0.0015	1.53E-03
37	5	33	1	36	5	32	0	952.147202	-0.0015	2.60E-03
38	3	35	1	37	3	34	0	952.147202	-0.0015	2.63E-03
38	4	35	1	37	3	34	0	952.147202	-0.0015	1.67E-03
38	4	35	1	37	4	34	0	952.147202	-0.0015	2.63E-03
39	2	37	1	38	2	36	0	952.147202	-0.0015	2.67E-03
39	3	37	1	38	2	36	0	952.147202	-0.0015	1.81E-03
39	3	37	1	38	3	36	0	952.147202	-0.0015	2.67E-03
40	1	39	1	39	1	38	0	952.147202	-0.0015	2.73E-03
40	2	39	1	39	1	38	0	952.147202	-0.0015	1.96E-03

Continued on next page

TABLE S9 – Continued from previous page

J'	K'_a	K'_c	v'	J''	K''_a	K''_c	v''	freq.	unc.	weigh
40	2	39	1	39	2	38	0	952.147202	-0.0015	2.73E-03
41	1	41	1	40	0	40	0	952.147202	-0.0015	2.11E-03
41	1	41	1	40	1	40	0	952.147202	-0.0015	2.80E-03
38	4	34	1	37	4	33	0	952.204618	-0.0015	2.38E-03
38	5	34	1	37	4	33	0	952.204618	-0.0015	1.41E-03
38	5	34	1	37	5	33	0	952.204618	-0.0015	2.38E-03
39	4	36	1	38	3	35	0	952.204618	-0.0015	1.54E-03
39	4	36	1	38	4	35	0	952.204618	-0.0015	2.40E-03
40	2	38	1	39	2	37	0	952.204618	-0.0015	2.43E-03
40	3	38	1	39	2	37	0	952.204618	-0.0015	1.66E-03
40	3	38	1	39	3	37	0	952.204618	-0.0015	2.43E-03
41	1	40	1	40	1	39	0	952.204618	-0.0015	2.48E-03
41	2	40	1	40	1	39	0	952.204618	-0.0015	1.79E-03
41	2	40	1	40	2	39	0	952.204618	-0.0015	2.48E-03
42	1	42	1	41	0	41	0	952.204618	-0.0015	1.92E-03
42	1	42	1	41	1	41	0	952.204618	-0.0015	2.55E-03
39	5	35	1	38	4	34	0	952.261218	-0.0015	1.29E-03
39	5	35	1	38	5	34	0	952.261218	-0.0015	2.16E-03
40	4	37	1	39	3	36	0	952.261218	-0.0015	1.40E-03
40	4	37	1	39	4	36	0	952.261218	-0.0015	2.18E-03
41	2	39	1	40	2	38	0	952.261218	-0.0015	2.21E-03
41	3	39	1	40	2	38	0	952.261218	-0.0015	1.51E-03
41	3	39	1	40	3	38	0	952.261218	-0.0015	2.21E-03
42	1	41	1	41	1	40	0	952.261218	-0.0015	2.25E-03
42	2	41	1	41	1	40	0	952.261218	-0.0015	1.62E-03
42	2	41	1	41	2	40	0	952.261218	-0.0015	2.25E-03
43	1	43	1	42	0	42	0	952.261218	-0.0015	1.74E-03
43	1	43	1	42	1	42	0	952.261218	-0.0015	2.31E-03
40	5	36	1	39	4	35	0	952.316513	-0.0015	1.18E-03
41	4	38	1	40	3	37	0	952.316513	-0.0015	1.28E-03
41	4	38	1	40	4	37	0	952.316513	-0.0015	1.97E-03
42	2	40	1	41	2	39	0	952.316513	-0.0015	2.00E-03
42	3	40	1	41	2	39	0	952.316513	-0.0015	1.37E-03
42	3	40	1	41	3	39	0	952.316513	-0.0015	2.00E-03
43	1	42	1	42	1	41	0	952.316513	-0.0015	2.04E-03
43	2	42	1	42	1	41	0	952.316513	-0.0015	1.47E-03
43	2	42	1	42	2	41	0	952.316513	-0.0015	2.04E-03
44	1	44	1	43	0	43	0	952.316513	-0.0015	1.58E-03
44	1	44	1	43	1	43	0	952.316513	-0.0015	2.09E-03
41	5	37	1	40	4	36	0	952.373259	-0.0015	1.08E-03
42	4	39	1	41	3	38	0	952.373259	-0.0015	1.16E-03
42	4	39	1	41	4	38	0	952.373259	-0.0015	1.78E-03
43	2	41	1	42	2	40	0	952.373259	-0.0015	1.80E-03
43	3	41	1	42	2	40	0	952.373259	-0.0015	1.24E-03
43	3	41	1	42	3	40	0	952.373259	-0.0015	1.80E-03
44	1	43	1	43	1	42	0	952.373259	-0.0015	1.83E-03
44	2	43	1	43	1	42	0	952.373259	-0.0015	1.33E-03
44	2	43	1	43	2	42	0	952.373259	-0.0015	1.83E-03

Continued on next page

TABLE S9 – Continued from previous page

J'	K'_a	K'_c	v'	J''	K''_a	K''_c	v''	freq.	unc.	weight
45	1	45	1	44	0	44	0	952.373259	-0.0015	1.42E-03
45	1	45	1	44	1	44	0	952.373259	-0.0015	1.88E-03
44	4	41	1	43	4	40	0	952.485034	-0.0015	1.43E-03
45	3	43	1	44	2	42	0	952.485034	-0.0015	1.00E-03
45	3	43	1	44	3	42	0	952.485034	-0.0015	1.45E-03
46	1	45	1	45	1	44	0	952.485034	-0.0015	1.47E-03
46	2	45	1	45	1	44	0	952.485034	-0.0015	1.07E-03
46	2	45	1	45	2	44	0	952.485034	-0.0015	1.47E-03
47	1	47	1	46	0	46	0	952.485034	-0.0015	1.14E-03
47	1	47	1	46	1	46	0	952.485034	-0.0015	1.51E-03
46	3	44	1	45	2	43	0	952.542273	-0.0015	8.97E-04
46	3	44	1	45	3	43	0	952.542273	-0.0015	1.29E-03
47	1	46	1	46	1	45	0	952.542273	-0.0015	1.31E-03
47	2	46	1	46	1	45	0	952.542273	-0.0015	9.54E-04
47	2	46	1	46	2	45	0	952.542273	-0.0015	1.31E-03
48	1	48	1	47	0	47	0	952.542273	-0.0015	1.02E-03
48	1	48	1	47	1	47	0	952.542273	-0.0015	1.34E-03
48	3	46	1	47	2	45	0	952.653574	-0.0015	7.10E-04
48	3	46	1	47	3	45	0	952.653574	-0.0015	1.02E-03
49	1	48	1	48	1	47	0	952.653574	-0.0015	1.03E-03
49	2	48	1	48	1	47	0	952.653574	-0.0015	7.53E-04
49	2	48	1	48	2	47	0	952.653574	-0.0015	1.03E-03
50	1	50	1	49	0	49	0	952.653574	-0.0015	7.99E-04
50	1	50	1	49	1	49	0	952.653574	-0.0015	1.06E-03
49	3	47	1	48	2	46	0	952.708552	-0.0015	6.29E-04
49	3	47	1	48	3	46	0	952.708552	-0.0015	8.99E-04
50	1	49	1	49	1	48	0	952.708552	-0.0015	9.12E-04
50	2	49	1	49	1	48	0	952.708552	-0.0015	6.65E-04
50	2	49	1	49	2	48	0	952.708552	-0.0015	9.12E-04
51	1	51	1	50	0	50	0	952.708552	-0.0015	7.05E-04
51	1	51	1	50	1	50	0	952.708552	-0.0015	9.31E-04
11	11	0	1	11	11	1	0	949.72226	-0.0015	9.14E-03
11	11	1	1	11	11	0	0	949.72226	-0.0015	9.14E-03
10	10	0	1	10	10	1	0	949.72226	-0.0015	9.12E-03
10	10	1	1	10	10	0	0	949.72226	-0.0015	9.12E-03
12	12	0	1	12	12	1	0	949.72226	-0.0015	8.99E-03
12	12	1	1	12	12	0	0	949.72226	-0.0015	8.99E-03
9	9	0	1	9	9	1	0	949.72226	-0.0015	8.92E-03
9	9	1	1	9	9	0	0	949.72226	-0.0015	8.92E-03
13	13	0	1	13	13	1	0	949.72226	-0.0015	8.70E-03
13	13	1	1	13	13	0	0	949.72226	-0.0015	8.70E-03
8	8	0	1	8	8	1	0	949.72226	-0.0015	8.53E-03
8	8	1	1	8	8	0	0	949.72226	-0.0015	8.53E-03
14	14	0	1	14	14	1	0	949.72226	-0.0015	8.29E-03
14	14	1	1	14	14	0	0	949.72226	-0.0015	8.29E-03
12	11	1	1	12	11	2	0	949.72226	-0.0015	8.04E-03
12	11	2	1	12	11	1	0	949.72226	-0.0015	8.04E-03
11	10	1	1	11	10	2	0	949.72226	-0.0015	7.99E-03

Continued on next page

TABLE S9 – *Continued from previous page*

J'	K'_a	K'_c	v'	J''	K''_a	K''_c	v''	freq.	unc.	weighth
11	10	2	1	11	10	1	0	949.72226	-0.0015	7.99E-03
13	12	1	1	13	12	2	0	949.72226	-0.0015	7.93E-03
13	12	2	1	13	12	1	0	949.72226	-0.0015	7.93E-03

TABLE S10: Assigned transitions in the ν_{18} band of 3MP-C4, experimental frequencies, uncertainties, and weight of each component (calculated at 30 K). $\nu' = 1$ refers to $\nu_{18} = 1$ and $\nu'' = 0$ to the vibrational ground state.

J'	K'_a	K'_c	ν'	J''	K''_a	K''_c	ν''	freq.	unc.	weight
18	3	16	1	19	2	17	0	948.353859	1.50E-03	4.01E-03
18	3	16	1	19	3	17	0	948.353859	1.50E-03	7.05E-03
19	1	18	1	20	1	19	0	948.353859	1.50E-03	7.48E-03
19	2	18	1	20	1	19	0	948.353859	1.50E-03	4.95E-03
19	2	18	1	20	2	19	0	948.353859	1.50E-03	7.48E-03
20	1	20	1	21	0	21	0	948.353859	1.50E-03	5.87E-03
17	3	15	1	18	2	16	0	948.415566	1.50E-03	3.94E-03
17	3	15	1	18	3	16	0	948.415566	1.50E-03	7.09E-03
18	1	17	1	19	1	18	0	948.415566	1.50E-03	7.54E-03
18	2	17	1	19	1	18	0	948.415566	1.50E-03	4.95E-03
18	2	17	1	19	2	18	0	948.415566	1.50E-03	7.54E-03
19	1	19	1	20	0	20	0	948.415566	1.50E-03	5.93E-03
16	3	14	1	17	2	15	0	948.478087	1.50E-03	3.83E-03
16	3	14	1	17	3	15	0	948.478087	1.50E-03	7.08E-03
17	1	16	1	18	1	17	0	948.478087	1.50E-03	7.57E-03
17	2	16	1	18	1	17	0	948.478087	1.50E-03	4.91E-03
17	2	16	1	18	2	17	0	948.478087	1.50E-03	7.57E-03
18	1	18	1	19	0	19	0	948.478087	1.50E-03	5.96E-03
18	1	18	1	19	1	19	0	948.478087	1.50E-03	8.12E-03
15	3	13	1	16	2	14	0	948.539004	1.50E-03	3.67E-03
15	3	13	1	16	3	14	0	948.539004	1.50E-03	7.02E-03
16	1	15	1	17	1	16	0	948.539004	1.50E-03	7.54E-03
16	2	15	1	17	1	16	0	948.539004	1.50E-03	4.83E-03
16	2	15	1	17	2	16	0	948.539004	1.50E-03	7.54E-03
17	1	17	1	18	0	18	0	948.539004	1.50E-03	5.95E-03
17	1	17	1	18	1	18	0	948.539004	1.50E-03	8.13E-03
14	3	12	1	15	2	13	0	948.601355	1.50E-03	3.47E-03
14	3	12	1	15	3	13	0	948.601355	1.50E-03	6.92E-03
15	1	14	1	16	1	15	0	948.601355	1.50E-03	7.47E-03
15	2	14	1	16	1	15	0	948.601355	1.50E-03	4.72E-03
15	2	14	1	16	2	15	0	948.601355	1.50E-03	7.47E-03
16	1	16	1	17	0	17	0	948.601355	1.50E-03	5.90E-03
16	1	16	1	17	1	17	0	948.601355	1.50E-03	8.09E-03
13	3	11	1	14	3	12	0	948.661181	1.50E-03	6.76E-03
14	1	13	1	15	1	14	0	948.661181	1.50E-03	7.35E-03
14	2	13	1	15	1	14	0	948.661181	1.50E-03	4.56E-03
14	2	13	1	15	2	14	0	948.661181	1.50E-03	7.35E-03
15	1	15	1	16	0	16	0	948.661181	1.50E-03	5.81E-03
15	1	15	1	16	1	16	0	948.661181	1.50E-03	8.00E-03
12	3	10	1	13	3	11	0	948.723362	1.50E-03	6.55E-03
13	1	12	1	14	1	13	0	948.723362	1.50E-03	7.17E-03
13	2	12	1	14	1	13	0	948.723362	1.50E-03	4.36E-03
13	2	12	1	14	2	13	0	948.723362	1.50E-03	7.17E-03

Continued on next page

TABLE S10 – *Continued from previous page*

J'	K'_a	K'_c	v'	J''	K''_a	K''_c	v''	freq.	unc.	weigh
14	1	14	1	15	0	15	0	948.723362	1.50E-03	5.68E-03
14	1	14	1	15	1	15	0	948.723362	1.50E-03	7.86E-03
10	4	6	1	11	4	7	0	948.783136	1.50E-03	5.53E-03
12	1	11	1	13	1	12	0	948.783136	1.50E-03	6.94E-03
12	2	11	1	13	1	12	0	948.783136	1.50E-03	4.12E-03
12	2	11	1	13	2	12	0	948.783136	1.50E-03	6.94E-03
13	1	13	1	14	0	14	0	948.783136	1.50E-03	5.51E-03
13	1	13	1	14	1	14	0	948.783136	1.50E-03	7.66E-03
11	3	9	1	12	2	10	0	948.810485	1.50E-03	2.54E-03
11	1	10	1	12	1	11	0	948.843423	1.50E-03	6.65E-03
11	2	10	1	12	1	11	0	948.843423	1.50E-03	3.83E-03
11	2	10	1	12	2	11	0	948.843423	1.50E-03	6.65E-03
12	1	12	1	13	0	13	0	948.843423	1.50E-03	5.30E-03
12	1	12	1	13	1	13	0	948.843423	1.50E-03	7.41E-03
9	4	5	1	10	4	6	0	948.871566	1.50E-03	5.06E-03
10	3	8	1	11	2	9	0	948.893628	1.50E-03	2.11E-03
10	2	9	1	11	1	10	0	948.906735	1.50E-03	3.50E-03
10	2	9	1	11	2	10	0	948.906735	1.50E-03	6.31E-03
11	1	11	1	12	0	12	0	948.906735	1.50E-03	5.04E-03
10	1	10	1	11	0	11	0	948.967979	1.50E-03	4.74E-03
9	1	9	1	10	0	10	0	949.025689	1.50E-03	4.40E-03
12	1	12	1	11	0	11	0	950.40104	1.50E-03	5.23E-03
12	1	12	1	11	1	11	0	950.40104	1.50E-03	7.37E-03
12	1	11	1	11	1	10	0	950.461337	1.50E-03	6.93E-03
13	1	13	1	12	0	12	0	950.461337	1.50E-03	5.51E-03
13	1	13	1	12	1	12	0	950.461337	1.50E-03	7.72E-03
13	1	12	1	12	1	11	0	950.520025	1.50E-03	7.25E-03
14	1	14	1	13	0	13	0	950.520025	1.50E-03	5.75E-03
14	1	14	1	13	1	13	0	950.520025	1.50E-03	8.00E-03
14	1	13	1	13	1	12	0	950.580138	1.50E-03	7.51E-03
15	1	15	1	14	0	14	0	950.580138	1.50E-03	5.95E-03
15	1	15	1	14	1	14	0	950.580138	1.50E-03	8.24E-03
15	1	14	1	14	1	13	0	950.637997	1.50E-03	7.72E-03
16	1	16	1	15	0	15	0	950.637997	1.50E-03	6.11E-03
16	1	16	1	15	1	15	0	950.637997	1.50E-03	8.41E-03
16	1	15	1	15	1	14	0	950.696372	1.50E-03	7.87E-03
17	1	17	1	16	0	16	0	950.696372	1.50E-03	6.22E-03
17	1	17	1	16	1	16	0	950.696372	1.50E-03	8.53E-03
17	1	16	1	16	1	15	0	950.755995	1.50E-03	7.97E-03
18	1	18	1	17	0	17	0	950.755995	1.50E-03	6.29E-03
18	1	18	1	17	1	17	0	950.755995	1.50E-03	8.60E-03
18	1	17	1	17	1	16	0	950.815167	1.50E-03	8.02E-03
19	1	19	1	18	0	18	0	950.815167	1.50E-03	6.32E-03
19	1	19	1	18	1	18	0	950.815167	1.50E-03	8.61E-03
17	3	14	1	16	3	13	0	950.875608	1.50E-03	7.15E-03
19	1	18	1	18	1	17	0	950.875608	1.50E-03	8.02E-03
20	1	20	1	19	0	19	0	950.875608	1.50E-03	6.31E-03
20	1	20	1	19	1	19	0	950.875608	1.50E-03	8.58E-03

Continued on next page

TABLE S10 – *Continued from previous page*

J'	K'_a	K'_c	v'	J''	K''_a	K''_c	v''	freq.	unc.	weight
18	3	15	1	17	3	14	0	950.931407	1.50E-03	7.15E-03
21	1	21	1	20	0	20	0	950.931407	1.50E-03	6.26E-03
21	1	21	1	20	1	20	0	950.931407	1.50E-03	8.50E-03
19	3	16	1	18	3	15	0	950.986396	1.50E-03	7.11E-03
22	1	22	1	21	0	21	0	950.990556	1.50E-03	6.18E-03
22	1	22	1	21	1	21	0	950.990556	1.50E-03	8.37E-03
23	1	23	1	22	0	22	0	951.048434	1.50E-03	6.08E-03
23	1	23	1	22	1	22	0	951.048434	1.50E-03	8.21E-03
24	1	24	1	23	0	23	0	951.104536	1.50E-03	5.94E-03
25	1	24	1	24	1	23	0	951.220641	1.50E-03	7.17E-03
25	2	24	1	24	1	23	0	951.220641	1.50E-03	4.91E-03
25	2	24	1	24	2	23	0	951.220641	1.50E-03	7.17E-03
26	1	26	1	25	0	25	0	951.220641	1.50E-03	5.60E-03
26	1	26	1	25	1	25	0	951.220641	1.50E-03	7.53E-03
26	1	25	1	25	1	24	0	951.278349	1.50E-03	6.91E-03
26	2	25	1	25	1	24	0	951.278349	1.50E-03	4.76E-03
26	2	25	1	25	2	24	0	951.278349	1.50E-03	6.91E-03
27	1	27	1	26	0	26	0	951.278349	1.50E-03	5.40E-03
27	1	27	1	26	1	26	0	951.278349	1.50E-03	7.25E-03
28	1	27	1	27	1	26	0	951.394905	1.50E-03	6.35E-03
28	2	27	1	27	1	26	0	951.394905	1.50E-03	4.41E-03
28	2	27	1	27	2	26	0	951.394905	1.50E-03	6.35E-03
29	1	29	1	28	0	28	0	951.394905	1.50E-03	4.95E-03
29	1	29	1	28	1	28	0	951.394905	1.50E-03	6.63E-03
29	1	28	1	28	1	27	0	951.452779	1.50E-03	6.05E-03
29	2	28	1	28	1	27	0	951.452779	1.50E-03	4.22E-03
29	2	28	1	28	2	27	0	951.452779	1.50E-03	6.05E-03
30	1	30	1	29	0	29	0	951.452779	1.50E-03	4.71E-03
30	1	30	1	29	1	29	0	951.452779	1.50E-03	6.31E-03
30	2	29	1	29	1	28	0	951.509239	1.50E-03	4.02E-03
30	2	29	1	29	2	28	0	951.509239	1.50E-03	5.74E-03
31	1	31	1	30	0	30	0	951.509239	1.50E-03	4.47E-03
31	1	31	1	30	1	30	0	951.509239	1.50E-03	5.97E-03
31	1	30	1	30	1	29	0	951.569515	1.50E-03	5.42E-03
31	2	30	1	30	1	29	0	951.569515	1.50E-03	3.81E-03
31	2	30	1	30	2	29	0	951.569515	1.50E-03	5.42E-03
32	1	32	1	31	1	31	0	951.569515	1.50E-03	5.63E-03
32	1	31	1	31	1	30	0	951.624818	1.50E-03	5.10E-03
32	2	31	1	31	1	30	0	951.624818	1.50E-03	3.60E-03
32	2	31	1	31	2	30	0	951.624818	1.50E-03	5.10E-03
33	1	33	1	32	0	32	0	951.624818	1.50E-03	3.97E-03
33	1	33	1	32	1	32	0	951.624818	1.50E-03	5.29E-03
30	4	26	1	29	4	25	0	951.672777	1.50E-03	4.46E-03
33	1	32	1	32	1	31	0	951.682377	1.50E-03	4.78E-03
33	2	32	1	32	1	31	0	951.682377	1.50E-03	3.38E-03
33	2	32	1	32	2	31	0	951.682377	1.50E-03	4.78E-03
34	1	34	1	33	0	33	0	951.682377	1.50E-03	3.72E-03
34	1	34	1	33	1	33	0	951.682377	1.50E-03	4.96E-03

Continued on next page

TABLE S10 – *Continued from previous page*

J'	K'_a	K'_c	v'	J''	K''_a	K''_c	v''	freq.	unc.	weigh
31	4	27	1	30	4	26	0	951.731481	1.50E-03	4.18E-03
34	1	33	1	33	1	32	0	951.741558	1.50E-03	4.47E-03
34	2	33	1	33	1	32	0	951.741558	1.50E-03	3.17E-03
34	2	33	1	33	2	32	0	951.741558	1.50E-03	4.47E-03
32	4	28	1	31	4	27	0	951.789692	1.50E-03	3.91E-03
35	1	34	1	34	1	33	0	951.799438	1.50E-03	4.16E-03
35	2	34	1	34	1	33	0	951.799438	1.50E-03	2.95E-03
35	2	34	1	34	2	33	0	951.799438	1.50E-03	4.16E-03
38	4	35	1	37	4	34	0	952.074777	1.50E-03	2.64E-03
40	1	39	1	39	1	38	0	952.082122	1.50E-03	2.74E-03
40	2	39	1	39	1	38	0	952.082122	1.50E-03	1.97E-03
39	4	36	1	38	4	35	0	952.131377	1.50E-03	2.41E-03
42	1	41	1	41	1	40	0	952.196281	1.50E-03	2.26E-03
42	2	41	1	41	1	40	0	952.196281	1.50E-03	1.63E-03
43	1	42	1	42	1	41	0	952.250334	1.50E-03	2.05E-03
43	2	42	1	42	1	41	0	952.250334	1.50E-03	1.48E-03
44	1	43	1	43	1	42	0	952.308213	1.50E-03	1.84E-03
44	2	43	1	43	1	42	0	952.308213	1.50E-03	1.33E-03
45	1	44	1	44	1	43	0	952.36385	1.50E-03	1.66E-03
46	1	45	1	45	1	44	0	952.418535	1.50E-03	1.48E-03
11	11	0	1	11	11	1	0	949.65196	1.50E-03	9.14E-03
11	11	1	1	11	11	0	0	949.65196	1.50E-03	9.14E-03
10	10	0	1	10	10	1	0	949.65196	1.50E-03	9.12E-03
10	10	1	1	10	10	0	0	949.65196	1.50E-03	9.12E-03
12	12	0	1	12	12	1	0	949.65196	1.50E-03	8.99E-03
12	12	1	1	12	12	0	0	949.65196	1.50E-03	8.99E-03
9	9	0	1	9	9	1	0	949.65196	1.50E-03	8.92E-03
9	9	1	1	9	9	0	0	949.65196	1.50E-03	8.92E-03
13	13	0	1	13	13	1	0	949.65196	1.50E-03	8.70E-03
13	13	1	1	13	13	0	0	949.65196	1.50E-03	8.70E-03
8	8	0	1	8	8	1	0	949.65196	1.50E-03	8.53E-03
8	8	1	1	8	8	0	0	949.65196	1.50E-03	8.53E-03
14	14	0	1	14	14	1	0	949.65196	1.50E-03	8.29E-03
14	14	1	1	14	14	0	0	949.65196	1.50E-03	8.29E-03
12	11	1	1	12	11	2	0	949.65196	1.50E-03	8.04E-03
12	11	2	1	12	11	1	0	949.65196	1.50E-03	8.04E-03
11	10	1	1	11	10	2	0	949.65196	1.50E-03	7.99E-03
11	10	2	1	11	10	1	0	949.65196	1.50E-03	7.99E-03
13	12	1	1	13	12	2	0	949.65196	1.50E-03	7.93E-03
13	12	2	1	13	12	1	0	949.65196	1.50E-03	7.93E-03