Probing intra- and inter-molecular interactions through rotational spectroscopy: the case of the odorant 2'-aminoacetophenone and its 1:1 water and neon complexes

SUPPLEMENTARY MATERIAL

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Table S1: Theoretical coordinates of 2AA(I).

	B3LYP-D3(BJ)/def2-TZVP			MP2/aug-cc-pVTZ		
	a/Å	b/Å	c/Å	a/Å	b/Å	c/Å
C1	−0.2085	−0.2271	0.0000	−0.2042	−0.2242	−0.0113
C2	0.5584	0.9750	0.0000	0.5532	0.9758	−0.0084
C3	1.9652	0.8741	0.0000	1.9569	0.8784	0.0117
C4	2.5931	−0.3500	0.0000	2.5980	−0.3475	0.0199
C5	1.8505	−1.5355	0.0000	1.8555	−1.5322	0.0052
C6	0.4750	−1.4557	0.0000	0.4734	−1.4571	−0.0097
C7	−1.6772	−0.1903	0.0000	−1.6790	−0.1977	0.0065
C8	−2.4486	−1.4953	0.0000	−2.4322	−1.5073	−0.0235
O9	−2.3098	0.8637	0.0000	−2.3165	0.8587	0.0517
N10	−0.0280	2.1946	0.0000	−0.0361	2.2082	−0.0663
H11	2.5498	1.7866	0.0000	2.5390	1.7930	0.0142
H12	3.6753	−0.3906	0.0000	3.6799	−0.3812	0.0356
H13	2.3463	−2.4960	0.0000	2.3509	−2.4932	0.0078
H14	−0.0993	−2.3707	0.0000	−0.1023	−2.3722	−0.0147
H15	−3.5102	−1.2623	0.0000	−3.4952	−1.2852	−0.0265
H16	−2.2101	−2.0947	−0.8800	−2.1751	−2.0837	−0.9118
H17	−2.2101	−2.0947	0.8800	−2.1894	−2.1132	0.8494
H18	−1.0369	2.2382	0.0000	−1.0333	2.2423	0.0901
H19	0.5361	3.0236	0.0000	0.5249	3.0077	0.1689

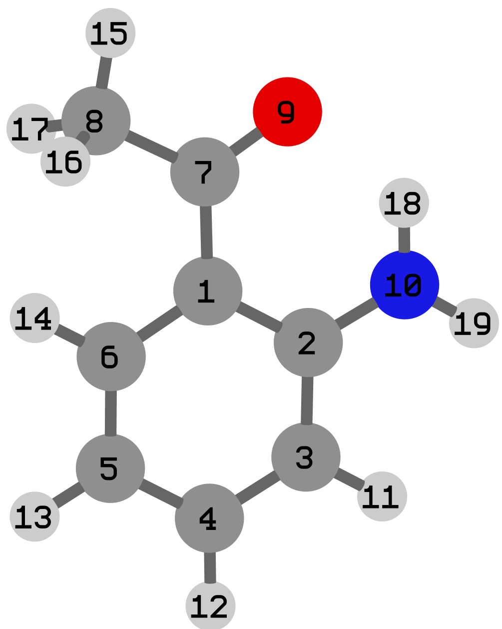

Table S2: Theoretical coordinates of 2AA(II).

	B3LYP-D3(BJ)/def2-TZVP			MP2/aug-cc-pVTZ		
	a/Å	b/Å	c/Å	a/Å	b/Å	c/Å
C1	−0.1925	0.2397	0.0225	−0.1853	0.2469	0.0238
C2	0.5169	−0.9817	0.0718	0.5083	−0.9771	0.0997
C3	1.9197	−0.9461	0.0133	1.9083	−0.9576	0.0341
C4	2.6076	0.2460	−0.0781	2.6116	0.2311	−0.0952
C5	1.9163	1.4569	−0.1020	1.9265	1.4463	−0.1449
C6	0.5389	1.4361	−0.0440	0.5424	1.4420	−0.0759
C7	−1.6779	0.3935	0.0138	−1.6722	0.3894	0.0181
C8	−2.5784	−0.7561	−0.3968	−2.5353	−0.7078	−0.5648
O9	−2.1861	1.4640	0.2895	−2.1932	1.4197	0.4260
N10	−0.0299	−2.3552	−0.0611	−0.1369	−2.2146	0.2048
H11	2.4644	−1.8826	0.0498	2.4456	−1.8876	0.0937
H12	3.6893	0.2335	−0.1231	3.6924	0.2076	−0.1475
H13	2.4493	2.3953	−0.1680	2.4664	2.3784	−0.2396
H14	−0.0299	2.3552	−0.0611	−0.0218	2.3649	−0.1101
H15	−3.1503	−0.3334	−0.7657	−3.3948	−0.2359	−1.0350
H16	−2.8252	−1.3671	0.4780	−2.9149	−1.3418	0.2401
H17	−2.1254	−1.4011	−1.1481	−1.9963	−1.3330	−1.2718
H18	−0.9900	−2.2821	0.5945	−1.0010	−2.2104	0.7227
H19	0.5213	−2.9781	0.4200	0.4723	−2.9477	0.5369

Table S3: Theoretical coordinates of 2AA·H_2O(I).

	B3LYP-D3(BJ)/def2-TZVP			MP2/aug-cc-pVTZ		
	a/Å	b/Å	c/Å	a/Å	b/Å	c/Å
C1	0.4156	−0.2710	−0.0108	0.4147	−0.2597	−0.0209
C2	1.0693	0.9973	−0.0020	1.0789	0.9949	−0.0095
C3	2.4798	1.0254	0.0135	2.4860	1.0037	0.0274
C4	3.2168	−0.1352	0.0169	3.2176	−0.1695	0.0449
C5	2.5863	−1.3848	0.0053	2.5672	−1.4076	0.0232
C6	1.2110	−1.4327	−0.0075	1.1848	−1.4384	−0.0086
C7	−1.0438	−0.3771	−0.0148	−1.0530	−0.3522	−0.0244
C8	−1.6926	−1.7431	−0.0108	−1.7039	−1.7122	−0.0551
O9	−1.7682	0.6251	−0.0180	−1.7662	0.6619	0.0039
N10	0.3798	2.1612	−0.0153	0.4040	2.1815	−0.0740
H11	2.9779	1.9875	0.0215	2.9969	1.9598	0.0359
H12	4.2980	−0.0762	0.0287	4.2986	−0.1210	0.0736
H13	3.1687	−2.2953	0.0077	3.1341	−2.3281	0.0337
H14	0.7234	−2.3964	−0.0139	0.6806	−2.3944	−0.0193
H15	−2.7732	−1.6246	−0.0214	−2.7832	−1.5921	−0.0775
H16	−1.4014	−2.3064	0.8776	−1.4209	−2.2876	0.8262
H17	−1.3824	−2.3229	−0.8819	−1.3799	−2.2698	−0.9335
H18	−0.6277	2.1224	0.0137	−0.5937	2.1499	0.0704
H19	0.8702	3.0337	0.0493	0.9057	3.0196	0.1614
O_w	−4.5764	0.1615	0.0771	−4.5501	0.0971	0.0743
H_{HB}	−3.6395	0.4281	0.0694	−3.6419	0.4418	0.0376
H_{free}	−4.9375	0.4827	−0.7545	−5.1090	0.8458	−0.1484

Table S4: Theoretical coordinates of $2AA \cdot H_2O$(II).

	B3LYP-D3(BJ)/def2-TZVP			MP2/aug-cc-pVTZ		
	a/Å	b/Å	c/Å	a/Å	b/Å	c/Å
C1	−0.4680	0.4530	−0.0134	−0.4731	0.4470	−0.0240
C2	−0.4137	−0.9740	−0.0303	−0.4162	−0.9723	−0.0708
C3	−1.6348	−1.6858	−0.0052	−1.6333	−1.6829	−0.0196
C4	−2.8454	−1.0377	0.0295	−2.8521	−1.0379	0.0684
C5	−2.9084	0.3610	0.0411	−2.9105	0.3595	0.1078
C6	−1.7323	1.0739	0.0203	−1.7301	1.0778	0.0615
C7	0.7451	1.2713	−0.0220	0.7436	1.2699	−0.0505
C8	0.6240	2.7821	−0.0002	0.6150	2.7750	−0.0218
O9	1.8738	0.7807	−0.0457	1.8734	0.7707	−0.0931
N10	0.7418	−1.6709	−0.0788	0.7445	−1.6722	−0.1988
H11	−1.5982	−2.7687	−0.0155	−1.5978	−2.7659	−0.0549
H12	−3.7581	−1.6202	0.0478	−3.7613	−1.6243	0.1061
H13	−3.8615	0.8702	0.0676	−3.8604	0.8711	0.1751
H14	−1.7799	2.1528	0.0321	−1.7724	2.1573	0.0960
H15	1.6258	3.2034	−0.0144	1.6132	3.2005	−0.0650
H16	0.1026	3.1230	0.8960	0.1190	3.1032	0.8913
H17	0.0664	3.1470	−0.8645	0.0278	3.1316	−0.8676
H18	1.6385	−1.2141	−0.0461	1.6335	−1.2142	−0.0803
H19	0.7124	−2.6722	−0.0179	0.7111	−2.6658	−0.0537
O_w	3.8915	−1.1736	0.1285	3.8928	−1.1547	0.2390
H_{HB}	3.4733	−0.3004	0.1670	3.5059	−0.2783	0.1063
H_{free}	4.3711	−1.1848	−0.7056	4.5959	−1.2117	−0.4135

Table S5: Theoretical coordinates (Å) of $2AA \cdot Ne$(I).

	B3LYP-D3(BJ)/def2-TZVP			MP2/aug-cc-pVTZ		
	a/Å	b/Å	c/Å	a/Å	b/Å	c/Å
C1	0.0182	−0.4807	−0.2342	0.0023	−0.4697	−0.2501
C2	0.6387	0.7391	−0.6338	0.6271	0.7490	−0.6210
C3	2.0222	0.8944	−0.4082	2.0098	0.8844	−0.3980
C4	2.7654	−0.1017	0.1820	2.7572	−0.1375	0.1599
C5	2.1670	−1.3026	0.5772	2.1474	−1.3444	0.5155
C6	0.8160	−1.4710	0.3650	0.7871	−1.4951	0.3081
C7	−1.4204	−0.7010	−0.4336	−1.4501	−0.6654	−0.4156
C8	−2.0363	−2.0110	0.0162	−2.0567	−1.9919	−0.0211
O9	−2.1503	0.1416	−0.9514	−2.1864	0.2220	−0.8570
N10	−0.0632	1.7378	−1.2177	−0.0620	1.7671	−1.2192
H11	2.4954	1.8211	−0.7107	2.4907	1.8144	−0.6795
H12	3.8257	0.0512	0.3403	3.8189	0.0049	0.3165
H13	2.7531	−2.0838	1.0405	2.7268	−2.1481	0.9484
H14	0.3529	−2.3978	0.6709	0.3129	−2.4252	0.5889
H15	−3.0976	−1.9850	−0.2164	−3.1207	−1.9533	−0.2347
H16	−1.9051	−2.1596	1.0896	−1.9053	−2.1855	1.0408
H17	−1.5753	−2.8596	−0.4926	−1.6001	−2.8099	−0.5778
H18	−1.0543	1.6043	−1.3584	−1.0698	1.7016	−1.2058
H19	0.3961	2.5912	−1.4748	0.3698	2.6739	−1.2437
Ne	−1.3295	1.6044	2.0118	−1.2049	1.5367	2.0259

Table S6: Theoretical coordinates (Å) of 2AA·Ne(II).

	B3LYP-D3(BJ)/def2-TZVP			MP2/aug-cc-pVTZ		
	a/Å	b/Å	c/Å	a/Å	b/Å	c/Å
C1	0.4011	−0.2076	0.3577	0.3846	−0.2100	0.3379
C2	−0.3449	1.0038	0.4511	−0.3543	0.9970	0.4377
C3	−1.7249	0.9232	0.7302	−1.7313	0.9151	0.7150
C4	−2.3477	−0.2907	0.9061	−2.3666	−0.3033	0.8763
C5	−1.6260	−1.4854	0.8148	−1.6446	−1.4954	0.7647
C6	−0.2762	−1.4252	0.5452	−0.2872	−1.4351	0.5001
C7	1.8407	−0.1917	0.0663	1.8380	−0.1984	0.0868
C8	2.5897	−1.5063	−0.0278	2.5664	−1.5163	−0.0392
O9	2.4666	0.8521	−0.1067	2.4781	0.8522	−0.0186
N10	0.2359	2.2136	0.2774	0.2738	−2.3559	0.4208
H11	−2.2933	1.8430	0.8016	−2.2992	1.8354	0.7926
H12	−3.4095	−0.3160	1.1174	−3.4281	−0.3254	1.0874
H13	−2.1179	−2.4380	0.9530	−2.1360	−2.4508	0.8859
H14	0.2819	−2.3474	0.4743	0.2738	−2.3559	0.4208
H15	3.6323	−1.2886	−0.2443	3.6126	−1.3059	−0.2403
H16	2.1805	−2.1370	−0.8193	2.1499	−2.1140	−0.8496
H17	2.5236	−2.0665	0.9066	2.4813	−2.0952	0.8803
H18	1.2261	2.2430	0.0807	1.2287	2.2494	0.2040
H19	−0.3122	3.0499	0.3526	−0.2852	3.0327	0.5380
Ne	−1.3316	−0.1493	−2.5986	−1.2594	−0.1107	−2.5414

Table S7: Experimental rotational transition frequencies of 2AA.

J'	K_a'	K_c'	F'	J"	K_a"	K_c"	F"	ν/MHz	$\Delta\nu_{o-c}$
1	1	1	0	0	0	0	1	3019.896	0.001
1	1	1	1	0	0	0	1	3021.851	0.001
1	1	1	2	0	0	0	1	3021.070	0.001
2	0	2	1	1	0	1	2	3879.577	-0.004
2	0	2	1	1	0	1	1	3879.224	0.001
2	0	2	1	1	0	1	0	3880.117	0.000
2	0	2	2	1	0	1	1	3880.317	0.003
2	0	2	2	1	0	1	2	3880.673	0.001
2	0	2	3	1	0	1	2	3879.972	0.002
2	0	2	1	1	1	1	0	2851.397	-0.005
2	0	2	1	1	1	1	1	2849.448	0.002
2	0	2	2	1	1	1	1	2850.539	0.002
2	0	2	2	1	1	1	2	2851.316	-0.004
2	0	2	3	1	1	1	2	2850.623	0.005
2	1	1	1	1	1	0	2	4401.662	0.007
2	1	1	1	1	1	0	0	4399.947	0.002
2	1	1	1	1	1	0	1	4402.797	0.002
2	1	1	2	1	1	0	2	4400.355	0.004
2	1	1	2	1	1	0	1	4401.493	0.003
2	1	1	3	1	1	0	2	4401.193	0.004
2	1	2	1	1	1	1	1	3564.309	-0.001
2	1	2	1	1	1	1	0	3566.264	-0.002
2	1	2	1	1	1	1	2	3565.089	-0.003
2	1	2	2	1	1	1	1	3566.216	0.006
2	1	2	2	1	1	1	2	3566.993	0.001
2	1	2	3	1	1	1	2	3565.772	0.002
2	1	2	1	1	0	1	1	4594.090	0.003
2	1	2	1	1	0	1	0	4594.982	0.001
2	1	2	1	1	0	1	2	4594.441	-0.003
2	1	2	2	1	0	1	1	4595.991	0.005
2	1	2	2	1	0	1	2	4596.345	0.001
2	1	2	3	1	0	1	2	4595.124	0.002
2	2	0	1	2	1	1	1	3191.655	0.008
2	2	0	1	2	1	1	2	3192.949	-0.003
2	2	0	2	2	1	1	2	3191.860	-0.001
2	2	0	2	2	1	1	3	3191.020	-0.002
2	2	0	2	2	1	1	1	3190.557	0.001
2	2	0	3	2	1	1	3	3191.720	-0.004
2	2	0	3	2	1	1	2	3192.567	0.005
2	2	0	2	1	1	1	1	8009.397	0.007
2	2	0	3	1	1	1	2	8010.879	0.006
2	2	1	1	1	1	0	0	7487.862	0.003
2	2	1	1	1	1	0	1	7490.711	0.001
2	2	1	2	1	1	0	1	7490.111	-0.002
2	2	1	2	1	1	0	2	7488.973	0.000
2	2	1	3	1	1	0	2	7489.356	0.000
2	2	1	1	2	0	2	1	5057.294	-0.008
2	2	1	3	2	0	2	3	5056.687	-0.011
2	2	1	2	2	0	2	2	5055.620	0.006
2	2	1	2	2	1	2	2	4339.943	0.002
2	2	1	2	2	1	2	2	4339.941	0.000
2	2	1	3	2	1	2	2	4340.316	-0.008
2	2	1	2	2	1	2	3	4341.162	0.000
2	2	1	3	2	1	2	3	4341.541	-0.005
2	2	1	2	2	1	2	1	4341.846	0.005
2	2	1	1	2	1	2	1	4342.441	0.003
3	0	3	2	2	1	2	2	4880.487	0.004

J'	K_a'	K_c'	F'	J"	K_a"	K_c"	F"	ν/MHz	$\Delta\nu_{o-c}$
3	0	3	2	2	1	2	1	4882.384	0.001
3	0	3	3	2	1	2	2	4881.995	0.002
3	0	3	3	2	1	2	3	4883.212	-0.003
3	0	3	4	2	1	2	3	4882.098	0.002
3	0	3	2	2	0	2	1	5597.250	0.003
3	0	3	2	2	0	2	2	5596.155	0.000
3	0	3	4	2	0	2	3	5597.250	0.001
3	0	3	3	2	0	2	2	5597.668	0.001
3	0	3	3	2	0	2	3	5598.369	0.002
3	1	2	3	2	1	1	3	6526.182	0.002
3	1	2	2	2	1	1	1	6526.580	0.001
3	1	2	4	2	1	1	3	6526.823	0.002
3	1	2	3	2	1	1	2	6527.020	0.002
3	1	2	2	2	1	1	2	6527.884	0.000
3	1	2	4	2	2	1	3	3438.659	0.000
3	1	2	2	2	2	1	1	3438.659	0.000
3	1	2	3	2	2	1	2	3438.392	-0.004
3	1	2	3	3	0	3	3	2896.346	0.002
3	1	2	4	3	0	3	4	2898.105	0.002
3	1	2	2	3	0	3	2	2898.725	0.005
3	1	2	4	3	1	3	4	2489.736	0.000
3	1	2	2	3	1	3	2	2490.474	0.004
3	1	2	3	3	1	3	3	2487.640	0.001
3	1	3	2	2	1	2	2	5288.733	0.000
3	1	3	4	2	1	2	3	5290.466	0.002
3	1	3	2	2	1	2	1	5290.634	0.001
3	1	3	3	2	1	2	2	5290.699	0.002
3	1	3	3	2	1	2	3	5291.921	0.001
3	1	3	2	2	0	2	1	6005.495	-0.001
3	1	3	4	2	0	2	3	6005.616	0.000
3	1	3	3	2	0	2	2	6006.370	-0.001
3	1	3	3	2	0	2	3	6007.066	-0.006
3	1	3	2	2	0	2	2	6004.405	-0.001
3	2	1	4	3	1	2	4	3018.205	-0.006
3	2	1	3	3	1	2	3	3018.128	-0.003
3	2	1	2	2	2	0	2	6354.266	0.003
3	2	1	4	2	2	0	3	6353.317	0.009
3	2	1	3	2	2	0	2	6353.277	-0.011
3	2	1	2	2	2	0	1	6353.169	-0.002
3	2	1	3	2	2	0	3	6352.590	0.003
3	2	2	2	2	2	1	1	5975.030	0.000
3	2	2	4	2	2	1	3	5975.247	0.004
3	2	2	3	2	2	1	2	5975.631	0.004
3	2	2	3	3	0	3	3	5433.575	0.001
3	2	2	4	3	0	3	4	5434.692	-0.001
3	2	2	2	3	0	3	2	5435.094	0.010
3	2	2	3	3	1	3	3	5024.872	0.002
3	2	2	4	3	1	3	4	5026.326	0.001
3	2	2	2	3	1	3	2	5026.841	0.007
3	3	0	4	3	2	1	4	5784.696	0.005
3	3	0	3	3	2	1	3	5784.785	-0.002
4	0	4	3	3	0	3	3	7174.319	-0.002
4	0	4	5	3	0	3	4	7175.822	-0.003
4	0	4	3	3	0	3	2	7175.822	-0.003
4	0	4	4	3	0	3	3	7176.178	-0.001
4	0	4	4	3	0	3	4	7177.296	-0.001
4	0	4	3	3	1	3	3	6765.618	0.001
4	0	4	5	3	1	3	4	6767.440	-0.012
4	0	4	3	3	1	3	2	6767.580	-0.001

J'	K_a'	K_c'	F'	J"	K_a"	K_c"	F"	ν/MHz	$\Delta\nu_{o-c}$
4	0	4	4	3	1	3	4	6768.919	-0.010
4	1	3	3	3	2	2	2	6003.887	-0.006
4	1	3	5	3	2	2	4	6003.794	-0.001
4	1	3	4	3	2	2	3	6003.410	0.000
4	1	3	4	4	0	4	4	4260.803	-0.002
4	1	3	5	4	0	4	5	4262.669	0.001
4	1	3	3	4	0	4	3	4263.140	-0.007
4	1	3	4	4	1	4	4	4062.862	0.000
4	1	3	5	4	1	4	5	4064.885	-0.002
4	1	3	3	4	1	4	3	4065.404	-0.003
4	1	4	5	3	1	3	4	6965.233	0.000
4	1	4	3	3	1	3	2	6965.320	-0.001
4	1	4	4	3	1	3	3	6965.418	0.000
4	1	4	4	3	1	3	4	6966.873	-0.001
4	1	4	3	3	1	3	3	6963.352	-0.004
4	1	4	3	3	0	3	3	7372.048	-0.012
4	1	4	5	3	0	3	4	7373.610	0.009
4	1	4	4	3	0	3	3	7374.121	-0.001
4	1	4	4	3	0	3	4	7375.241	-0.001
4	2	2	4	4	1	3	4	3151.777	0.000
4	2	2	5	4	1	3	5	3152.218	0.002
4	2	2	3	4	1	3	3	3152.329	-0.001
4	2	3	3	3	2	2	2	7885.256	0.001
4	2	3	5	3	2	2	4	7885.315	-0.003
4	2	3	4	3	2	2	3	7885.564	0.002
4	2	3	4	4	0	4	4	6142.959	0.002
4	2	3	5	4	0	4	5	6144.195	0.003
4	2	3	3	4	0	4	3	6144.507	-0.002
4	2	3	4	4	1	4	4	5945.012	-0.002
4	2	3	5	4	1	4	5	5946.414	0.004
4	2	3	3	4	1	4	3	5946.775	0.005
4	3	1	3	4	2	2	3	5339.246	0.000
4	3	1	5	4	2	2	5	5339.325	-0.003
4	3	1	4	4	2	2	4	5339.649	0.002
4	3	2	4	4	2	3	4	6497.331	-0.002
4	3	2	5	4	2	3	5	6497.917	-0.004
5	1	4	6	5	0	5	6	5935.950	-0.009
5	1	4	5	5	0	5	4	5936.300	0.006
5	1	4	4	5	0	5	4	5936.300	0.006
5	2	3	5	5	1	4	5	3729.978	-0.003
5	2	3	6	5	1	4	6	3730.768	-0.007
5	2	3	4	5	1	4	4	3730.943	0.006
5	2	3	5	5	2	4	5	2501.139	-0.007
5	2	3	6	5	2	4	6	2502.432	-0.005
5	2	4	5	5	0	5	5	7163.021	0.000
5	2	4	6	5	0	5	6	7164.296	-0.001
5	3	2	6	5	2	3	6	4856.093	-0.010
5	3	2	5	5	2	3	5	4856.351	-0.005
5	3	2	4	5	2	3	4	4856.051	-0.001
6	3	3	7	6	2	4	7	4579.948	-0.004
6	3	3	5	6	2	4	5	4579.948	-0.004
6	3	3	6	6	2	4	6	4579.948	-0.004

Table S8: Experimental rotational transition frequencies of 2AA·H_2O.

J'	K_a'	K_c'	F'	J"	K_a"	K_c"	F"	ν/MHz	$\Delta\nu_{o-c}$
1	1	1	2	0	0	0	1	2666.881	-0.001
2	0	2	1	1	0	1	1	2125.566	-0.002
2	0	2	3	1	0	1	2	2126.202	0.000
2	0	2	2	1	0	1	1	2126.307	0.003
2	0	2	1	1	0	1	0	2126.492	-0.003
2	0	2	2	1	0	1	2	2126.676	0.001
2	1	1	1	1	1	0	0	2257.257	0.002
2	1	1	2	1	1	0	2	2257.685	0.001
2	1	1	3	1	1	0	2	2258.507	0.002
2	1	1	2	1	1	0	1	2258.820	-0.002
2	1	1	1	1	1	0	1	2260.098	-0.003
2	1	2	2	1	0	1	2	3609.465	-0.001
2	1	2	2	1	0	1	1	3609.089	-0.006
2	1	2	3	1	0	1	2	3608.243	-0.003
2	1	2	1	1	0	1	0	3608.124	-0.002
2	1	2	1	1	0	1	1	3607.190	-0.008
2	1	2	3	1	1	1	2	2007.959	0.001
2	1	2	2	1	1	1	1	2008.399	-0.012
2	1	2	2	1	1	1	2	2009.176	-0.002
2	1	2	1	1	1	1	1	2006.508	-0.006
2	2	0	3	1	1	1	2	7192.079	0.004
2	2	1	3	1	1	0	2	7059.481	0.009
3	0	3	2	2	0	2	2	3171.124	-0.002
3	0	3	4	2	0	2	3	3171.814	0.002
3	0	3	3	2	0	2	2	3171.944	-0.002
3	0	3	3	2	0	2	3	3172.418	-0.002
3	1	2	3	2	1	1	3	3382.499	0.002
3	1	2	2	2	1	1	1	3383.016	0.000
3	1	2	4	2	1	1	3	3383.220	0.000
3	1	2	3	2	1	1	2	3383.318	0.000
3	1	2	2	2	1	1	2	3384.293	-0.002
3	1	3	4	2	0	2	3	4489.823	0.001
3	1	3	2	2	0	2	1	4489.599	0.001
3	1	3	3	2	0	2	2	4490.736	-0.004
3	1	3	2	2	1	2	2	3006.070	-0.001
3	1	3	4	2	1	2	3	3007.776	-0.002
3	1	3	3	2	1	2	2	3007.944	-0.006
3	1	3	3	2	1	2	3	3009.166	-0.003
3	2	1	2	2	2	0	1	3227.796	-0.008
3	2	1	4	2	2	0	3	3228.003	0.004
3	2	1	3	2	2	0	2	3228.279	0.001
3	2	1	2	2	2	0	2	3228.538	-0.003
3	2	1	2	3	1	2	2	4652.634	-0.006
3	2	1	4	3	1	2	4	4652.832	0.007
3	2	1	3	3	1	2	3	4653.357	0.003
3	2	2	2	2	2	1	1	3199.643	-0.001
3	2	2	4	2	2	1	3	3199.871	0.006
3	2	2	2	2	2	1	3	3199.871	0.006
3	2	2	3	2	2	1	2	3200.268	0.005
3	2	2	4	3	1	3	4	5369.126	0.001
3	2	2	2	3	1	3	2	5369.609	-0.003
3	2	2	3	3	1	3	3	5367.734	0.000
4	0	4	3	3	0	3	3	4196.438	-0.002
4	0	4	5	3	0	3	4	4197.245	-0.008
4	0	4	3	3	0	3	2	4197.245	-0.008
4	0	4	4	3	0	3	3	4197.411	-0.002

J'	K_a'	K_c'	F'	J"	K_a"	K_c"	F"	ν/MHz	$\Delta\nu_{o-c}$
4	0	4	4	3	0	3	4	4198.020	0.000
4	0	4	4	3	1	3	3	2878.627	0.009
4	0	4	5	3	1	3	4	2879.238	0.002
4	0	4	3	3	1	3	2	2879.529	0.004
4	1	3	5	3	1	2	4	4502.116	0.001
4	1	3	4	3	1	2	3	4502.186	0.004
4	1	3	3	3	1	2	2	4502.032	0.001
4	1	3	4	3	1	2	4	4501.459	0.001
4	1	3	3	3	1	2	3	4503.010	0.002
4	1	3	4	4	0	4	4	2372.964	0.001
4	1	3	4	4	0	4	4	2372.962	-0.001
4	1	3	5	4	0	4	5	2374.397	0.005
4	1	4	3	3	0	3	2	5320.576	-0.001
4	1	4	5	3	0	3	4	5320.751	0.002
4	1	4	4	3	0	3	3	5321.641	-0.002
4	1	4	3	3	1	3	3	4000.957	-0.006
4	1	4	5	3	1	3	4	4002.737	-0.002
4	1	4	3	3	1	3	2	4002.842	-0.002
4	1	4	4	3	1	3	3	4002.842	-0.002
4	1	4	4	3	1	3	4	4004.234	-0.006
4	2	2	5	3	2	1	4	4330.427	0.008
4	2	2	4	3	2	1	3	4330.427	0.008
4	2	2	3	3	2	1	3	4330.636	-0.005
4	2	2	4	3	2	1	4	4330.238	-0.001
4	2	2	4	4	1	3	4	4481.601	-0.003
4	2	2	5	4	1	3	5	4481.115	0.002
4	2	2	3	4	1	3	3	4480.975	-0.012
4	2	3	3	3	2	2	2	4261.012	0.006
4	2	3	5	3	2	2	4	4261.050	-0.005
4	2	3	4	3	2	2	3	4261.245	0.003
4	2	3	3	4	1	4	3	5627.786	0.009
4	2	3	5	4	1	4	5	5627.438	-0.002
5	0	5	5	4	1	4	4	4074.227	-0.003
5	0	5	6	4	1	4	5	4074.765	0.000
5	0	5	4	4	1	4	3	4074.947	-0.007
5	0	5	6	4	0	4	5	5198.269	0.001
5	0	5	5	4	0	4	4	5198.460	0.000
5	0	5	5	4	0	4	5	5199.231	-0.002
5	0	5	4	4	0	4	4	5197.292	-0.005
5	1	4	6	4	1	3	5	5612.658	-0.006
5	1	4	5	4	1	3	4	5612.735	0.001
5	1	4	5	4	1	3	5	5612.077	0.000
5	1	4	4	4	1	3	4	5613.439	-0.001
5	1	4	6	5	0	5	6	2788.790	0.002
5	1	4	5	5	0	5	5	2787.225	-0.012
5	1	5	6	4	1	4	5	4991.815	0.002
5	1	5	5	4	1	4	5	4993.401	0.001
5	1	5	4	4	1	4	4	4989.998	0.009
5	1	5	5	4	1	4	4	4991.909	0.009
5	1	5	6	4	0	4	5	6115.315	0.000
5	1	5	4	4	0	4	3	6115.192	0.000
5	1	5	5	4	0	4	4	6116.128	-0.001
5	2	3	5	4	2	2	4	5452.388	0.004
5	2	3	6	4	2	2	5	5452.455	0.004
5	2	3	4	4	2	2	4	5452.663	0.000
5	2	3	5	4	2	2	5	5452.215	-0.005
5	2	3	4	5	1	4	4	4320.830	0.003
5	2	3	6	5	1	4	6	4320.906	0.006
5	2	3	5	5	1	4	5	4321.257	0.001

J'	K_a'	K_c'	F'	J"	K_a"	K_c"	F"	ν/MHz	$\Delta\nu_{o-c}$
5	2	4	4	4	2	3	4	5317.269	-0.004
5	2	4	4	4	2	3	3	5317.521	0.005
5	2	4	6	4	2	3	5	5317.521	0.005
5	2	4	5	4	2	3	4	5317.642	0.000
5	2	4	5	4	2	3	5	5317.831	0.002
5	3	2	6	4	3	1	5	5360.158	-0.001
5	3	2	5	4	3	1	4	5360.309	0.003
5	3	3	6	4	3	2	5	5354.953	0.003
5	3	3	5	4	3	2	4	5355.110	-0.002
6	0	6	5	5	0	5	5	6172.959	-0.004
6	0	6	6	5	0	5	6	6175.295	0.002
6	0	6	6	5	0	5	5	6174.328	0.001
6	0	6	7	5	0	5	6	6174.127	0.001
6	0	6	6	5	1	5	5	5256.659	0.001
6	0	6	7	5	1	5	6	5257.079	0.001
6	0	6	5	5	1	5	4	5257.210	0.006
6	1	5	5	5	1	4	4	6711.785	-0.016
6	1	5	6	5	1	4	5	6711.918	0.001
6	1	5	7	5	1	4	6	6711.836	0.001
6	1	5	5	5	1	4	5	6712.506	-0.001
6	1	5	7	6	1	6	7	2609.220	0.000
6	1	6	7	5	1	5	6	5974.364	0.007
6	1	6	6	5	1	5	5	5974.440	0.005
6	1	6	5	5	1	5	5	5972.488	0.000
6	1	6	6	5	1	5	6	5976.020	-0.003
6	1	6	7	5	0	5	6	6891.405	0.001
6	1	6	6	5	0	5	5	6892.106	0.001
6	1	6	5	5	0	5	4	6891.315	-0.004
6	2	4	7	5	2	3	6	6593.672	0.004
6	2	4	5	5	2	3	5	6593.958	0.003
6	2	4	5	5	2	3	4	6593.672	-0.006
6	2	4	6	5	2	3	5	6593.563	0.001
6	2	4	5	6	1	5	5	4202.698	-0.006
6	2	4	7	6	1	5	7	4202.730	-0.002
6	2	4	6	6	1	5	6	4202.905	0.003
6	2	5	5	5	2	4	4	6368.153	0.004
6	2	5	7	5	2	4	6	6368.153	0.004
6	2	5	6	5	2	4	5	6368.243	0.006
6	2	5	5	5	2	4	5	6367.784	0.005
6	2	5	6	5	2	4	6	6368.534	-0.009
6	3	3	7	5	3	2	6	6445.837	-0.003
6	3	3	6	5	3	2	5	6445.908	0.008
6	3	4	5	5	3	3	4	6432.054	0.001
6	3	4	7	5	3	3	6	6432.054	0.001
6	3	4	6	5	3	3	5	6432.148	-0.001
7	0	7	7	6	1	6	6	6410.707	0.005
7	0	7	8	6	1	6	7	6411.011	0.010
7	0	7	8	6	0	6	7	7128.285	0.003
7	0	7	6	6	0	6	5	7128.285	0.003
7	0	7	7	6	0	6	6	7128.483	0.003
7	1	6	8	6	1	5	7	7796.032	-0.001
7	1	6	7	6	1	5	6	7796.132	0.000
7	1	7	8	6	1	6	7	6950.161	-0.007
7	1	7	7	6	1	6	6	6950.240	-0.001
7	1	7	6	6	0	6	5	7667.399	0.006
7	1	7	8	6	0	6	7	7667.458	0.012
7	1	7	7	6	0	6	6	7668.013	-0.007
7	2	5	8	6	2	4	7	7749.274	-0.003
7	2	5	6	6	2	4	5	7749.274	-0.003

J'	K_a'	K_c'	F'	J"	K_a"	K_c"	F"	ν/MHz	$\Delta\nu_{o-c}$
7	2	5	7	6	2	4	6	7749.162	-0.002
7	2	5	7	7	1	6	7	4155.961	0.000
7	2	5	8	7	1	6	8	4155.961	0.000
7	2	5	6	7	1	6	6	4155.961	0.000
7	2	6	8	6	2	5	7	7411.885	0.006
7	2	6	7	6	2	5	6	7411.971	0.008
7	3	5	6	6	3	4	5	7510.602	0.003
7	3	5	8	6	3	4	7	7510.602	0.003
7	3	5	7	6	3	4	6	7510.602	0.003
7	3	4	8	6	3	3	7	7541.161	-0.006
7	3	4	6	6	3	3	5	7541.161	-0.009
7	3	4	7	6	3	3	6	7541.161	-0.009
8	0	8	7	7	0	7	6	8067.281	-0.004
8	0	8	9	7	0	7	8	8067.281	-0.004
8	0	8	8	7	0	7	7	8067.453	-0.007
8	1	8	9	7	1	7	8	7919.438	-0.013
8	1	8	7	7	1	7	6	7919.502	0.004
8	1	8	8	7	1	7	7	7919.502	0.004

Table S9: Experimental rotational transition frequencies of 2AA·Ne.

J'	K_a'	K_c'	F'	J"	K_a"	K_c"	F"	ν/MHz	$\Delta\nu_{o-c}$
2	0	2	1	1	0	1	1	3111.222	0.001
2	0	2	3	1	0	1	2	3111.761	0.001
2	0	2	2	1	0	1	1	3111.911	0.004
2	0	2	2	1	0	1	2	3112.192	-0.009
2	1	2	1	1	1	1	1	3023.336	-0.006
2	1	2	3	1	1	1	2	3024.165	-0.002
2	1	2	1	1	1	1	0	3024.372	0.011
2	1	2	2	1	1	1	1	3024.515	0.004
2	1	2	2	1	1	1	2	3024.911	-0.008
2	1	1	1	1	1	0	0	3233.990	-0.012
2	1	1	2	1	1	0	2	3234.382	0.006
2	1	1	3	1	1	0	2	3234.814	0.002
2	1	1	2	1	1	0	1	3235.078	0.001
2	1	1	1	1	1	0	1	3235.751	-0.005
2	2	0	3	1	1	0	2	4485.307	0.004
2	2	1	3	1	1	1	2	4572.995	0.003
2	2	1	2	1	1	1	1	4572.269	-0.001
3	0	3	4	2	0	2	3	4626.165	-0.009
3	0	3	3	2	0	2	2	4626.366	0.000
3	1	2	4	2	0	2	3	5479.263	0.003
3	1	2	2	2	0	2	1	5479.627	0.008
3	1	2	2	2	1	1	1	4839.693	0.003
3	1	2	4	2	1	1	3	4839.824	0.003
3	1	2	3	2	1	1	2	4839.934	0.001
3	1	2	3	2	1	1	3	4839.507	0.011
3	1	2	2	2	1	1	2	4840.364	-0.006
3	1	3	4	2	1	2	3	4525.874	-0.001
3	1	3	3	2	1	2	2	4526.009	-0.012
3	1	3	2	2	1	2	1	4526.009	0.031
3	2	1	3	2	1	1	2	6012.569	0.011
3	2	1	4	2	1	1	3	6012.422	-0.005
3	2	1	2	2	1	1	1	6012.289	-0.003
3	2	1	3	2	2	0	3	4761.629	-0.001
3	2	1	2	2	2	0	1	4761.797	-0.001
3	2	1	4	2	2	0	3	4761.938	0.002
3	2	1	3	2	2	0	2	4762.072	0.002
3	2	1	2	2	2	0	2	4762.481	-0.004
3	2	2	4	2	1	2	3	6242.780	-0.016
3	2	2	2	2	1	2	2	6242.040	-0.004
3	2	2	2	2	2	1	1	4693.794	-0.001
3	2	2	4	2	2	1	3	4693.974	0.003
3	2	2	3	2	2	1	2	4694.287	0.001
4	0	4	5	3	0	3	4	6104.819	-0.005
4	0	4	3	3	0	3	2	6104.819	-0.005
4	0	4	4	3	0	3	3	6105.011	-0.005
4	1	4	5	3	1	3	4	6017.433	-0.002
4	1	4	4	3	1	3	3	6017.518	0.003
4	1	4	3	3	1	3	2	6017.518	0.003
4	1	3	3	3	1	2	2	6427.206	0.006
4	1	3	5	3	1	2	4	6427.260	0.002
4	1	3	4	3	1	2	3	6427.369	0.002
4	2	3	3	3	2	2	2	6244.422	0.009
4	2	3	5	3	2	2	4	6244.422	0.009
4	2	3	4	3	2	2	3	6244.597	-0.002
4	2	2	5	3	1	2	4	7570.547	0.008
4	2	2	4	3	1	2	3	7570.547	0.008

J'	K_a'	K_c'	F'	J"	K_a"	K_c"	F"	ν/MHz	$\Delta\nu_{o-c}$
4	2	2	4	3	2	1	3	6397.900	-0.019
4	2	2	3	3	2	1	2	6397.900	-0.019
4	2	2	5	3	2	1	4	6397.900	-0.019
4	3	2	3	3	3	1	2	6288.488	0.005
4	3	2	5	3	3	1	4	6288.584	-0.001
4	3	2	4	3	3	1	3	6288.825	-0.002
5	0	5	6	4	0	4	5	7560.068	-0.006
5	0	5	4	4	0	4	3	7560.068	-0.006
5	0	5	5	4	0	4	4	7560.231	-0.001
5	1	5	6	4	1	4	5	7498.863	-0.004
5	1	5	5	4	1	4	4	7498.943	0.015
5	1	5	4	4	1	4	3	7498.943	0.015
5	1	4	5	4	1	3	4	7987.575	0.002
5	1	4	4	4	1	3	3	7987.392	-0.009
5	1	4	6	4	1	3	5	7987.444	0.005
5	2	4	6	4	2	3	5	7783.048	-0.001
5	2	4	4	4	2	3	3	7783.048	-0.001

Table S10: Experimental rotational transition frequencies of ^{13}C1-2AA.

J'	K_a'	K_c'	F'	J"	K_a"	K_c"	F"	ν/MHz	$\Delta\nu_{o-c}$
2	0	2	1	1	0	1	0	3879.790	0.000
2	1	1	3	1	1	0	2	4400.919	0.005
2	1	1	1	1	1	0	1	4402.511	-0.009
2	1	2	3	1	1	1	2	3565.465	0.001
2	1	2	2	1	1	1	1	3565.906	0.002
3	0	3	4	2	0	2	3	5596.698	0.000
3	0	3	3	2	0	2	2	5597.116	-0.001
3	1	2	4	2	1	1	3	6526.380	0.002
3	1	3	4	2	1	2	3	5289.989	0.004
3	1	3	3	2	1	2	2	5290.220	0.001
4	0	4	5	3	0	3	4	7175.059	-0.001
4	0	4	4	3	0	3	3	7175.421	0.002
4	1	4	3	3	1	3	2	6964.654	-0.005
4	1	4	5	3	1	3	4	6964.570	-0.001

Table S11: Experimental rotational transition frequencies of ^{13}C2-2AA.

J'	K_a'	K_c'	F'	J"	K_a"	K_c"	F"	ν/MHz	$\Delta\nu_{o-c}$
2	0	2	2	1	0	1	1	3874.634	0.001
2	0	2	3	1	0	1	2	3874.289	0.002
2	1	1	3	1	1	0	2	4397.118	0.001
2	1	1	2	1	1	0	1	4397.416	-0.003
2	1	2	3	1	1	1	2	3560.408	0.003
2	1	2	2	1	1	1	1	3560.852	0.008
3	0	3	4	2	0	2	3	5587.132	0.000
3	0	3	3	2	0	2	2	5587.546	-0.005
3	1	2	4	2	1	1	3	6519.915	0.001
3	1	2	2	2	1	1	1	6519.671	-0.002
3	1	2	3	2	1	1	2	6520.118	0.005
3	1	3	4	2	1	2	3	5281.905	-0.006
3	1	3	3	2	1	2	2	5282.142	-0.002
3	1	3	2	2	1	2	1	5282.069	-0.010
3	2	2	4	2	2	1	3	5968.161	-0.004
4	0	4	4	3	0	3	3	7161.872	0.005
4	0	4	3	3	0	3	2	7161.513	-0.007
4	0	4	5	3	0	3	4	7161.513	0.004
4	1	4	5	3	1	3	4	6953.215	0.004
4	1	4	4	3	1	3	3	6953.402	0.005

Table S12: Experimental rotational transition frequencies of ^{13}C3-2AA.

J'	K_a'	K_c'	F'	J"	K_a"	K_c"	F"	ν/MHz	$\Delta\nu_{o-c}$
2	0	2	2	1	0	1	1	3849.818	0.008
2	0	2	3	1	0	1	2	3849.471	0.000
2	0	2	1	1	0	1	0	3849.614	-0.006
2	1	1	3	1	1	0	2	4362.651	-0.002
2	1	1	2	1	1	0	1	4362.955	0.000
2	1	2	2	1	1	1	1	3538.425	0.006
2	1	2	3	1	1	1	2	3537.990	0.011
3	0	3	2	2	0	2	1	5556.455	0.006
3	0	3	3	2	0	2	2	5556.871	0.004
3	1	2	4	2	1	1	3	6471.107	-0.003
3	1	3	4	2	1	2	3	5250.212	-0.002
3	1	3	4	2	1	2	3	5250.212	-0.002
3	1	3	3	2	1	2	2	5250.447	-0.001
3	1	3	2	2	1	2	1	5250.384	0.001
3	2	2	4	2	2	1	3	5925.498	0.001
4	0	4	5	3	0	3	4	7125.794	0.004
4	0	4	3	3	0	3	2	7125.794	-0.002
4	0	4	4	3	0	3	3	7126.146	-0.002
4	1	4	5	3	1	3	4	6913.506	-0.004
4	1	4	4	3	1	3	3	6913.690	-0.003

Table S13: Experimental rotational transition frequencies of ^{13}C4-2AA.

J'	K_a'	K_c'	F'	J"	K_a"	K_c"	F"	ν/MHz	$\Delta\nu_{o-c}$
2	0	2	3	1	0	1	2	3831.337	0.003
2	1	1	3	1	1	0	2	4335.711	0.005
2	1	1	2	1	1	0	1	4336.009	0.001
2	1	2	3	1	1	1	2	3521.762	-0.002
3	0	3	4	2	0	2	3	5535.468	-0.004
3	0	3	4	2	0	2	3	5535.468	-0.004
3	0	3	3	2	0	2	2	5535.879	-0.003
3	1	2	3	2	1	1	2	6433.620	-0.004
3	1	2	4	2	1	1	3	6433.432	0.000
3	1	2	4	2	1	1	3	6433.432	0.000
3	1	3	4	2	1	2	3	5227.742	0.008
3	1	3	4	2	1	2	3	5227.742	0.008
3	1	3	3	2	1	2	2	5227.966	-0.001
4	0	4	5	3	0	3	4	7102.694	-0.004
4	0	4	4	3	0	3	3	7103.066	0.009
4	1	4	5	3	1	3	4	6885.960	-0.003
4	1	4	4	3	1	3	3	6886.142	-0.003

Table S14: Experimental rotational transition frequencies of ^{13}C5-2AA.

J'	K_a'	K_c'	F'	J"	K_a"	K_c"	F"	ν/MHz	$\Delta\nu_{o-c}$
2	0	2	1	1	0	1	0	3846.504	-0.004
2	0	2	2	1	0	1	1	3846.702	-0.004
2	0	2	3	1	0	1	2	3846.365	0.003
2	1	1	2	1	1	0	1	4364.780	-0.004
2	1	1	3	1	1	0	2	4364.487	0.006
2	1	2	3	1	1	1	2	3534.778	0.007
3	0	3	4	2	0	2	3	5547.641	0.003
3	0	3	3	2	0	2	2	5548.066	0.009
3	1	2	2	2	1	1	1	6471.629	-0.008
3	1	2	4	2	1	1	3	6471.882	0.003
3	1	2	3	2	1	1	2	6472.079	0.001
3	1	3	4	2	1	2	3	5244.130	0.005
3	1	3	2	2	1	2	1	5244.292	-0.002
3	1	3	3	2	1	2	2	5244.364	0.006
4	0	4	4	3	0	3	3	7111.766	-0.008
4	0	4	5	3	0	3	4	7111.419	0.003
4	1	4	5	3	1	3	4	6903.779	0.001
4	1	4	4	3	1	3	3	6903.951	-0.012

Table S15: Experimental rotational transition frequencies of ^{13}C6-2AA.

J'	K_a'	K_c'	F'	J"	K_a"	K_c"	F"	ν/MHz	$\Delta\nu_{o-c}$
2	0	2	3	1	0	1	2	3870.350	-0.005
2	0	2	2	1	0	1	1	3870.710	0.006
2	1	1	3	1	1	0	2	4396.451	0.001
2	1	2	3	1	1	1	2	3556.572	-0.002
3	0	3	4	2	0	2	3	5578.400	-0.005
3	0	3	3	2	0	2	2	5578.823	-0.004
3	1	2	4	2	1	1	3	6517.530	0.002
3	1	2	3	2	1	1	2	6517.733	0.005
3	1	2	2	2	1	1	1	6517.279	-0.006
3	1	3	4	2	1	2	3	5275.277	-0.001
3	1	3	3	2	1	2	2	5275.516	0.002
3	1	3	2	2	1	2	1	5275.447	0.000
4	0	4	5	3	0	3	4	7148.227	0.006
4	1	4	5	3	1	3	4	6943.268	0.000
4	1	4	5	3	1	3	4	6943.268	0.000

Table S16: Experimental rotational transition frequencies of ^{13}C7-2AA.

J'	K_a'	K_c'	F'	J"	K_a"	K_c"	F"	ν/MHz	$\Delta\nu_{o-c}$
2	0	2	3	1	0	1	2	3859.653	-0.001
2	1	1	3	1	1	0	2	4373.710	-0.002
2	1	1	2	1	1	0	1	4374.009	-0.005
2	1	2	3	1	1	1	2	3547.373	-0.003
2	1	2	2	1	1	1	1	3547.799	-0.017
2	1	2	2	1	1	1	2	3548.617	0.019
2	1	2	1	1	1	1	0	3547.883	0.012
3	0	3	4	2	0	2	3	5571.534	-0.002
3	0	3	3	2	0	2	2	5571.952	0.001
3	1	2	4	2	1	1	3	6487.684	0.000
3	1	2	3	2	1	1	2	6487.883	0.003
3	1	2	2	2	1	1	1	6487.445	0.001
3	1	3	4	2	1	2	3	5264.276	-0.001
3	1	3	2	2	1	2	1	5264.446	-0.002
3	1	3	3	2	1	2	2	5264.507	-0.003
4	0	4	5	3	0	3	4	7145.417	0.000
4	1	4	5	3	1	3	4	6932.182	0.000
4	1	4	4	3	1	3	3	6932.366	0.001
4	1	4	3	3	1	3	2	6932.267	-0.002

Table S17: Experimental rotational transition frequencies of ^{13}C8-2AA.

J'	K_a'	K_c'	F'	J"	K_a"	K_c"	F"	ν/MHz	$\Delta\nu_{o-c}$
2	0	2	1	0	1	1	1	3827.819	-0.008
2	0	2	1	0	1	3	2	3828.573	0.000
2	0	2	1	0	1	2	2	3829.269	-0.002
2	1	1	1	1	0	3	2	4339.687	-0.001
2	1	2	1	1	1	2	1	3519.143	-0.002
2	1	2	1	1	1	3	2	3518.709	0.003
3	0	3	2	0	2	4	3	5525.721	0.004
3	1	2	2	1	1	4	3	6436.797	0.002
3	1	2	2	1	1	3	2	6436.991	0.000
3	1	2	2	1	1	2	1	6436.555	0.001
3	1	3	2	1	2	4	3	5221.440	0.001
3	1	3	2	1	2	3	2	5221.670	-0.003
3	1	3	2	1	2	2	1	5221.604	-0.005
3	1	3	2	1	2	4	3	5221.440	0.001
4	0	4	3	0	3	4	3	7086.312	-0.002
4	1	4	3	1	3	5	4	6875.397	0.004
4	1	4	3	1	3	4	3	6875.579	0.002

Table S18: Experimental rotational transition frequencies of ^{15}N-2AA.

J'	K_a'	K_c'	J'	'K_a"	K_c"	ν/MHz	$\Delta\nu_{o-c}$
2	0	2	1	0	1	3861.783	0.009
2	1	1	1	1	0	4395.349	0.005
2	1	2	1	1	1	3548.339	-0.004
3	0	3	2	0	2	5559.003	0.004
3	1	2	2	1	1	6512.622	-0.006
3	1	3	2	1	2	5260.746	-0.001
3	2	2	2	2	1	5957.763	-0.001
4	0	4	3	0	3	7118.662	-0.004
4	1	4	3	1	3	6921.301	0.002

Table S19: Experimental rotational transition frequencies of ^{13}C1-2AA·H_2O.

J'	K_a'	K_c'	F'	J"	K_a"	K_c"	F"	ν/MHz	$\Delta\nu_{o-c}$
3	0	3	3	2	0	2	2	3171.341	-0.005
3	0	3	4	2	0	2	3	3171.208	-0.003
3	1	2	4	2	1	1	3	3382.609	0.003
3	1	2	3	2	1	1	2	3382.696	-0.009
4	0	4	4	3	0	3	3	4196.611	0.001
4	1	3	5	3	1	2	4	4501.292	-0.003
5	0	5	5	4	0	4	4	5197.452	-0.002
5	1	4	6	4	1	3	5	5611.635	-0.003
5	1	4	4	4	1	3	3	5611.591	0.002
5	2	3	6	4	2	2	5	5451.469	0.005
5	2	3	4	4	2	2	3	5451.469	0.005
5	2	3	5	4	2	2	4	5451.400	0.004
6	0	6	7	5	0	5	6	6172.927	0.010
6	1	6	7	5	1	5	6	5973.183	-0.006
6	1	6	6	5	1	5	5	5973.267	0.001

Table S20: Experimental rotational transition frequencies of ^{13}C2-2AA·H_2O.

J'	K_a'	K_c'	F'	J"	K_a"	K_c"	F"	ν/MHz	$\Delta\nu_{o-c}$
3	0	3	4	2	0	2	3	3166.450	0.005
3	1	2	3	2	1	1	2	3378.298	-0.006
3	1	2	4	2	1	1	3	3378.216	0.010
4	0	4	5	3	0	3	4	4189.878	-0.005
4	0	4	3	3	0	3	2	4189.878	-0.005
4	0	4	4	3	0	3	3	4190.051	0.007
4	1	4	5	3	1	3	4	3995.509	0.000
4	1	4	3	3	1	3	2	3995.605	-0.009
4	1	4	4	3	1	3	3	3995.605	-0.009
5	0	5	6	4	0	4	5	5188.770	0.005
5	0	5	4	4	0	4	3	5188.770	0.005
5	0	5	5	4	0	4	4	5188.960	0.004
5	1	4	6	4	1	3	5	5604.092	-0.013
5	1	5	6	4	1	4	5	4982.701	0.000
5	2	3	6	4	2	2	5	5444.626	0.007
5	2	3	4	4	2	2	3	5444.626	0.007
6	1	6	7	5	1	5	6	5963.329	-0.001
6	1	6	6	5	1	5	5	5963.408	-0.001

Table S21: Experimental rotational transition frequencies of ^{13}C3-2AA·H_2O.

J'	K_a'	K_c'	F'	J"	K_a"	K_c"	F"	ν/MHz	$\Delta\nu_{o-c}$
3	0	3	4	2	0	2	3	3149.916	0.000
3	0	3	3	2	0	2	2	3150.063	0.014
3	1	2	3	2	1	1	2	3359.333	-0.004
3	1	2	4	2	1	1	3	3359.241	0.002
4	0	4	5	3	0	3	4	4168.508	-0.007
4	0	4	3	3	0	3	2	4168.508	-0.007
4	0	4	4	3	0	3	3	4168.678	0.005
4	1	3	5	3	1	2	4	4470.274	0.001
4	1	4	5	3	1	3	4	3975.506	-0.004
4	1	4	3	3	1	3	2	3975.616	0.001
4	1	4	4	3	1	3	3	3975.616	0.001
5	0	5	6	4	0	4	5	5163.010	-0.001
5	0	5	4	4	0	4	3	5163.010	-0.001
5	0	5	5	4	0	4	4	5163.200	0.000
5	1	4	6	4	1	3	5	5573.090	-0.002

Table S22: Experimental rotational transition frequencies of ^{13}C4-2AA·H_2O.

J'	K_a'	K_c'	F'	J"	K_a"	K_c"	F"	ν/MHz	$\Delta\nu_{o-c}$
3	0	3	4	2	0	2	3	3137.846	0.005
3	0	3	2	2	0	2	1	3137.898	0.007
3	0	3	3	2	0	2	2	3137.970	-0.001
4	0	4	5	3	0	3	4	4153.367	-0.001
4	0	4	3	3	0	3	2	4153.367	-0.001
4	0	4	4	3	0	3	3	4153.512	-0.012
4	1	4	5	3	1	3	4	3961.731	-0.005
4	1	4	3	3	1	3	2	3961.838	-0.002
4	1	4	4	3	1	3	3	3961.838	-0.002
5	0	5	6	4	0	4	5	5145.436	0.009
5	0	5	4	4	0	4	3	5145.436	0.009
5	0	5	5	4	0	4	4	5145.616	0.002
5	1	4	6	4	1	3	5	5548.749	-0.01
5	1	4	4	4	1	3	3	5548.703	-0.007
5	1	4	5	4	1	3	4	5548.838	0.011
5	2	3	6	4	2	2	5	5388.510	0.005
5	2	3	4	4	2	2	3	5388.510	0.005
6	1	6	5	5	1	5	4	5914.109	-0.007
6	1	6	7	5	1	5	6	5914.109	-0.007
6	1	6	6	5	1	5	5	5914.179	0.007

Table S23: Experimental rotational transition frequencies of ^{13}C5-2AA·H_2O.

J'	K_a'	K_c'	F'	J"	K_a"	K_c"	F"	ν/MHz	$\Delta\nu_{o-c}$
3	0	3	4	2	0	2	3	3146.595	-0.014
3	0	3	2	2	0	2	1	3146.595	-0.014
3	0	3	3	2	0	2	2	3146.706	-0.012
3	1	2	3	2	1	1	2	3356.510	0.004
3	1	2	4	2	1	1	3	3356.415	0.007
4	0	4	5	3	0	3	4	4163.844	0.007
4	0	4	3	3	0	3	2	4163.844	0.007
4	0	4	4	3	0	3	3	4163.987	-0.009
4	1	3	5	3	1	2	4	4466.420	-0.005
4	1	4	5	3	1	3	4	3970.845	0.014
4	1	4	3	3	1	3	2	3970.925	-0.011
4	1	4	4	3	1	3	3	3970.925	-0.011
5	0	5	6	4	0	4	5	5156.840	0.002
5	0	5	4	4	0	4	3	5156.840	0.002
5	0	5	5	4	0	4	4	5157.026	-0.003
5	1	4	6	4	1	3	5	5568.129	-0.001
5	1	4	4	4	1	3	3	5568.129	-0.001
5	1	5	6	4	1	4	5	4951.995	-0.013
5	2	3	6	4	2	2	5	5409.258	0.006
5	2	3	4	4	2	2	3	5409.258	0.006
6	0	6	6	5	0	5	5	6125.073	0.007
6	0	6	7	5	0	5	6	6124.866	0.002
6	1	6	7	5	1	5	6	5926.713	0.010

Table S24: Experimental rotational transition frequencies of ^{13}C6-2AA·H_2O.

J'	K_a'	K_c'	F'	J"	K_a"	K_c"	F"	ν/MHz	$\Delta\nu_{o-c}$
3	0	3	4	2	0	2	3	3163.560	0.001
3	0	3	2	2	0	2	1	3163.609	-0.001
3	0	3	3	2	0	2	2	3163.690	-0.005
3	1	2	3	2	1	1	2	3376.273	0.000
3	1	2	4	2	1	1	3	3376.177	0.003
4	0	4	5	3	0	3	4	4185.678	0.007
4	0	4	3	3	0	3	2	4185.678	0.007
4	0	4	4	3	0	3	3	4185.836	0.002
4	1	3	5	3	1	2	4	4492.541	0.000
4	1	4	5	3	1	3	4	3991.191	0.003
4	1	4	3	3	1	3	2	3991.294	0.000
4	1	4	4	3	1	3	3	3991.294	0.000
5	0	5	6	4	0	4	5	5182.997	-0.001
5	0	5	4	4	0	4	3	5182.997	-0.001
5	0	5	5	4	0	4	4	5183.193	0.002
5	1	4	6	4	1	3	5	5600.376	-0.006
5	1	5	6	4	1	4	5	4977.165	-0.009
5	2	3	6	4	2	2	5	5441.699	0.003
5	2	3	4	4	2	2	3	5441.699	0.003
6	1	6	7	5	1	5	6	5956.542	0.003

Table S25: Experimental rotational transition frequencies of ^{13}C7-2AA·H_2O.

J'	K_a'	K_c'	F'	J"	K_a"	K_c"	F"	ν/MHz	$\Delta\nu_{o-c}$
3	0	3	4	2	0	2	3	3168.093	0.001
3	1	2	3	2	1	1	2	3379.204	0.007
3	1	2	4	2	1	1	3	3379.102	0.003
4	0	4	5	3	0	3	4	4192.378	-0.011
4	0	4	3	3	0	3	2	4192.378	-0.011
4	0	4	4	3	0	3	3	4192.546	-0.002
4	1	4	5	3	1	3	4	3998.145	-0.001
4	1	4	3	3	1	3	2	3998.253	0.002
4	1	4	4	3	1	3	3	3998.253	0.002
5	0	5	6	4	0	4	5	5192.332	0.006
5	0	5	4	4	0	4	3	5192.332	0.006
5	0	5	5	4	0	4	4	5192.522	0.005
5	1	4	6	4	1	3	5	5605.872	-0.007
5	1	5	6	4	1	4	5	4986.103	-0.002
5	2	3	6	4	2	2	5	5445.762	0.002
5	2	3	4	4	2	2	3	5445.762	0.002
6	1	6	7	5	1	5	6	5967.552	0.000

Table S26: Experimental rotational transition frequencies of ^{13}C8-2AA·H_2O.

J'	K_a'	K_c'	F'	J"	K_a"	K_c"	F"	ν/MHz	$\Delta\nu_{o-c}$
3	0	3	4	2	0	2	3	3157.438	0.001
3	0	3	3	2	0	2	2	3157.562	-0.012
3	1	2	4	2	1	1	3	3370.273	0.000
3	1	2	3	2	1	1	2	3370.371	0.000
4	0	4	5	3	0	3	4	4177.346	0.013
4	0	4	3	3	0	3	2	4177.346	0.013
4	0	4	4	3	0	3	3	4177.501	0.005
4	1	4	5	3	1	3	4	3983.06	0.004
4	1	4	3	3	1	3	2	3983.159	-0.002
4	1	4	4	3	1	3	3	3983.159	-0.002
5	0	5	6	4	0	4	5	5172.337	-0.001
5	0	5	4	4	0	4	3	5172.337	-0.001
5	0	5	5	4	0	4	4	5172.531	-0.001
5	1	4	6	4	1	3	5	5590.375	-0.004
5	1	5	6	4	1	4	5	4966.943	-0.005
5	2	3	6	4	2	2	5	5432.404	0.003
5	2	3	4	4	2	2	3	5432.404	0.003

Table S27: Experimental rotational transition frequencies of 2AA·$H_2^{18}O$.

J'	K_a'	K_c'	F'	J"	K_a"	K_c"	F"	ν/MHz	$\Delta\nu_{o-c}$
4	0	4	4	3	0	3	3	4025.785	-0.003
4	0	4	5	3	0	3	4	4025.633	-0.002
4	1	3	4	3	1	2	3	4300.816	0.005
4	1	3	5	3	1	2	4	4300.750	0.001
4	1	3	3	3	1	2	2	4300.668	0.003
4	2	2	4	3	2	1	3	4136.560	-0.003
4	2	2	5	3	2	1	4	4136.560	-0.003
4	2	3	4	3	2	2	3	4078.974	0.003
4	2	3	5	3	2	2	4	4078.783	-0.002
5	0	5	5	4	0	4	4	4991.487	-0.001
5	0	5	4	4	0	4	3	4991.311	-0.001
5	0	5	6	4	0	4	5	4991.311	-0.001
5	1	4	5	4	1	3	4	5363.706	0.003
5	1	4	6	4	1	3	5	5363.634	-0.006
5	1	5	6	4	1	4	5	4793.386	-0.005
5	1	5	5	4	1	4	4	4793.482	0.007
5	2	3	4	4	2	2	3	5204.079	-0.006
5	2	3	6	4	2	2	5	5204.079	-0.002
5	2	4	5	4	2	3	4	5091.301	0.001
5	2	4	6	4	2	3	5	5091.182	0.005
5	2	4	4	4	2	3	3	5091.182	0.005
5	3	2	5	4	3	1	4	5126.502	-0.001
5	3	2	6	4	3	1	5	5126.337	0.007
5	3	2	4	4	3	1	3	5126.337	0.007
5	3	3	5	4	3	2	4	5122.606	0.007
5	3	3	6	4	3	2	5	5122.409	-0.003
5	3	3	4	4	3	2	3	5122.409	-0.003
6	0	6	5	5	0	5	4	5934.833	0.000
6	0	6	7	5	0	5	6	5934.833	-0.001
6	0	6	6	5	0	5	5	5935.024	-0.001
6	1	6	6	5	1	5	5	5738.751	-0.001
6	1	6	7	5	1	5	6	5738.681	0.003
6	2	5	6	5	2	4	5	6098.809	-0.006
6	2	5	7	5	2	4	6	6098.724	0.000
6	2	5	5	5	2	4	4	6098.724	0.000

Table S28: Experimental rotational transition frequencies of 2AA·^{22}Ne.

J'	K_a'	K_c'	F'	J"	K_a"	K_c"	F"	ν/MHz	$\Delta\nu_{o-c}$
2	0	2	3	1	0	1	2	3058.620	0.002
2	0	2	2	1	0	1	1	3058.736	-0.001
2	0	2	1	1	0	1	0	3058.808	-0.002
2	0	2	2	1	0	1	2	3059.009	0.000
2	1	1	3	1	1	0	2	3174.698	0.001
2	1	1	2	1	1	0	1	3174.946	-0.003
2	1	1	3	1	0	1	2	3663.333	0.008
2	1	2	3	1	1	1	2	2975.913	-0.001
2	1	2	2	1	1	1	1	2976.232	0.005
2	2	0	3	1	1	0	2	4358.736	0.002
2	2	0	2	1	1	0	1	4358.914	-0.003
3	0	3	4	2	0	2	3	4548.875	-0.004
3	0	3	3	2	0	2	2	4549.031	0.000
3	0	3	2	2	0	2	2	4548.307	0.009
3	0	3	3	2	0	2	3	4549.431	0.009
3	1	2	4	2	1	1	3	4750.363	-0.001
3	1	2	3	2	1	1	2	4750.464	0.000
3	1	2	2	2	1	1	1	4750.262	0.000
3	1	2	3	2	1	1	3	4750.135	-0.006
3	1	2	2	2	1	1	2	4750.760	-0.004
3	1	3	3	2	1	2	2	4454.205	-0.011
3	1	3	4	2	1	2	3	4454.087	-0.001
3	1	3	2	2	1	2	2	4453.214	0.001
3	1	3	3	2	1	2	3	4454.834	0.003
3	2	1	3	2	1	1	2	5860.791	0.000
3	2	1	4	2	1	1	3	5860.704	-0.004
3	2	1	2	2	1	1	1	5860.613	0.002
3	2	2	4	2	2	1	3	4612.738	0.001
3	2	2	3	2	2	1	2	4613.028	0.000
3	2	2	2	2	2	1	1	4612.570	-0.004
3	2	1	2	2	2	0	1	4676.535	-0.003
3	2	1	4	2	2	0	3	4676.669	-0.002
3	2	1	3	2	2	0	2	4676.820	-0.002
4	0	4	5	3	0	3	4	6005.402	-0.003
4	0	4	3	3	0	3	2	6005.402	-0.003
4	1	3	5	3	1	2	4	6309.475	0.011
4	1	3	3	3	1	2	2	6309.475	0.011
4	1	3	4	3	1	2	3	6309.573	-0.003
4	1	4	5	3	1	3	4	5922.698	0.005
4	1	4	4	3	1	3	3	5922.774	-0.006
4	2	3	3	3	2	2	2	6136.928	0.009
4	2	3	5	3	2	2	4	6136.928	0.009
4	2	3	4	3	2	2	3	6137.084	-0.004
4	2	2	5	3	2	1	4	6281.394	0.003
4	2	2	4	3	2	1	3	6281.394	0.002
5	0	5	6	4	0	4	5	7439.769	0.002
5	0	5	5	4	0	4	4	7439.896	-0.002
5	1	4	5	4	1	3	4	7843.082	0.002
5	1	4	6	4	1	3	5	7842.972	-0.001
5	1	5	5	4	1	4	4	7381.796	0.013
5	1	5	4	4	1	4	3	7381.796	0.013
5	1	5	6	4	1	4	5	7381.722	-0.011
5	2	3	6	4	2	2	5	7895.810	-0.004
5	2	3	4	4	2	2	3	7895.810	-0.004
5	2	3	5	4	2	2	4	7895.810	-0.004
5	2	4	6	4	2	3	5	7649.972	-0.006
5	2	4	4	4	2	3	3	7649.972	-0.006
5	2	4	5	4	2	3	4	7650.088	-0.001
5	3	3	5	4	3	2	4	7728.044	0.002
5	3	3	6	4	3	2	5	7727.927	0.003