Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Where's Water?
The many binding sites of hydantoin

Supplementary materials

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Table 1: Line list of hydantoin monomer. Frequencies are in MHz.

J'	K_a'	K_c'	F_1'	F_2'		J"	K_a"	K_c"	F_1"	F_2"	Obs.	Obs. – Calc.	Exp. Error
b-type transitions													
2	2	0	3	3	←	3	1	3	4	4	3387.6794	-0.0099	0.010
2	2	0	2	1	←	3	1	3	2	2	3387.9970	-0.0212	0.010
2	2	0	2	3	←	3	1	3	3	4	3389.2425	-0.0123	0.010
2	2	0	3	4	←	3	1	3	4	5	3390.8422	-0.0056	0.010
2	0	2	1	0	←	1	1	1	1	1	3712.9659	-0.0038	0.010
2	0	2	3	2	←	1	1	1	1	2	3713.2636	-0.0004	0.010
2	0	2	3	2	←	1	1	1	1	1	3713.3515	-0.0022	0.010
2	0	2	1	1	←	1	1	1	1	2	3713.4606	0.0013	0.010
2	0	2	1	1	←	1	1	1	1	1	3713.5487	-0.0002	0.010
2	0	2	3	2	←	1	1	1	2	2	3713.8534	-0.0134	0.010
2	0	2	1	2	←	1	1	1	2	2	3714.1316	-0.0066	0.010
2	0	2	2	3	←	1	1	1	1	2	3714.2557	0.0020	0.010
2	0	2	2	1	←	1	1	1	1	0	3714.4846	-0.0046	0.010
2	0	2	3	4	←	1	1	1	2	3	3714.6585	-0.0046	0.010
2	0	2	1	2	←	1	1	1	2	1	3714.7251	0.0018	0.010
2	0	2	2	3	←	1	1	1	2	2	3714.8445	-0.0120	0.010
2	0	2	2	2	←	1	1	1	1	2	3715.2026	-0.0068	0.010
2	0	2	2	2	←	1	1	1	1	1	3715.2932	-0.0059	0.010
2	0	2	1	1	←	1	1	1	0	1	3715.4642	-0.0032	0.010
2	0	2	3	3	←	1	1	1	2	3	3715.7680	-0.0041	0.010
2	0	2	2	1	←	1	1	1	2	1	3715.9680	-0.0032	0.010
2	0	2	2	2	←	1	1	1	2	3	3716.0999	-0.0062	0.010
1	1	0	1	2	←	1	0	1	1	2	4819.0438	0.0040	0.010
1	1	0	1	2	←	1	0	1	1	1	4819.1419	0.0049	0.010
1	1	0	1	1	←	1	0	1	1	2	4819.2277	0.0016	0.010
1	1	0	1	1	←	1	0	1	1	1	4819.3269	0.0036	0.010
1	1	0	1	0	←	1	0	1	0	1	4819.7031	0.0005	0.010
1	1	0	1	1	←	1	0	1	2	2	4819.8979	-0.0091	0.010
1	1	0	1	2	←	1	0	1	2	3	4820.0169	0.0029	0.010
1	1	0	2	2	←	1	0	1	1	2	4820.3147	-0.0019	0.010
1	1	0	2	2	←	1	0	1	1	1	4820.4079	-0.0059	0.010
1	1	0	1	1	←	1	0	1	0	1	4820.4800	0.0006	0.010
1	1	0	1	0	←	1	0	1	2	1	4820.6525	-0.0024	0.010
1	1	0	2	3	←	1	0	1	1	2	4820.9097	0.0026	0.010
1	1	0	2	2	←	1	0	1	2	2	4820.9976	0.0000	0.010
1	1	0	1	2	←	1	0	1	2	1	4821.2484	0.0029	0.010
1	1	0	1	1	←	1	0	1	2	1	4821.4331	0.0013	0.010
1	1	0	2	2	←	1	0	1	0	1	4821.5700	0.0000	0.010
1	1	0	2	3	←	1	0	1	2	3	4821.8842	0.0029	0.010
1	1	0	0	1	←	1	0	1	2	2	4822.1652	0.0015	0.010
1	1	0	0	1	←	1	0	1	0	1	4822.7393	0.0033	0.010

1	1	0	2	1	←	1	0	1	1	0	4822.9516	0.0031	0.010
1	1	0	2	1	←	1	0	1	1	2	4823.2377	-0.0040	0.010
1	1	0	2	1	←	1	0	1	1	1	4823.3350	-0.0039	0.010
4	1	3	4	4	←	3	2	2	3	3	5148.8621	-0.0020	0.010
4	1	3	4	5	←	3	2	2	4	4	5149.1072	0.0111	0.010
4	1	3	5	5	←	3	2	2	3	4	5149.2201	-0.0023	0.010
4	1	3	3	3	←	3	2	2	2	2	5149.3378	-0.0004	0.010
4	1	3	5	6	←	3	2	2	4	5	5149.4658	-0.0057	0.010
4	1	3	3	2	←	3	2	2	2	1	5149.6336	0.0012	0.010
2	1	1	2	2	←	2	0	2	2	2	5448.7202	0.0003	0.010
2	1	1	2	3	←	2	0	2	3	3	5449.3485	0.0039	0.010
2	1	1	2	1	←	2	0	2	2	1	5449.5113	0.0026	0.010
2	1	1	2	2	←	2	0	2	2	3	5449.6713	-0.0043	0.010
2	1	1	3	3	←	2	0	2	3	3	5449.7874	0.0030	0.010
2	1	1	2	3	←	2	0	2	2	3	5449.9711	0.0046	0.010
2	1	1	1	1	←	2	0	2	2	2	5450.0889	0.0006	0.010
2	1	1	3	4	←	2	0	2	3	3	5450.2086	0.0064	0.010
2	1	1	3	3	←	2	0	2	2	3	5450.4121	0.0058	0.010
2	1	1	3	2	←	2	0	2	3	3	5450.5817	0.0039	0.010
2	1	1	2	1	←	2	0	2	1	2	5450.7586	0.0021	0.010
2	1	1	2	3	←	2	0	2	3	2	5450.9569	0.0009	0.010
2	1	1	1	2	←	2	0	2	2	3	5451.0365	0.0060	0.010
2	1	1	3	3	←	2	0	2	1	2	5451.1268	0.0022	0.010
2	1	1	3	4	←	2	0	2	3	4	5451.3145	0.0033	0.010
2	1	1	1	2	←	2	0	2	1	2	5451.7521	0.0033	0.010
2	1	1	3	2	←	2	0	2	3	2	5452.1906	0.0013	0.010
2	1	1	1	0	←	2	0	2	1	1	5452.3291	0.0018	0.010
2	1	1	1	1	←	2	0	2	1	0	5452.4186	0.0008	0.010
3	1	2	3	3	←	3	0	3	3	3	6490.0054	-0.0013	0.010
3	1	2	3	4	←	3	0	3	3	3	6490.2998	0.0037	0.010
3	1	2	3	3	←	3	0	3	4	4	6490.6043	0.0024	0.010
3	1	2	2	2	←	3	0	3	3	3	6490.7601	-0.0044	0.010
3	1	2	3	4	←	3	0	3	4	4	6490.8939	0.0026	0.010
3	1	2	3	2	←	3	0	3	2	2	6491.1104	0.0024	0.010
3	1	2	4	5	←	3	0	3	4	4	6491.4501	0.0031	0.010
3	1	2	3	4	←	3	0	3	3	4	6491.5330	0.0050	0.010
3	1	2	4	3	←	3	0	3	4	4	6491.6123	0.0069	0.010
3	1	2	4	4	←	3	0	3	3	4	6491.7564	0.0042	0.010
3	1	2	3	2	←	3	0	3	3	2	6492.1516	0.0026	0.010
3	1	2	3	4	←	3	0	3	4	5	6492.2262	0.0106	0.010
3	1	2	2	2	←	3	0	3	3	2	6492.5476	-0.0031	0.010
3	1	2	4	5	←	3	0	3	4	5	6492.7710	-0.0003	0.010
3	1	2	2	1	←	3	0	3	3	2	6492.9451	-0.0038	0.010
3	1	2	2	3	←	3	0	3	2	3	6493.1046	0.0049	0.010
3	1	2	4	3	←	3	0	3	4	3	6493.3166	-0.0069	0.010

3	1	2	2	1	←	3	0	3	2	1	6493.7821	-0.0043	0.010
a-type transitions													
1	0	1	2	1	←	0	0	0	1	2	4006.4049	0.0033	0.010
1	0	1	0	1	←	0	0	0	1	1	4007.3531	-0.0008	0.010
1	0	1	2	3	←	0	0	0	1	2	4007.6333	0.0001	0.010
1	0	1	2	2	←	0	0	0	1	1	4007.9249	-0.0013	0.010
1	0	1	1	1	←	0	0	0	1	0	4008.5121	0.0018	0.010
1	0	1	1	2	←	0	0	0	1	2	4008.6083	0.0010	0.010
2	1	2	1	2	←	1	1	1	2	2	7439.7009	-0.0021	0.010
2	1	2	1	2	←	1	1	1	2	1	7440.2836	-0.0044	0.010
2	1	2	3	4	←	1	1	1	2	3	7440.4023	0.0023	0.010
2	1	2	3	2	←	1	1	1	0	1	7440.7074	-0.0018	0.010
2	1	2	2	3	←	1	1	1	2	2	7440.9424	0.0027	0.010
2	1	2	3	3	←	1	1	1	1	2	7441.3160	0.0127	0.010
2	1	2	2	2	←	1	1	1	1	2	7441.8711	-0.0077	0.010
2	1	2	2	2	←	1	1	1	1	1	7441.9619	-0.0066	0.010
2	1	2	3	3	←	1	1	1	2	3	7442.2111	0.0111	0.010
2	0	2	3	2	←	1	0	1	1	2	7959.5648	0.0070	0.010
2	0	2	3	2	←	1	0	1	1	1	7959.6522	-0.0027	0.010
2	0	2	1	2	←	1	0	1	2	2	7960.5153	0.0052	0.010
2	0	2	2	1	←	1	0	1	1	0	7960.7761	-0.0076	0.010
2	0	2	3	4	←	1	0	1	2	3	7961.0391	0.0046	0.010
2	0	2	2	3	←	1	0	1	2	2	7961.2172	-0.0111	0.010
2	0	2	2	2	←	1	0	1	1	2	7961.5059	0.0027	0.010
2	0	2	2	2	←	1	0	1	1	1	7961.5971	-0.0032	0.010
2	0	2	3	2	←	1	0	1	2	1	7961.7617	-0.0017	0.010
2	0	2	1	1	←	1	0	1	2	1	7961.9560	-0.0026	0.010
2	0	2	3	3	←	1	0	1	2	3	7962.1444	0.0010	0.010
2	0	2	2	1	←	1	0	1	0	1	7962.3255	-0.0048	0.010

Table 2: Experimental rotational parameters for hydantoin monomer. Values in parenthesis are standard errors.

Parameters	Parent fit
A (MHz)	6537.73154(80)
B (MHz)	2291.37309(21)
C (MHz)	1716.47119(31)
χ_{aa} (MHz)	1.6316(57)
X_{bb-cc} (MHz)	5.227(20)
χ_{ab} (MHz)	[0.0918]
χ_{aa} (MHz)	2.5927(43)
X_{bb-cc} (MHz)	6.935(16)
χ_{ab} (MHz)	[-0.2235]
Nlines	114
RMS (kHz)	5.3

Table 3: Line list of hydantoin-$H_2{}^{16}O$ complex (I). Frequencies are in MHz.

J'	K_a'	K_c'	F_1'	F_2'		J"	K_a"	K_c"	F_1"	F_2"	Obs.	Obs. – Calc.	Exp. Error
b-type transitions													
3	0	3	3	3	←	2	1	2	2	2	2472.2443	0.0053	0.010
3	0	3	4	5	←	2	1	2	3	4	2473.0761	-0.0043	0.010
3	0	3	2	3	←	2	1	2	1	2	2473.3039	0.0033	0.010
3	0	3	4	3	←	2	1	2	3	2	2473.5630	0.0041	0.010
3	0	3	2	2	←	2	1	2	1	1	2473.6661	0.0039	0.010
3	0	3	2	1	←	2	1	2	1	0	2473.9512	-0.0070	0.010
1	1	0	1	1	←	1	0	1	1	1	4095.0746	-0.0033	0.010
1	1	0	1	0	←	1	0	1	2	1	4095.3712	0.0016	0.010
1	1	0	1	2	←	1	0	1	2	3	4095.6717	0.0012	0.010
1	1	0	2	2	←	1	0	1	2	2	4096.6012	0.0009	0.010
1	1	0	2	2	←	1	0	1	2	1	4097.1627	0.0045	0.010
1	1	0	2	3	←	1	0	1	2	3	4097.4590	0.0005	0.010
1	1	0	2	1	←	1	0	1	2	1	4098.3012	-0.0032	0.010
1	1	0	0	1	←	1	0	1	1	2	4098.8248	0.0013	0.010
1	1	0	0	1	←	1	0	1	1	1	4098.9145	0.0054	0.010
2	1	1	2	2	←	2	0	2	2	2	4304.9037	0.0026	0.010
2	1	1	2	2	←	2	0	2	2	3	4305.2004	0.0003	0.010
2	1	1	3	3	←	2	0	2	2	3	4305.4941	0.0039	0.010
2	1	1	2	1	←	2	0	2	2	1	4305.6410	0.0022	0.010
2	1	1	1	1	←	2	0	2	2	2	4306.3228	-0.0007	0.010
2	1	1	2	3	←	2	0	2	3	3	4306.4181	-0.0032	0.010
2	1	1	2	1	←	2	0	2	1	2	4306.6670	0.0055	0.010
2	1	1	3	4	←	2	0	2	3	4	4307.2756	0.0054	0.010
2	1	1	1	2	←	2	0	2	1	2	4307.6903	0.0055	0.010
2	1	1	1	1	←	2	0	2	3	2	4307.8992	0.0053	0.010
2	1	1	3	2	←	2	0	2	3	2	4308.0586	0.0041	0.010
2	1	1	1	1	←	2	0	2	1	0	4308.2360	0.0014	0.010
3	1	2	3	3	←	3	0	3	3	3	4633.8333	0.0007	0.010
3	1	2	4	4	←	3	0	3	4	4	4634.6252	0.0027	0.010
3	1	2	2	2	←	3	0	3	3	2	4634.8179	0.0055	0.010
3	1	2	3	3	←	3	0	3	2	2	4635.1299	-0.0059	0.010
3	1	2	3	4	←	3	0	3	3	4	4635.3335	0.0017	0.010
3	1	2	3	2	←	3	0	3	2	2	4636.0278	0.0009	0.010
3	1	2	4	5	←	3	0	3	4	5	4636.2468	0.0064	0.010
3	1	2	2	3	←	3	0	3	2	3	4636.5389	0.0034	0.010
3	1	2	4	3	←	3	0	3	4	3	4636.7206	0.0092	0.010
3	1	2	2	1	←	3	0	3	2	1	4637.1229	-0.0020	0.010
4	0	4	4	4	←	3	1	3	3	3	4771.8540	0.0017	0.010
4	0	4	5	5	←	3	1	3	4	4	4772.1646	0.0044	0.010
4	0	4	3	3	←	3	1	3	3	2	4772.2579	-0.0013	0.010
4	0	4	4	5	←	3	1	3	3	4	4772.5920	0.0038	0.010
4	0	4	5	6	←	3	1	3	4	5	4772.9920	0.0039	0.010

4	0	4	4	3	←	3	1	3	2	2	4773.0813	0.0006	0.010
4	0	4	3	4	←	3	1	3	2	3	4773.1814	0.0086	0.010
4	0	4	5	4	←	3	1	3	4	3	4773.3159	0.0128	0.010
4	0	4	3	2	←	3	1	3	2	1	4773.5835	0.0039	0.010
4	1	3	4	4	←	4	0	4	4	4	5098.1758	0.0016	0.010
4	1	3	5	5	←	4	0	4	4	4	5098.4668	0.0010	0.010
4	1	3	5	5	←	4	0	4	5	5	5099.0967	0.0037	0.010
4	1	3	3	3	←	4	0	4	3	3	5099.2833	0.0054	0.010
4	1	3	4	5	←	4	0	4	4	5	5099.7190	0.0038	0.010
4	1	3	4	3	←	4	0	4	4	3	5100.2017	0.0017	0.010
4	1	3	5	6	←	4	0	4	5	6	5100.7068	0.0016	0.010
4	1	3	3	4	←	4	0	4	3	4	5100.9487	0.0029	0.010
4	1	3	5	4	←	4	0	4	5	4	5101.0662	0.0031	0.010
4	1	3	3	2	←	4	0	4	3	2	5101.3742	-0.0005	0.010
5	1	4	5	5	←	5	0	5	5	5	5718.0393	0.0013	0.010
5	1	4	6	6	←	5	0	5	6	6	5719.0689	-0.0020	0.010
5	1	4	5	6	←	5	0	5	5	6	5719.6511	-0.0057	0.010
5	1	4	5	4	←	5	0	5	5	4	5720.0396	-0.0016	0.010
5	1	4	4	5	←	5	0	5	4	5	5720.9351	-0.0141	0.010
1	1	1	0	1	←	0	0	0	1	2	5961.2804	-0.0027	0.010
1	1	1	2	1	←	0	0	0	1	1	5962.1488	-0.0041	0.010
1	1	1	2	3	←	0	0	0	1	2	5962.4410	-0.0023	0.010
1	1	1	2	2	←	0	0	0	1	1	5962.7371	-0.0026	0.010
1	1	1	1	1	←	0	0	0	1	0	5963.2768	-0.0029	0.010
1	1	1	1	2	←	0	0	0	1	2	5963.3692	-0.0037	0.010
1	1	1	1	0	←	0	0	0	1	1	5963.6642	-0.0057	0.010
5	0	5	6	6	←	4	1	4	5	5	7109.1124	-0.0057	0.010
5	0	5	4	4	←	4	1	4	3	3	7109.2134	-0.0039	0.010
5	0	5	5	6	←	4	1	4	4	5	7109.4607	-0.0044	0.010
5	0	5	5	4	←	4	1	4	4	3	7109.7777	-0.0043	0.010
5	0	5	6	7	←	4	1	4	5	6	7109.8839	-0.0076	0.010
5	0	5	4	5	←	4	1	4	3	4	7110.0287	-0.0056	0.010
5	0	5	6	5	←	4	1	4	5	4	7110.1074	-0.0054	0.010
5	0	5	4	3	←	4	1	4	3	2	7110.3050	-0.0026	0.010
2	1	2	3	2	←	1	0	1	1	2	7826.4296	-0.0017	0.010
2	1	2	3	2	←	1	0	1	1	1	7826.5197	0.0027	0.010
2	1	2	1	1	←	1	0	1	1	2	7826.7357	-0.0061	0.010
2	1	2	1	1	←	1	0	1	1	1	7826.8329	0.0055	0.010
2	1	2	1	2	←	1	0	1	2	2	7827.3624	-0.0001	0.010
2	1	2	1	0	←	1	0	1	0	1	7827.7002	0.0006	0.010
2	1	2	1	2	←	1	0	1	2	1	7827.9177	-0.0028	0.010
2	1	2	3	4	←	1	0	1	2	3	7828.0414	-0.0023	0.010
2	1	2	3	2	←	1	0	1	0	1	7828.3480	-0.0030	0.010
2	1	2	2	1	←	1	0	1	1	0	7828.4719	-0.0050	0.010
2	1	2	1	1	←	1	0	1	0	1	7828.6532	-0.0082	0.010
2	1	2	2	2	←	1	0	1	1	2	7829.4636	-0.0046	0.010

2	1	2	2	2	←	1	0	1	1	1	7829.5442	-0.0097	0.010
2	1	2	2	1	←	1	0	1	2	1	7829.8892	-0.0028	0.010
a-type transitions													
1	0	1	2	1	←	0	0	0	1	1	2067.4479	-0.0020	0.010
1	0	1	2	3	←	0	0	0	1	2	2067.7270	-0.0005	0.010
1	0	1	2	2	←	0	0	0	1	1	2068.0171	0.0092	0.010
1	0	1	1	2	←	0	0	0	1	2	2068.5671	-0.0175	0.010
1	0	1	1	0	←	0	0	0	1	1	2068.8695	0.0045	0.010
2	1	2	3	2	←	1	1	1	1	2	3931.6441	0.0009	0.010
2	1	2	3	2	←	1	1	1	1	1	3931.7344	-0.0021	0.010
2	1	2	1	1	←	1	1	1	1	2	3931.9520	-0.0014	0.010
2	1	2	1	1	←	1	1	1	1	1	3932.0448	-0.0021	0.010
2	1	2	1	2	←	1	1	1	2	2	3932.6340	0.0033	0.010
2	1	2	1	0	←	1	1	1	0	1	3933.0838	0.0023	0.010
2	1	2	1	2	←	1	1	1	2	1	3933.2181	0.0006	0.010
2	1	2	3	4	←	1	1	1	2	3	3933.3300	0.0018	0.010
2	1	2	2	1	←	1	1	1	1	0	3933.6730	0.0009	0.010
2	1	2	3	2	←	1	1	1	0	1	3933.7355	0.0025	0.010
2	1	2	1	1	←	1	1	1	0	1	3934.0431	-0.0002	0.010
2	1	2	2	2	←	1	1	1	1	2	3934.6844	0.0043	0.010
2	1	2	2	2	←	1	1	1	1	1	3934.7735	0.0000	0.010
2	1	2	2	1	←	1	1	1	2	1	3935.1877	-0.0013	0.010
2	0	2	3	2	←	1	0	1	1	2	4126.8261	0.0068	0.010
2	0	2	3	2	←	1	0	1	1	1	4126.8953	-0.0095	0.010
2	0	2	1	1	←	1	0	1	1	2	4126.9789	-0.0010	0.010
2	0	2	1	1	←	1	0	1	1	1	4127.0634	-0.0021	0.010
2	0	2	1	2	←	1	0	1	2	2	4127.5735	0.0022	0.010
2	0	2	2	1	←	1	0	1	1	0	4127.7366	-0.0003	0.010
2	0	2	3	4	←	1	0	1	2	3	4128.0600	-0.0024	0.010
2	0	2	3	3	←	1	0	1	2	2	4128.2123	0.0004	0.010
2	0	2	2	2	←	1	0	1	1	2	4128.3963	0.0067	0.010
2	0	2	2	2	←	1	0	1	1	1	4128.4746	-0.0005	0.010
2	0	2	3	2	←	1	0	1	0	1	4128.7384	-0.0004	0.010
2	0	2	2	1	←	1	0	1	2	1	4129.1523	0.0003	0.010
2	1	1	1	1	←	1	1	0	0	1	4335.8887	-0.0008	0.010
2	1	1	3	2	←	1	1	0	0	1	4336.0517	0.0015	0.010
2	1	1	1	0	←	1	1	0	0	1	4336.3768	-0.0055	0.010
2	1	1	2	1	←	1	1	0	2	1	4336.4878	0.0015	0.010
2	1	1	3	3	←	1	1	0	2	3	4336.9816	0.0021	0.010
2	1	1	1	2	←	1	1	0	2	1	4337.5088	-0.0007	0.010
2	1	1	3	4	←	1	1	0	2	3	4337.8749	0.0007	0.010
2	1	1	2	3	←	1	1	0	2	2	4338.0339	0.0010	0.010
2	1	1	2	2	←	1	1	0	1	1	4338.3027	0.0043	0.010
2	1	1	2	2	←	1	1	0	1	2	4338.4776	0.0003	0.010
2	1	1	1	2	←	1	1	0	2	2	4338.6543	-0.0014	0.010
2	1	1	3	3	←	1	1	0	1	2	4338.7692	0.0017	0.010

2	1	1	2	1	←	1	1	0	1	0	4339.4241	0.0029	0.010
2	1	1	1	1	←	1	1	0	1	1	4339.7243	0.0035	0.010
2	1	1	3	2	←	1	1	0	1	2	4340.0646	0.0043	0.010
2	1	1	1	0	←	1	1	0	1	1	4340.2232	0.0096	0.010
3	1	3	2	2	←	2	1	2	2	2	5893.6142	-0.0004	0.010
3	1	3	2	1	←	2	1	2	1	1	5895.0405	-0.0018	0.010
3	1	3	4	5	←	2	1	2	3	4	5895.6421	0.0043	0.010
3	1	3	2	1	←	2	1	2	1	0	5895.9976	-0.0067	0.010
3	1	3	3	3	←	2	1	2	2	2	5896.1861	-0.0027	0.010
3	1	3	2	2	←	2	1	2	1	1	5896.3390	-0.0021	0.010
3	1	3	2	2	←	2	1	2	3	2	5896.6499	-0.0017	0.010
3	1	3	4	4	←	2	1	2	3	4	5897.5351	-0.0001	0.010
3	1	3	3	2	←	2	1	2	1	2	5897.7099	-0.0026	0.010
3	0	3	4	3	←	2	0	2	2	3	6171.8919	-0.0077	0.010
3	0	3	2	2	←	2	0	2	2	2	6172.0139	-0.0005	0.010
3	0	3	2	1	←	2	0	2	1	1	6172.7585	0.0003	0.010
3	0	3	4	5	←	2	0	2	3	4	6173.0539	-0.0079	0.010
3	0	3	3	3	←	2	0	2	2	2	6173.3159	-0.0018	0.010
3	0	3	2	2	←	2	0	2	1	1	6173.4252	0.0011	0.010
3	0	3	4	4	←	2	0	2	3	4	6174.0209	-0.0004	0.010
3	0	3	3	2	←	2	0	2	1	2	6174.1282	0.0097	0.010
3	2	1	4	3	←	2	2	0	3	2	6233.7550	-0.0033	0.010
3	2	1	3	2	←	2	2	0	1	1	6233.8384	-0.0138	0.010
3	2	1	2	3	←	2	2	0	1	2	6233.9150	-0.0018	0.010
3	2	1	4	5	←	2	2	0	3	4	6234.0996	0.0000	0.010
3	2	1	3	4	←	2	2	0	3	3	6234.4343	-0.0057	0.010
3	2	1	4	4	←	2	2	0	2	3	6234.8168	-0.0091	0.010
3	2	1	3	3	←	2	2	0	2	2	6235.0345	-0.0126	0.010
3	1	2	2	2	←	2	1	1	1	2	6501.2367	-0.0094	0.010
3	1	2	4	4	←	2	1	1	3	4	6501.3759	0.0022	0.010
3	1	2	3	2	←	2	1	1	3	2	6501.5587	0.0016	0.010
3	1	2	3	2	←	2	1	1	1	1	6501.7151	-0.0025	0.010
3	1	2	4	3	←	2	1	1	3	2	6501.8300	0.0020	0.010
3	1	2	2	3	←	2	1	1	1	2	6501.9449	0.0023	0.010
3	1	2	4	5	←	2	1	1	3	4	6502.0364	0.0045	0.010
3	1	2	3	4	←	2	1	1	2	3	6502.0901	-0.0045	0.010
3	1	2	4	4	←	2	1	1	3	3	6502.2753	0.0070	0.010
3	1	2	2	3	←	2	1	1	2	3	6502.5641	-0.0013	0.010
4	1	4	5	4	←	3	1	3	4	4	7850.1044	0.0072	0.010
4	1	4	4	3	←	3	1	3	3	3	7850.2544	0.0184	0.010
4	1	4	3	2	←	3	1	3	2	2	7851.3588	0.0112	0.010
4	1	4	4	5	←	3	1	3	3	4	7852.5948	0.0039	0.010
4	1	4	4	4	←	3	1	3	3	3	7852.7362	0.0093	0.010
4	1	4	4	3	←	3	1	3	2	2	7852.8181	0.0079	0.010
4	1	4	4	4	←	3	1	3	4	4	7853.6614	-0.0006	0.010
4	1	4	5	5	←	3	1	3	4	5	7854.4223	0.0079	0.010

Table 4: Line list of hydantoin-$H_2{}^{18}O$ complex (I). Frequencies are in MHz.

J'	K_a'	K_c'	F_1'	F_2'		J"	K_a"	K_c"	F_1"	F_2"	Obs.	Obs. – Calc.	Exp. Error
b-type transitions													
3	0	3	3	3	←	2	1	2	2	2	2179.8299	-0.0019	0.010
3	0	3	4	4	←	2	1	2	2	3	2179.9278	0.0044	0.010
3	0	3	3	4	←	2	1	2	3	3	2180.4158	-0.0006	0.010
3	0	3	4	5	←	2	1	2	3	4	2180.6894	0.0012	0.010
3	0	3	2	3	←	2	1	2	1	2	2180.9113	0.0014	0.010
3	0	3	4	3	←	2	1	2	3	2	2181.1678	-0.0015	0.010
3	0	3	2	2	←	2	1	2	1	1	2181.2639	-0.0045	0.010
1	1	0	1	1	←	1	0	1	1	1	4092.6778	-0.0165	0.010
1	1	0	1	0	←	1	0	1	2	1	4092.9803	-0.0100	0.010
1	1	0	1	2	←	1	0	1	2	3	4093.2893	0.0007	0.010
1	1	0	2	2	←	1	0	1	2	2	4094.2229	0.0082	0.010
1	1	0	2	2	←	1	0	1	2	1	4094.7766	0.0024	0.010
1	1	0	2	1	←	1	0	1	2	2	4095.3645	0.0042	0.010
1	1	0	0	1	←	1	0	1	1	2	4096.4167	-0.0171	0.010
1	1	0	0	1	←	1	0	1	1	1	4096.5077	-0.0117	0.010
2	1	1	2	2	←	2	0	2	2	2	4285.8433	-0.0023	0.010
2	1	1	3	3	←	2	0	2	2	2	4286.1265	-0.0082	0.010
2	1	1	3	3	←	2	0	2	2	3	4286.4326	0.0002	0.010
2	1	1	2	1	←	2	0	2	2	1	4286.5830	0.0021	0.010
2	1	1	2	3	←	2	0	2	3	3	4287.3622	0.0031	0.010
2	1	1	3	4	←	2	0	2	3	4	4288.2339	0.0291	0.010
2	1	1	1	2	←	2	0	2	1	2	4288.6100	-0.0093	0.010
3	1	2	3	3	←	3	0	3	3	3	4587.6750	0.0065	0.010
3	1	2	4	4	←	3	0	3	4	4	4588.4618	0.0093	0.010
3	1	2	2	2	←	3	0	3	3	2	4588.6425	0.0017	0.010
3	1	2	3	4	←	3	0	3	3	4	4589.1555	-0.0002	0.010
3	1	2	4	5	←	3	0	3	4	5	4590.0648	0.0074	0.010
3	1	2	2	3	←	3	0	3	2	3	4590.3606	0.0101	0.010
4	1	3	5	5	←	4	0	4	5	5	5013.0165	-0.0091	0.010
4	1	3	4	5	←	4	0	4	4	5	5013.6374	-0.0028	0.010
4	1	3	4	3	←	4	0	4	4	3	5014.1228	0.0035	0.010
4	1	3	5	6	←	4	0	4	5	6	5014.6227	0.0041	0.010
4	1	3	3	4	←	4	0	4	3	4	5014.8566	0.0002	0.010
4	1	3	5	4	←	4	0	4	5	4	5014.9762	0.0041	0.010
4	1	3	3	2	←	4	0	4	3	2	5015.2673	-0.0128	0.010
1	1	1	0	1	←	0	0	0	1	2	5884.6235	-0.0130	0.010
1	1	1	2	1	←	0	0	0	1	1	5885.4980	-0.0067	0.010
1	1	1	2	3	←	0	0	0	1	2	5885.7894	-0.0045	0.010
1	1	1	2	2	←	0	0	0	1	1	5886.0853	-0.0040	0.010

1	1	1	1	1	←	0	0	0	1	0	5886.6273	-0.0008	0.010
1	1	1	1	2	←	0	0	0	1	2	5886.7206	-0.0004	0.010
1	1	1	1	0	←	0	0	0	1	1	5887.0163	-0.0008	0.010
5	0	5	5	5	←	4	1	4	4	4	6612.6494	-0.0101	0.010
5	0	5	6	6	←	4	1	4	5	5	6613.0574	0.0069	0.010
5	0	5	4	4	←	4	1	4	3	3	6613.1575	0.0051	0.010
5	0	5	5	6	←	4	1	4	4	5	6613.4115	0.0049	0.010
5	0	5	6	7	←	4	1	4	5	6	6613.8474	-0.0026	0.010
5	0	5	4	5	←	4	1	4	3	4	6613.9875	-0.0085	0.010
5	0	5	6	5	←	4	1	4	5	4	6614.0838	0.0080	0.010
5	0	5	4	3	←	4	1	4	3	2	6614.2709	-0.0035	0.010
2	1	2	1	2	←	1	0	1	2	1	7677.0144	0.0060	0.010
2	1	2	3	4	←	1	0	1	2	3	7677.1352	0.0043	0.010
2	1	2	3	2	←	1	0	1	0	1	7677.4515	0.0119	0.010
2	1	2	3	3	←	1	0	1	2	2	7677.6726	0.0042	0.010
2	1	2	2	3	←	1	0	1	1	2	7677.9955	0.0105	0.010
2	1	2	2	2	←	1	0	1	1	1	7678.6270	-0.0111	0.010
2	1	2	2	3	←	1	0	1	2	3	7678.8394	-0.0031	0.010
2	1	2	2	1	←	1	0	1	2	1	7678.9872	0.0092	0.010
a-type transitions													
2	0	2	1	2	←	1	0	1	2	2	3949.1071	-0.0071	0.010
2	0	2	2	1	←	1	0	1	1	0	3949.2847	0.0101	0.010
2	0	2	3	4	←	1	0	1	2	3	3949.6001	-0.0066	0.010
2	0	2	1	2	←	1	0	1	2	1	3949.6702	-0.0035	0.010
2	0	2	3	3	←	1	0	1	2	2	3949.7543	0.0003	0.010
2	0	2	2	2	←	1	0	1	1	1	3950.0166	0.0041	0.010
2	0	2	3	2	←	1	0	1	0	1	3950.2951	0.0108	0.010
2	0	2	2	3	←	1	0	1	2	3	3950.4746	-0.0121	0.010
2	0	2	2	1	←	1	0	1	2	1	3950.6781	-0.0136	0.010
2	1	1	1	1	←	1	1	0	0	1	4140.7527	-0.0046	0.010
2	1	1	3	2	←	1	1	0	0	1	4140.9173	-0.0001	0.010
2	1	1	3	3	←	1	1	0	2	3	4141.8355	-0.0110	0.010
2	1	1	1	2	←	1	1	0	2	1	4142.3710	-0.0023	0.010
2	1	1	3	4	←	1	1	0	2	3	4142.7335	-0.0055	0.010
2	1	1	2	3	←	1	1	0	2	2	4142.8931	-0.0052	0.010
2	1	1	2	2	←	1	1	0	1	1	4143.1593	-0.0044	0.010
2	1	1	2	2	←	1	1	0	1	2	4143.3222	-0.0192	0.010
2	1	1	3	3	←	1	1	0	1	2	4143.6256	-0.0049	0.010
2	1	1	2	1	←	1	1	0	1	0	4144.2922	0.0098	0.010
3	1	3	4	3	←	2	1	2	2	3	5647.9844	0.0066	0.010
3	1	3	2	2	←	2	1	2	2	2	5648.2179	-0.0006	0.010
3	1	3	2	3	←	2	1	2	3	3	5649.0816	0.0116	0.010

3	1	3	2	1	←	2	1	2	1	1	5649.6409	-0.0027	0.010
3	1	3	4	5	←	2	1	2	3	4	5650.2482	0.0097	0.010
3	1	3	4	4	←	2	1	2	2	3	5650.4072	-0.0129	0.010
3	1	3	3	4	←	2	1	2	3	3	5650.4922	-0.0024	0.010
3	1	3	2	1	←	2	1	2	1	0	5650.6138	0.0085	0.010
3	1	3	3	3	←	2	1	2	2	2	5650.7887	0.0012	0.010
3	1	3	2	2	←	2	1	2	1	1	5650.9432	0.0015	0.010
3	1	3	2	2	←	2	1	2	3	2	5651.2461	-0.0056	0.010
3	1	3	4	4	←	2	1	2	3	4	5652.1336	0.0018	0.010
3	0	3	4	3	←	2	0	2	2	3	5907.0603	0.0008	0.010
3	0	3	2	2	←	2	0	2	2	2	5907.1647	-0.0063	0.010
3	0	3	2	3	←	2	0	2	3	3	5907.5980	-0.0068	0.010
3	0	3	2	1	←	2	0	2	1	1	5907.9166	0.0017	0.010
3	0	3	4	5	←	2	0	2	3	4	5908.2105	-0.0017	0.010
3	0	3	3	3	←	2	0	2	2	2	5908.4500	-0.0075	0.010
3	0	3	2	2	←	2	0	2	1	1	5908.5707	-0.0031	0.010
3	0	3	3	3	←	2	0	2	2	3	5908.7693	0.0141	0.010
3	0	3	4	4	←	2	0	2	3	4	5909.1511	-0.0081	0.010
3	0	3	3	2	←	2	0	2	1	2	5909.2583	-0.0001	0.010
3	1	2	4	4	←	2	1	1	3	4	6209.4047	-0.0021	0.010
3	1	2	3	2	←	2	1	1	1	1	6209.7515	-0.0005	0.010
3	1	2	4	3	←	2	1	1	3	2	6209.8636	0.0017	0.010
3	1	2	2	3	←	2	1	1	1	2	6209.9789	0.0031	0.010
3	1	2	4	5	←	2	1	1	3	4	6210.0634	-0.0014	0.010
3	1	2	3	4	←	2	1	1	2	3	6210.1271	-0.0004	0.010
3	1	2	4	4	←	2	1	1	3	3	6210.3060	0.0067	0.010
3	1	2	3	2	←	2	1	1	2	2	6211.1683	-0.0025	0.010
4	1	4	5	6	←	3	1	3	4	5	7526.4768	0.0000	0.010
4	1	4	5	5	←	3	1	3	4	4	7526.5612	0.0026	0.010
4	1	4	4	5	←	3	1	3	3	4	7526.6239	-0.0101	0.010
4	1	4	4	4	←	3	1	3	3	3	7526.7638	-0.0038	0.010
4	1	4	4	3	←	3	1	3	2	2	7526.8497	-0.0038	0.010
4	0	4	3	2	←	3	0	3	2	2	7847.0056	-0.0036	0.010
4	0	4	5	6	←	3	0	3	4	5	7847.5853	-0.0003	0.010
4	0	4	4	4	←	3	0	3	3	3	7847.8430	0.0158	0.010
4	0	4	4	3	←	3	0	3	4	3	7848.2009	-0.0038	0.010
4	0	4	4	4	←	3	0	3	4	4	7848.2977	-0.0053	0.010
4	2	3	4	5	←	3	2	2	3	4	7907.4367	0.0068	0.010
4	2	3	4	4	←	3	2	2	4	3	7907.7392	-0.0049	0.010
4	2	2	4	4	←	3	2	1	3	3	7972.4009	0.0222	0.010
4	2	2	3	4	←	3	2	1	4	4	7972.1836	0.0105	0.010

Table 5: Experimental rotational parameters for hydantoin-H_2O complex (I). Values in parenthesis are standard errors.

Parameters	Hydantoin-$H_2{}^{16}O$ (I)	Hydantoin-$H_2{}^{18}O$ (I)
A (MHz)	5029.76179(63)	4990.2437(11)
B (MHz)	1135.03113(20)	1082.36369(21)
C (MHz)	932.88647(16)	895.75461(24)
Δ_J (kHz)	0.1305(62)	[0.1305]
χ_{aa} (MHz)	1.7100(73)	1.721(15)
X_{bb-cc} (MHz)	5.185(10)	5.180(22)
χ_{ab} (MHz)	[0.1360]	[0.1360]
χ_{aa} (MHz)	2.0814(62)	2.075(13)
X_{bb-cc} (MHz)	6.7832(76)	6..769(17)
χ_{ab} (MHz)	[-0.5956]	[-0.5956]
Nlines	179	121
RMS (kHz)	5.0	7.8

Table 6: Line list of hydantoin-$H_2{}^{16}O$ complex (II). Frequencies are in MHz.

J'	K_a'	K_c'	F_1'	F_2'		J"	K_a"	K_c"	F_1"	F_2"	Obs.	Obs. – Calc.	Exp. Error
b-type transitions													
2	1	1	2	2	←	2	0	2	2	2	2557.2579	-0.0042	0.010
2	1	1	2	3	←	2	0	2	3	3	2557.9205	0.0150	0.010
2	1	1	2	1	←	2	0	2	2	1	2558.0972	0.0186	0.010
2	1	1	3	3	←	2	0	2	2	3	2559.0626	0.0101	0.010
2	1	1	3	4	←	2	0	2	3	4	2560.0013	0.0138	0.010
2	1	1	1	2	←	2	0	2	1	2	2560.4484	0.0122	0.010
2	1	1	3	2	←	2	0	2	3	2	2560.9307	0.0065	0.010
2	0	2	3	2	←	1	1	1	1	2	3522.8854	0.0005	0.010
2	0	2	1	2	←	1	1	1	2	2	3523.7751	-0.0084	0.010
2	0	2	3	4	←	1	1	1	2	3	3524.3085	-0.0067	0.010
2	0	2	2	3	←	1	1	1	2	2	3524.5713	-0.0041	0.010
2	0	2	3	3	←	1	1	1	1	2	3524.7356	0.0015	0.010
2	0	2	3	2	←	1	1	1	0	1	3524.7801	-0.0085	0.010
2	0	2	1	1	←	1	1	1	0	1	3525.0043	-0.0042	0.010
2	0	2	2	2	←	1	1	1	1	2	3525.0954	-0.0063	0.010
2	0	2	2	2	←	1	1	1	1	1	3525.1813	-0.0055	0.010
2	0	2	3	3	←	1	1	1	2	3	3525.5816	-0.0025	0.010
2	0	2	2	1	←	1	1	1	2	1	3525.7564	0.0008	0.010
3	1	2	3	3	←	3	0	3	3	3	3665.7799	0.0031	0.010
3	1	2	3	4	←	3	0	3	3	3	3666.0202	0.0086	0.010
3	1	2	3	4	←	3	0	3	4	4	3666.7459	0.0009	0.010
3	1	2	3	2	←	3	0	3	2	2	3666.9912	0.0052	0.010
1	1	1	0	1	←	0	0	0	1	2	3953.7994	0.0040	0.010
1	1	1	2	1	←	0	0	0	1	1	3954.5792	0.0064	0.010
1	1	1	2	3	←	0	0	0	1	2	3954.8557	0.0065	0.010

1	1	1	2	2	←	0	0	0	1	1	3955.1340	0.0063	0.010
1	1	1	1	1	←	0	0	0	1	0	3955.6224	0.0082	0.010
1	1	1	1	2	←	0	0	0	1	2	3955.7046	0.0054	0.010
1	1	1	1	0	←	0	0	0	1	1	3955.9814	0.0033	0.010
3	1	2	2	3	←	2	2	1	3	2	4006.8417	0.0004	0.010
3	1	2	4	5	←	2	2	1	3	4	4007.1384	-0.0057	0.010
3	1	2	4	4	←	2	2	1	2	3	4007.2416	-0.0087	0.010
3	1	2	4	3	←	2	2	1	1	2	4007.0701	0.0099	0.010
3	2	1	3	3	←	3	1	2	2	2	4124.8272	-0.0027	0.010
3	2	1	4	4	←	3	1	2	2	3	4125.0000	0.0069	0.010
3	2	1	2	2	←	3	1	2	4	3	4125.1186	-0.0002	0.010
3	2	1	3	3	←	3	1	2	3	4	4125.2075	0.0004	0.010
3	2	1	3	3	←	3	1	2	3	3	4125.4432	0.0012	0.010
3	2	1	4	4	←	3	1	2	3	4	4125.5756	0.0067	0.010
3	2	1	3	4	←	3	1	2	4	4	4125.7264	-0.0008	0.010
3	2	1	4	5	←	3	1	2	4	5	4125.8894	0.0145	0.010
3	2	1	4	3	←	3	1	2	2	2	4126.1760	0.0088	0.010
3	2	1	3	2	←	3	1	2	3	3	4126.4554	-0.0082	0.010
2	2	0	2	2	←	2	1	1	2	2	4385.1271	0.0009	0.010
2	2	0	3	3	←	2	1	1	2	3	4385.2176	-0.0006	0.010
2	2	0	1	1	←	2	1	1	1	0	4385.3599	-0.0026	0.010
2	2	0	2	3	←	2	1	1	3	3	4385.5208	-0.0105	0.010
2	2	0	3	4	←	2	1	1	3	4	4385.6639	-0.0100	0.010
2	2	0	3	2	←	2	1	1	3	2	4385.8966	-0.0018	0.010
4	1	3	4	4	←	4	0	4	4	4	5312.4902	-0.0022	0.010
4	1	3	4	4	←	4	0	4	5	5	5313.5313	-0.0113	0.010
4	1	3	4	5	←	4	0	4	5	5	5313.6066	0.0014	0.010
4	1	3	5	5	←	4	0	4	5	5	5313.7081	-0.0029	0.010
4	1	3	4	3	←	4	0	4	3	3	5313.8541	0.0138	0.010
4	1	3	3	3	←	4	0	4	3	3	5313.9842	0.0043	0.010
4	1	3	4	5	←	4	0	4	4	5	5314.5040	-0.0016	0.010
4	1	3	5	5	←	4	0	4	4	5	5314.6021	-0.0094	0.010
4	1	3	3	3	←	4	0	4	4	3	5315.2630	0.0089	0.010
4	1	3	5	6	←	4	0	4	5	6	5315.8113	-0.0031	0.010
2	2	1	2	2	←	2	1	2	2	2	5800.1417	-0.0087	0.010
2	2	1	3	3	←	2	1	2	2	2	5800.3950	-0.0106	0.010
2	2	1	2	2	←	2	1	2	3	3	5800.6831	-0.0049	0.010
2	2	1	3	3	←	2	1	2	3	3	5800.9343	-0.0088	0.010
2	2	1	2	1	←	2	1	2	2	1	5801.1584	-0.0057	0.010
2	2	1	1	1	←	2	1	2	2	2	5801.6051	-0.0023	0.010
2	2	1	3	4	←	2	1	2	3	3	5801.8749	0.0034	0.010
2	2	1	1	2	←	2	1	2	2	1	5802.1844	-0.0052	0.010
2	2	1	3	2	←	2	1	2	3	3	5802.2909	-0.0109	0.010
2	2	1	2	3	←	2	1	2	2	3	5802.4486	0.0019	0.010
2	2	1	3	3	←	2	1	2	3	4	5802.6755	0.0007	0.010
2	2	1	2	2	←	2	1	2	1	1	5802.8819	-0.0076	0.010

2	2	1	3	3	←	2	1	2	3	2	5803.4391	-0.0138	0.010
2	2	1	3	4	←	2	1	2	3	4	5803.6039	0.0009	0.010
2	2	1	1	2	←	2	1	2	1	2	5804.1328	-0.0181	0.010
2	2	1	3	2	←	2	1	2	1	1	5804.5023	-0.0010	0.010
2	2	1	1	1	←	2	1	2	3	2	5804.6425	-0.0123	0.010
2	2	1	3	2	←	2	1	2	3	2	5804.8067	-0.0048	0.010
2	2	1	1	1	←	2	1	2	1	0	5805.2685	-0.0039	0.010
2	1	2	3	2	←	1	0	1	1	2	5973.7326	-0.0049	0.010
2	1	2	3	2	←	1	0	1	1	1	5973.8396	0.0080	0.010
2	1	2	1	1	←	1	0	1	1	2	5974.0495	0.0037	0.010
2	1	2	1	1	←	1	0	1	1	1	5974.1429	0.0031	0.010
2	1	2	1	2	←	1	0	1	2	2	5974.8199	0.0033	0.010
2	1	2	1	2	←	1	0	1	0	1	5975.3415	0.0021	0.010
2	1	2	3	4	←	1	0	1	2	3	5975.4649	0.0033	0.010
2	1	2	3	2	←	1	0	1	2	1	5975.8871	-0.0043	0.010
2	1	2	2	3	←	1	0	1	2	2	5975.9754	0.0032	0.010
2	1	2	3	3	←	1	0	1	1	2	5976.2458	-0.0014	0.010
2	1	2	2	2	←	1	0	1	1	2	5976.7887	0.0038	0.010
2	1	2	2	2	←	1	0	1	1	1	5976.8823	0.0034	0.010
2	1	2	3	3	←	1	0	1	2	3	5977.1967	0.0035	0.010
2	1	2	2	1	←	1	0	1	0	1	5977.3031	0.0024	0.010
2	1	2	2	2	←	1	0	1	2	3	5977.7315	0.0007	0.010
3	0	3	4	3	←	2	1	2	3	3	6139.6378	-0.0098	0.010
3	0	3	3	2	←	2	1	2	2	2	6139.7578	-0.0065	0.010
3	0	3	2	3	←	2	1	2	2	3	6140.8269	-0.0040	0.010
3	0	3	2	1	←	2	1	2	1	1	6141.4623	-0.0048	0.010
3	0	3	4	5	←	2	1	2	3	4	6141.8654	-0.0142	0.010
3	0	3	3	4	←	2	1	2	2	3	6141.9505	0.0037	0.010
3	0	3	4	3	←	2	1	2	3	2	6142.1524	-0.0050	0.010
3	0	3	2	1	←	2	1	2	1	0	6142.3873	-0.0055	0.010
3	0	3	3	2	←	2	1	2	1	1	6142.5076	0.0040	0.010
3	0	3	3	2	←	2	1	2	3	2	6142.8019	-0.0098	0.010
3	0	3	4	4	←	2	1	2	3	4	6143.5471	-0.0068	0.010
3	0	3	2	2	←	2	1	2	1	2	6143.7381	-0.0030	0.010
3	2	2	3	3	←	3	1	3	3	3	6631.4782	0.0032	0.010
3	2	2	4	4	←	3	1	3	4	4	6632.3920	0.0006	0.010
3	2	2	2	2	←	3	1	3	2	2	6632.6191	-0.0027	0.010
3	2	2	3	4	←	3	1	3	3	4	6633.3672	0.0046	0.010
3	2	2	3	2	←	3	1	3	3	2	6634.2176	0.0045	0.010
3	2	2	4	5	←	3	1	3	4	5	6634.4296	0.0091	0.010
3	2	2	2	3	←	3	1	3	2	3	6634.7588	0.0025	0.010
3	2	2	4	3	←	3	1	3	4	3	6635.0274	0.0036	0.010
3	2	2	2	1	←	3	1	3	2	1	6635.5016	0.0003	0.010
5	3	2	6	7	←	5	2	3	6	7	6768.5292	-0.0166	0.010
5	3	2	5	5	←	5	2	3	5	5	6768.7418	-0.0186	0.010
4	1	3	5	5	←	3	2	2	4	4	7276.1313	0.0013	0.010

4	1	3	4	4	←	3	2	2	3	3	7275.9526	-0.0091	0.010
4	1	3	4	5	←	3	2	2	3	4	7276.0179	-0.0061	0.010
4	1	3	5	6	←	3	2	2	4	5	7276.2165	0.0184	0.010
5	1	4	5	5	←	5	0	5	5	5	7382.9883	-0.0015	0.010
5	1	4	6	6	←	5	0	5	6	6	7384.2067	-0.0090	0.010
5	1	4	5	6	←	5	0	5	5	6	7384.9658	0.0049	0.010
5	1	4	5	4	←	5	0	5	5	4	7385.4113	-0.0098	0.010
5	1	4	6	7	←	5	0	5	6	7	7386.2480	0.0016	0.010
5	1	4	4	5	←	5	0	5	4	5	7386.4856	-0.0066	0.010
5	1	4	6	5	←	5	0	5	6	5	7386.6043	-0.0121	0.010
5	1	4	4	3	←	5	0	5	4	3	7386.9258	0.0037	0.010
4	2	3	5	5	←	4	1	4	4	4	7750.2220	0.0055	0.010
4	2	3	4	4	←	4	1	4	4	4	7750.4355	0.0050	0.010
4	2	3	5	5	←	4	1	4	5	5	7751.3844	0.0064	0.010
4	2	3	3	3	←	4	1	4	3	3	7751.5855	0.0106	0.010
4	2	3	4	5	←	4	1	4	4	5	7752.1373	0.0073	0.010
4	2	3	4	3	←	4	1	4	4	3	7752.6548	0.0020	0.010
4	2	3	5	6	←	4	1	4	5	6	7753.1603	0.0075	0.010
4	2	3	3	4	←	4	1	4	3	4	7753.4002	0.0031	0.010
4	2	3	5	4	←	4	1	4	5	4	7753.5615	0.0086	0.010
4	2	3	3	2	←	4	1	4	3	2	7753.8732	0.0008	0.010
3	1	3	3	2	←	2	0	2	2	2	7788.9642	0.0092	0.010
3	1	3	2	3	←	2	0	2	2	3	7789.5094	0.0005	0.010
3	1	3	2	1	←	2	0	2	1	1	7789.6717	0.0080	0.010
3	1	3	2	3	←	2	0	2	1	2	7790.3107	0.0099	0.010
3	1	3	4	5	←	2	0	2	3	4	7790.3981	0.0145	0.010
3	1	3	3	4	←	2	0	2	2	3	7790.9121	0.0094	0.010
3	1	3	2	2	←	2	0	2	2	1	7791.0170	-0.0013	0.010
3	1	3	4	4	←	2	0	2	3	3	7791.1460	0.0021	0.010
3	1	3	3	3	←	2	0	2	2	2	7791.6968	0.0044	0.010
3	1	3	3	3	←	2	0	2	3	3	7792.0699	0.0098	0.010
3	1	3	4	4	←	2	0	2	3	4	7792.4073	-0.0055	0.010
a-type transitions													
2	1	2	3	4	←	1	1	1	2	3	4551.7745	0.0086	0.010
2	1	2	2	3	←	1	1	1	2	2	4552.2678	-0.0008	0.010
2	1	2	3	3	←	1	1	1	1	2	4552.6485	0.0010	0.010
2	0	2	3	4	←	1	0	1	2	3	4948.0176	0.0067	0.010
2	0	2	2	3	←	1	0	1	2	2	4948.2887	0.0097	0.010
2	0	2	2	2	←	1	0	1	1	1	4948.8103	0.0147	0.010
2	1	1	3	2	←	1	1	0	2	1	5571.2423	-0.0188	0.010
2	1	1	2	3	←	1	1	0	2	3	5572.3306	-0.0083	0.010
2	1	1	1	2	←	1	1	0	0	1	5572.8083	-0.0027	0.010
2	1	1	3	4	←	1	1	0	2	3	5573.1471	-0.0049	0.010
2	1	1	3	3	←	1	1	0	2	2	5573.3045	-0.0069	0.010
2	1	1	2	2	←	1	1	0	1	1	5573.6765	0.0021	0.010
2	1	1	2	3	←	1	1	0	1	2	5574.1213	-0.0073	0.010

3	1	3	4	5	←	2	1	2	3	4	6762.9351	0.0022	0.010
3	1	3	4	3	←	2	1	2	3	2	6763.1009	-0.0071	0.010
3	1	3	3	4	←	2	1	2	2	3	6763.1879	-0.0215	0.010
3	1	3	3	3	←	2	1	2	2	2	6763.6038	-0.0052	0.010
3	1	3	4	4	←	2	1	2	3	4	6764.9725	0.0104	0.010
3	0	3	4	5	←	2	0	2	3	4	7169.3354	0.0051	0.010
3	0	3	4	3	←	2	0	2	3	2	7169.4138	0.0035	0.010
3	0	3	3	4	←	2	0	2	2	3	7169.6332	-0.0068	0.010
3	0	3	4	4	←	2	0	2	3	3	7169.7342	-0.0015	0.010
3	0	3	3	2	←	2	0	2	1	1	7169.8401	-0.0045	0.010
3	0	3	3	3	←	2	0	2	2	2	7170.0943	-0.0071	0.010
3	2	2	4	3	←	2	2	1	3	2	7593.3234	0.0031	0.010
3	2	2	3	2	←	2	2	1	1	1	7593.4911	0.0139	0.010
3	2	2	2	3	←	2	2	1	1	2	7593.5712	-0.0053	0.010
3	2	2	4	5	←	2	2	1	3	4	7593.7537	0.0033	0.010
3	2	2	3	4	←	2	2	1	2	3	7594.1270	0.0015	0.010
3	2	2	2	2	←	2	2	1	2	1	7594.6062	0.0038	0.010
3	2	2	4	4	←	2	2	1	3	3	7594.6866	0.0080	0.010
3	2	2	3	3	←	2	2	1	2	2	7594.9364	0.0028	0.010

Table 7: Line list of hydantoin-$H_2{}^{18}O$ complex (II). Frequencies are in MHz.

J'	K_a'	K_c'	F_1'	F_2'		J"	K_a"	K_c"	F_1"	F_2"	Obs.	Obs. – Calc.	Exp. Error
b-type transitions													
2	1	1	2	2	←	2	0	2	2	2	2501.4706	0.0040	0.010
2	1	1	2	3	←	2	0	2	3	3	2502.0989	-0.0018	0.010
2	1	1	3	4	←	2	0	2	3	4	2504.1651	0.0031	0.010
2	1	1	1	2	←	2	0	2	1	2	2504.6071	0.0029	0.010
2	1	1	3	2	←	2	0	2	3	2	2505.0980	0.0077	0.010
2	0	2	3	4	←	1	1	1	2	3	3300.5541	-0.0010	0.010
2	0	2	2	3	←	1	1	1	2	2	3300.7890	-0.0096	0.010
2	0	2	3	3	←	1	1	1	1	2	3300.9410	-0.0058	0.010
2	0	2	3	2	←	1	1	1	0	1	3301.0363	-0.0055	0.010
2	0	2	2	2	←	1	1	1	1	1	3301.3895	0.0004	0.010
1	1	1	0	1	←	0	0	0	1	2	3874.3259	-0.0071	0.010
1	1	1	2	1	←	0	0	0	1	1	3875.1130	0.0005	0.010
1	1	1	2	3	←	0	0	0	1	2	3875.3907	0.0001	0.010
1	1	1	2	2	←	0	0	0	1	1	3875.6727	0.0020	0.010
1	1	1	1	1	←	0	0	0	1	0	3876.1617	0.0029	0.010
1	1	1	1	2	←	0	0	0	1	2	3876.2463	0.0023	0.010
1	1	1	1	0	←	0	0	0	1	1	3876.5360	0.0115	0.010
3	2	1	3	3	←	3	1	2	3	3	4177.4793	-0.0038	0.010
3	2	1	4	4	←	3	1	2	3	4	4177.5761	-0.0089	0.010
3	2	1	3	4	←	3	1	2	4	4	4177.7186	-0.0024	0.010
3	2	1	4	5	←	3	1	2	4	5	4177.8442	0.0041	0.010
4	2	2	5	6	←	4	1	3	5	6	4197.5912	-0.0012	0.010

2	2	0	3	3	←	2	1	1	2	3	4450.0838	-0.0054	0.010
2	2	0	2	3	←	2	1	1	3	3	4450.3902	-0.0030	0.010
2	2	0	1	1	←	2	1	1	3	2	4450.5223	0.0049	0.010
2	2	1	3	3	←	2	1	2	3	3	5779.5823	-0.0120	0.010
2	2	1	2	3	←	2	1	2	2	3	5781.1019	-0.0016	0.010
2	2	1	3	4	←	2	1	2	3	4	5782.2445	-0.0069	0.010
2	2	1	3	2	←	2	1	2	3	2	5783.4549	-0.0062	0.010
2	1	2	3	2	←	1	0	1	1	2	5821.9509	0.0094	0.010
2	1	2	3	2	←	1	0	1	1	1	5822.0490	0.0140	0.010
2	1	2	1	2	←	1	0	1	2	2	5823.0334	0.0122	0.010
2	1	2	1	2	←	1	0	1	0	1	5823.5426	0.0067	0.010
2	1	2	3	4	←	1	0	1	2	3	5823.6697	0.0085	0.010
2	1	2	3	2	←	1	0	1	2	1	5824.0895	0.0014	0.010
2	1	2	2	3	←	1	0	1	2	2	5824.1807	0.0072	0.010
2	1	2	3	3	←	1	0	1	1	2	5824.4660	0.0159	0.010
2	1	2	2	2	←	1	0	1	1	1	5825.0903	0.0107	0.010
2	1	2	3	3	←	1	0	1	2	3	5825.4120	0.0202	0.010
3	0	3	4	4	←	2	1	2	3	3	5830.2675	-0.0235	0.010
3	0	3	4	5	←	2	1	2	3	4	5830.3787	-0.0059	0.010
3	0	3	4	3	←	2	1	2	3	2	5830.6624	-0.0134	0.010
3	2	2	3	3	←	3	1	3	3	3	6551.3556	-0.0016	0.010
3	2	2	3	4	←	3	1	3	4	4	6552.2581	-0.0093	0.010
3	2	2	2	2	←	3	1	3	2	2	6552.4990	0.0020	0.010
3	2	2	4	4	←	3	1	3	3	4	6553.2349	-0.0043	0.010
3	2	2	3	2	←	3	1	3	3	2	6554.0831	-0.0031	0.010
3	2	2	4	5	←	3	1	3	4	5	6554.2920	0.0017	0.010
3	2	2	2	3	←	3	1	3	2	3	6554.6129	-0.0106	0.010
3	2	2	4	3	←	3	1	3	4	3	6554.8907	-0.0015	0.010
4	1	3	4	4	←	3	2	2	3	3	6705.8485	0.0030	0.010
4	1	3	4	5	←	3	2	2	3	4	6705.9346	0.0056	0.010
4	1	3	5	5	←	3	2	2	4	4	6706.0553	0.0140	0.010
3	1	3	4	3	←	2	0	2	3	3	7574.4752	0.0079	0.010
3	1	3	3	2	←	2	0	2	2	2	7574.9142	-0.0024	0.010
3	1	3	2	3	←	2	0	2	2	3	7575.4404	-0.0165	0.010
3	1	3	2	1	←	2	0	2	1	1	7575.5909	-0.0034	0.010
3	1	3	2	3	←	2	0	2	1	2	7576.2340	0.0084	0.010
3	1	3	4	5	←	2	0	2	3	4	7576.3179	0.0040	0.010
3	1	3	3	4	←	2	0	2	2	3	7576.8340	-0.0073	0.010
3	1	3	2	2	←	2	0	2	2	1	7576.9636	-0.0014	0.010
3	1	3	4	4	←	2	0	2	3	3	7577.0917	0.0000	0.010
3	1	3	3	3	←	2	0	2	2	2	7577.6464	0.0014	0.010
3	1	3	3	3	←	2	0	2	3	3	7577.9974	-0.0042	0.010
3	1	3	4	4	←	2	0	2	3	4	7578.3425	0.0057	0.010
4	2	3	4	4	←	4	1	4	4	4	7592.3488	0.0161	0.010
4	2	3	5	5	←	4	1	4	5	5	7593.2845	0.0090	0.010
4	2	3	3	3	←	4	1	4	3	3	7593.4728	0.0012	0.010

4	2	3	4	5	←	4	1	4	4	5	7594.0289	0.0014	0.010
4	2	3	4	3	←	4	1	4	4	3	7594.5496	0.0011	0.010
4	2	3	5	6	←	4	1	4	5	6	7595.0468	0.0016	0.010
a-type transitions													
3	1	2	3	4	←	2	1	1	2	3	7921.1747	-0.0063	0.010
3	1	2	4	4	←	2	1	1	3	3	7920.9473	-0.0013	0.010
3	1	2	4	5	←	2	1	1	3	4	7920.8238	-0.0037	0.010
3	1	2	4	3	←	2	1	1	1	2	7920.7052	-0.0177	0.010
3	1	2	2	3	←	2	1	1	3	2	7920.5928	-0.0089	0.010
3	2	1	4	4	←	2	2	0	3	3	7648.6862	0.0093	0.010
3	2	1	3	4	←	2	2	0	2	3	7648.2684	-0.0081	0.010
3	2	1	4	5	←	2	2	0	3	4	7648.1495	0.0002	0.010
2	1	1	3	3	←	1	1	0	2	2	5327.4507	0.0028	0.010
2	1	1	3	4	←	1	1	0	2	3	5327.2925	0.0004	0.010
2	0	2	3	4	←	1	0	1	2	3	4750.8521	-0.0066	0.010
2	0	2	2	3	←	1	0	1	2	2	4751.1133	-0.0020	0.010

Table 8: Experimental rotational parameters for hydantoin-H_2O complex (II). Values in parenthesis are standard errors.

Parameters	Hydantoin-$H_2{}^{16}O$ (II)	Hydantoin-$H_2{}^{18}O$ (II)
A (MHz)	2944.64549(47)	2901.35875(55)
B (MHz)	1520.96485(56)	1451.06795(33)
C (MHz)	1010.39251(44)	974.22152(27)
Δ_J (kHz)	0.300(23)	[0.300]
δ_J (kHz)	0.1039(54)	[0.1039]
χ_{aa} (MHz)	1.4634(59)	1.437(11)
X_{bb-cc} (MHz)	4.873(11)	4.877(20)
χ_{ab} (MHz)	[0.3275]	[0.3275]
χ_{aa} (MHz)	2.5916(44)	2.5920(73)
X_{bb-cc} (MHz)	6.7080(92)	6.711(16)
χ_{ab} (MHz)	[0.1606]	[0.1606]
Nlines	181	83
RMS (kHz)	7.5	7.8

Table 9: Line list of hydantoin-$H_2{}^{16}O$ complex (III). Frequencies are in MHz.

J'	K_a'	K_c'	F_1'	F_2'		J"	K_a"	K_c"	F_1"	F_2"	Obs.	Obs. – Calc.	Exp. Error
b-type transitions													
2	1	2	3	4	←	1	0	1	2	3	5972.7359	-0.0006	0.010
2	1	2	3	2	←	1	0	1	2	1	5972.6467	0.0058	0.010
2	1	2	1	2	←	1	0	1	0	1	5973.0010	-0.0019	0.010
2	1	2	3	3	←	1	0	1	2	2	5973.2241	-0.0026	0.010
2	1	2	1	1	←	1	0	1	0	1	5973.3142	0.0055	0.010
2	1	2	3	2	←	1	0	1	0	1	5973.4142	-0.0184	0.010

2	1	2	3	3	←	1	0	1	2	3	5973.5037	0.0065	0.010
2	1	2	2	3	←	1	0	1	1	2	5973.6313	0.0009	0.010
2	1	2	2	2	←	1	0	1	1	2	5974.1429	-0.0085	0.010
2	1	2	2	2	←	1	0	1	1	1	5974.2396	0.0033	0.010
2	1	2	2	3	←	1	0	1	2	3	5974.4799	0.0026	0.010
2	1	2	3	2	←	1	0	1	2	2	5972.1040	-0.0017	0.010
2	1	2	1	0	←	1	0	1	0	1	5972.4019	-0.0015	0.010
2	1	2	1	1	←	1	0	1	1	1	5971.4713	-0.0187	0.010
2	1	2	1	1	←	1	0	1	1	2	5971.4033	-0.0020	0.010
2	1	2	1	2	←	1	0	1	1	1	5971.1863	0.0019	0.010
2	1	2	1	2	←	1	0	1	1	2	5971.0949	-0.0047	0.010
4	1	3	4	4	←	3	2	2	3	3	7116.7283	-0.0114	0.010
3	2	2	3	2	←	3	1	3	2	1	6667.7997	-0.0088	0.010
3	2	2	3	3	←	3	1	3	3	3	6663.8374	0.0060	0.010
3	2	2	3	3	←	3	1	3	3	4	6664.7261	0.0031	0.010
3	2	2	4	3	←	3	1	3	3	2	6664.9540	0.0042	0.010
3	2	2	4	5	←	3	1	3	4	4	6665.7242	0.0136	0.010
3	2	2	4	5	←	3	1	3	4	5	6666.7411	-0.0001	0.010
3	2	2	3	3	←	3	1	3	2	3	6667.3533	0.0095	0.010
3	2	2	3	3	←	3	1	3	4	3	6667.0540	-0.0125	0.010
3	2	2	3	2	←	3	1	3	2	1	6667.7995	-0.0090	0.010
3	0	3	2	2	←	2	1	2	1	2	6077.4931	0.0037	0.010
3	0	3	2	2	←	2	1	2	1	1	6077.1855	0.0018	0.010
3	0	3	2	3	←	2	1	2	1	2	6076.8483	-0.0029	0.010
3	0	3	3	4	←	2	1	2	2	3	6076.3747	-0.0113	0.010
3	2	1	3	3	←	3	1	2	3	3	4186.5220	0.0046	0.010
1	1	1	2	3	←	0	0	0	1	2	3961.5079	-0.0008	0.010
1	1	1	1	2	←	0	0	0	1	2	3962.4412	-0.0149	0.010
3	1	3	2	3	←	2	0	2	2	3	7778.5182	0.0064	0.010
3	1	3	2	2	←	2	0	2	2	2	7778.9475	0.0108	0.010
3	1	3	2	1	←	2	0	2	1	1	7779.5327	0.0007	0.010
3	1	3	4	5	←	2	0	2	3	4	7780.2909	0.0065	0.010
3	1	3	4	4	←	2	0	2	3	3	7780.7871	0.0065	0.010
3	1	3	3	2	←	2	0	2	2	1	7781.0027	-0.0009	0.010
3	1	3	3	4	←	2	0	2	2	3	7781.1450	0.0123	0.010
3	1	3	3	3	←	2	0	2	2	2	7781.6646	0.0086	0.010
3	1	3	3	3	←	2	0	2	2	3	7782.0319	0.0077	0.010
4	2	3	3	4	←	4	1	4	3	4	7765.0914	-0.0099	0.010
4	2	3	5	4	←	4	1	4	5	4	7764.9217	-0.0003	0.010
4	2	3	5	6	←	4	1	4	5	6	7764.7010	0.0117	0.010
4	2	3	5	5	←	4	1	4	5	5	7763.7069	0.0022	0.010
4	2	3	4	5	←	4	1	4	4	5	7762.8778	-0.0021	0.010
3	2	2	2	2	←	3	1	3	2	2	6666.5476	-0.0038	0.010
2	1	2	2	1	←	1	0	1	2	1	5974.6090	0.0116	0.010
4	2	2	4	4	←	4	1	3	4	4	4241.4849	0.0038	0.010
4	2	2	4	5	←	4	1	3	4	5	4241.7627	0.0115	0.010

4	2	2	5	5	←	4	1	3	5	5	4241.9582	-0.0002	0.010
4	2	2	3	3	←	4	1	3	3	3	4242.1046	0.0004	0.010
4	2	2	5	6	←	4	1	3	5	6	4242.2601	0.0095	0.010
1	1	1	1	1	←	0	0	0	1	0	3962.3544	-0.0076	0.010
1	1	1	2	2	←	0	0	0	1	1	3961.7723	-0.0060	0.010
3	1	2	3	3	←	3	0	3	3	3	3641.5078	0.0155	0.010
3	1	2	3	4	←	3	0	3	3	4	3642.4303	0.0070	0.010
3	1	2	4	4	←	3	0	3	4	4	3643.5484	0.0136	0.010
3	1	2	4	3	←	3	0	3	4	3	3644.9662	0.0144	0.010
2	0	2	3	3	←	1	1	1	2	2	3468.7190	0.0023	0.010
2	0	2	3	4	←	1	1	1	2	3	3468.4556	0.0035	0.010
2	1	1	2	1	←	2	0	2	2	1	2560.2905	0.0071	0.010
2	1	1	3	4	←	2	0	2	3	4	2562.2287	0.0186	0.010
2	1	1	1	2	←	2	0	2	1	2	2563.1878	0.0215	0.010
3	1	3	3	4	←	2	0	2	3	4	7782.3008	-0.0017	0.010
3	1	3	4	3	←	2	0	2	3	2	7780.2155	-0.0003	0.010
4	1	3	5	5	←	3	2	2	4	4	7117.0111	-0.0117	0.010
4	1	3	4	5	←	3	2	2	3	4	7116.8317	0.0088	0.010
3	0	3	3	2	←	2	1	2	3	2	6078.3030	-0.0034	0.010
3	0	3	3	4	←	2	1	2	3	4	6078.1230	-0.0038	0.010
3	0	3	2	1	←	2	1	2	1	0	6077.0742	-0.0010	0.010
2	2	0	2	2	←	2	1	1	2	2	4454.5135	-0.0091	0.010
2	2	0	3	3	←	2	1	1	3	3	4454.6989	-0.0172	0.010
2	2	0	2	3	←	2	1	1	2	3	4454.6142	-0.0235	0.010
2	2	0	3	4	←	2	1	1	3	4	4454.8567	-0.0202	0.010
3	2	1	4	4	←	3	1	2	4	4	4186.7027	0.0036	0.010
3	1	2	4	5	←	3	0	3	4	5	3644.6303	0.0173	0.010
4	1	3	3	2	←	4	0	4	3	2	5257.4706	-0.0086	0.010
4	1	3	3	4	←	4	0	4	3	4	5257.1091	0.0027	0.010
4	1	3	5	4	←	4	0	4	5	4	5256.8648	-0.0052	0.010
4	1	3	5	5	←	4	0	4	5	5	5255.3814	-0.0101	0.010
4	1	3	4	5	←	4	0	4	4	5	5254.3008	-0.0143	0.010
4	1	3	4	4	←	4	0	4	4	4	5253.2020	-0.0076	0.010
2	2	0	3	2	←	2	1	1	3	2	4454.9604	-0.0011	0.010

Table 10: Line list of hydantoin-$H_2{}^{18}O$ complex (III). Frequencies are in MHz.

J'	K_a'	K_c'	F_1'	F_2'		J"	K_a"	K_c"	F_1"	F_2"	Obs.	Obs. – Calc.	Exp. Error
b-type transitions													
3	1	3	4	5	←	2	0	2	3	4	7566.7803	0.0043	0.010
3	1	3	4	4	←	2	0	2	3	3	7567.2834	0.0051	0.010
3	1	3	3	2	←	2	0	2	2	1	7567.5238	-0.0019	0.010
3	1	3	3	4	←	2	0	2	2	3	7567.6551	-0.0005	0.010
2	1	2	3	4	←	1	0	1	2	3	5821.3794	0.0005	0.010
2	1	2	2	1	←	1	0	1	1	0	5821.8694	-0.0013	0.010

1	1	1	0	1	←	0	0	0	1	2	3881.2625	-0.0078	0.010
1	1	1	2	1	←	0	0	0	1	1	3882.2364	-0.0017	0.010
1	1	1	2	3	←	0	0	0	1	2	3882.4916	-0.0006	0.010
1	1	1	2	2	←	0	0	0	1	1	3882.7693	0.0041	0.010
2	0	2	3	2	←	1	1	1	2	1	3244.6165	-0.0003	0.010
1	1	1	1	1	←	0	0	0	1	0	3883.3527	-0.0004	0.010
1	1	1	1	2	←	0	0	0	1	2	3883.4497	0.0016	0.010
2	1	2	1	2	←	1	0	1	0	1	5821.6647	0.0132	0.010
2	1	2	1	1	←	1	0	1	0	1	5821.9522	-0.0072	0.010
2	1	2	2	3	←	1	0	1	1	2	5822.2898	0.0037	0.010
2	1	2	2	2	←	1	0	1	1	1	5822.8888	-0.0021	0.010
3	1	3	3	3	←	2	0	2	2	2	7568.1763	-0.0057	0.010
3	1	3	3	3	←	2	0	2	2	3	7568.5374	-0.0019	0.010
3	1	3	2	3	←	2	0	2	1	2	7566.6863	-0.0025	0.010
2	1	2	3	2	←	1	0	1	2	1	5821.2824	0.0009	0.010

Table 11: Experimental rotational parameters for hydantoin-H_2O complex (III). Values in parenthesis are standard errors.

Parameters	Hydantoin-$H_2{}^{16}O$ (III)	Hydantoin-$H_2{}^{18}O$ (III)
A (MHz)	2956.01125(78)	2913.1665(24)
B (MHz)	1507.54475(93)	1437.9473(29)
C (MHz)	1005.70153(76)	969.53176(66)
Δ_J (kHz)	0.305(42)	[0.305]
χ_{aa} (MHz)	2.137(10)	2.223(27)
X_{bb-cc} (MHz)	7.346(14)	7.470(31)
χ_{ab} (MHz)	[-0.2493]	[-0.2493]
χ_{aa} (MHz)	1.587(14)	1.541(23)
X_{bb-cc} (MHz)	4.494(18)	4.488(27)
χ_{ab} (MHz)	[-0.2506]	[-0.2506]
Nlines	86	21
RMS (kHz)	9.2	4.5

Table 12: Line list of hydantoin-$(H_2{}^{16}O)_2$ complex (I). Frequencies are in MHz.

J'	K_a'	K_c'	F_1'	F_2'		J"	K_a"	K_c"	F_1"	F_2"	Obs.	Obs. – Calc.	Exp. Error
b-type transitions													
4	2	3	3	2	←	4	1	4	3	2	7540.3338	0.0052	0.010
4	2	3	5	4	←	4	1	4	5	4	7540.0118	0.0035	0.010
4	2	3	3	4	←	4	1	4	3	4	7539.9043	-0.0050	0.010
4	2	3	5	6	←	4	1	4	5	6	7539.6589	-0.0017	0.010
4	2	3	3	3	←	4	1	4	4	3	7539.1281	-0.0025	0.010
4	2	3	5	5	←	4	1	4	4	5	7538.6492	0.0013	0.010
4	2	3	4	3	←	4	1	4	3	3	7538.2584	-0.0029	0.010
4	2	3	4	5	←	4	1	4	5	5	7538.0860	0.0099	0.010

4	2	3	4	4	←	4	1	4	4	4	7537.1277	-0.0074	0.010
3	2	2	4	3	←	3	1	3	4	3	7231.5802	-0.0066	0.010
3	2	2	2	3	←	3	1	3	2	3	7231.4115	-0.0010	0.010
3	2	2	2	2	←	3	1	3	2	2	7230.7940	-0.0061	0.010
3	2	2	3	4	←	3	1	3	3	4	7230.0231	0.0113	0.010
3	2	2	3	2	←	3	1	3	3	2	7229.4560	-0.0135	0.010
3	2	2	4	4	←	3	1	3	4	4	7229.2552	0.0009	0.010
3	2	2	3	3	←	3	1	3	3	3	7228.3372	0.0011	0.010
4	1	4	4	4	←	3	0	3	3	3	6963.7969	-0.0027	0.010
4	1	4	5	5	←	3	0	3	3	4	6963.1515	-0.0020	0.010
4	1	4	3	3	←	3	0	3	3	2	6963.0483	0.0050	0.010
4	1	4	4	5	←	3	0	3	4	4	6962.8576	0.0004	0.010
4	1	4	4	3	←	3	0	3	2	2	6962.6996	0.0096	0.010
4	1	4	5	6	←	3	0	3	4	5	6962.1949	-0.0015	0.010
4	1	4	3	4	←	3	0	3	2	3	6962.0845	0.0033	0.010
4	1	4	3	2	←	3	0	3	2	1	6961.9289	0.0100	0.010
6	0	6	7	8	←	5	1	5	6	7	6572.2302	0.0050	0.010
6	0	6	6	5	←	5	1	5	5	4	6572.0944	-0.0086	0.010
6	0	6	6	7	←	5	1	5	5	6	6571.9187	0.0013	0.010
6	0	6	5	5	←	5	1	5	4	4	6571.7639	-0.0002	0.010
6	0	6	7	7	←	5	1	5	6	6	6571.6885	-0.0057	0.010
6	0	6	6	6	←	5	1	5	5	5	6571.4142	-0.0003	0.010
6	0	6	5	6	←	5	1	5	4	5	6572.3215	0.0026	0.010
6	0	6	5	4	←	5	1	5	4	3	6572.4842	0.0030	0.010
3	2	1	3	3	←	3	1	2	3	3	6367.8356	-0.0044	0.010
3	2	1	4	4	←	3	1	2	4	4	6367.6250	-0.0058	0.010
3	2	1	3	4	←	3	1	2	3	4	6367.4266	0.0215	0.010
3	2	1	4	5	←	3	1	2	4	5	6367.1720	0.0082	0.010
4	2	2	4	4	←	4	1	3	4	4	6151.2321	0.0001	0.010
4	2	2	5	5	←	4	1	3	5	5	6150.9616	0.0081	0.010
4	2	2	4	5	←	4	1	3	4	5	6150.7645	0.0092	0.010
4	2	2	5	6	←	4	1	3	5	6	6150.4484	-0.0066	0.010
4	2	2	3	2	←	4	1	3	3	2	6150.2426	-0.0071	0.010
3	1	3	3	3	←	2	0	2	2	3	5889.7507	0.0041	0.010
3	1	3	4	4	←	2	0	2	3	4	5889.6612	-0.0057	0.010
3	1	3	3	3	←	2	0	2	2	2	5889.4547	-0.0012	0.010
3	1	3	4	4	←	2	0	2	2	3	5888.8258	-0.0027	0.010
3	1	3	3	2	←	2	0	2	2	1	5888.6789	-0.0038	0.010
3	1	3	3	4	←	2	0	2	3	3	5888.4911	-0.0010	0.010
3	1	3	2	2	←	2	0	2	1	1	5888.3260	-0.0058	0.010
3	1	3	4	5	←	2	0	2	3	4	5887.8565	0.0015	0.010
3	1	3	2	1	←	2	0	2	1	0	5887.5437	-0.0050	0.010
5	0	5	5	5	←	4	1	4	4	4	5050.0766	0.0163	0.010
5	0	5	5	6	←	4	1	4	4	5	5050.6705	0.0040	0.010
5	0	5	4	5	←	4	1	4	3	4	5051.1434	-0.0067	0.010
5	0	5	6	5	←	4	1	4	5	4	5051.2167	0.0009	0.010

2	1	2	3	3	←	1	0	1	2	2	4751.6307	-0.0117	0.010
2	1	2	3	4	←	1	0	1	2	3	4751.1021	-0.0039	0.010
1	1	1	0	1	←	0	0	0	1	2	3541.1618	-0.0014	0.010
1	1	1	2	1	←	0	0	0	1	1	3542.0294	0.0005	0.010
1	1	1	2	3	←	0	0	0	1	2	3542.3189	-0.0003	0.010
1	1	1	2	2	←	0	0	0	1	1	3542.6141	-0.0013	0.010
1	1	1	1	1	←	0	0	0	1	0	3543.1525	-0.0004	0.010
1	1	1	1	2	←	0	0	0	1	2	3543.2441	-0.0018	0.010
4	0	4	5	6	←	3	1	3	4	5	3521.7424	0.0017	0.010
4	0	4	4	5	←	3	1	3	3	4	3521.3895	0.0008	0.010
4	0	4	4	3	←	3	1	3	3	2	3521.0879	-0.0016	0.010
4	0	4	5	5	←	3	1	3	4	4	3520.9987	-0.0022	0.010
4	0	4	4	4	←	3	1	3	3	3	3520.7428	0.0073	0.010
3	1	2	4	5	←	3	0	3	4	5	2741.8600	0.0040	0.010
3	1	2	3	4	←	3	0	3	4	4	2740.9612	0.0166	0.010
3	1	2	2	2	←	3	0	3	3	2	2740.4492	0.0078	0.010
3	1	2	4	4	←	3	0	3	3	4	2740.2542	0.0015	0.010
3	1	2	3	3	←	3	0	3	3	3	2739.4681	0.0084	0.010
4	0	4	3	4	←	3	1	3	2	3	3521.9112	-0.0018	0.010
4	0	4	5	4	←	3	1	3	4	3	3522.0334	0.0049	0.010
2	1	2	2	3	←	1	0	1	1	2	4751.9493	-0.0067	0.010
2	1	2	3	2	←	1	0	1	0	1	4751.3514	-0.0154	0.010
2	1	2	2	3	←	1	0	1	2	3	4752.7407	-0.0087	0.010
5	0	5	6	6	←	4	1	4	5	5	5050.3734	0.0060	0.010
5	0	5	4	4	←	4	1	4	3	3	5050.4505	-0.0028	0.010
4	2	2	4	3	←	4	1	3	4	3	6150.5984	-0.0094	0.010
5	1	5	4	3	←	4	0	4	3	2	7989.1184	0.0025	0.010
5	1	5	6	7	←	4	0	4	5	6	7989.3284	-0.0010	0.010
5	1	5	5	4	←	4	0	4	3	3	7989.8424	0.0065	0.010
5	1	5	5	6	←	4	0	4	4	5	7989.9705	0.0073	0.010
5	1	5	4	4	←	4	0	4	4	3	7990.1289	0.0056	0.010
5	1	5	6	6	←	4	0	4	5	5	7990.2162	0.0067	0.010
5	1	5	5	5	←	4	0	4	4	4	7990.8431	0.0099	0.010
a-type transitions													
2	1	2	1	0	←	1	1	1	0	1	2567.4408	-0.0010	0.010
2	1	2	1	2	←	1	1	1	2	1	2567.5372	-0.0009	0.010
2	1	2	3	4	←	1	1	1	2	3	2567.6429	-0.0001	0.010
2	1	2	2	1	←	1	1	1	1	0	2567.9220	-0.0034	0.010
2	1	2	3	2	←	1	1	1	0	1	2568.0740	-0.0064	0.010
2	1	2	3	3	←	1	1	1	2	2	2568.1511	0.0041	0.010
2	1	2	2	3	←	1	1	1	1	2	2568.3511	-0.0085	0.010
2	1	2	2	2	←	1	1	1	1	2	2568.9174	0.0015	0.010
2	1	2	2	2	←	1	1	1	1	1	2569.0075	-0.0016	0.010
2	1	2	2	3	←	1	1	1	2	3	2569.2921	0.0057	0.010
2	0	2	3	2	←	1	0	1	1	1	2709.4078	-0.0017	0.010
2	0	2	1	1	←	1	0	1	1	2	2709.4834	0.0002	0.010

2	0	2	1	1	←	1	0	1	1	1	2709.5748	0.0123	0.010
2	0	2	1	2	←	1	0	1	2	2	2710.0118	-0.0034	0.010
2	0	2	2	1	←	1	0	1	1	0	2710.1952	-0.0029	0.010
2	0	2	3	4	←	1	0	1	2	3	2710.4918	0.0049	0.010
2	0	2	3	3	←	1	0	1	2	2	2710.6442	0.0042	0.010
2	0	2	2	2	←	1	0	1	1	1	2710.9045	0.0026	0.010
2	0	2	3	2	←	1	0	1	0	1	2711.1080	0.0049	0.010
2	0	2	1	1	←	1	0	1	0	1	2711.2595	0.0035	0.010
2	0	2	2	3	←	1	0	1	2	3	2711.3337	0.0084	0.010
2	0	2	2	1	←	1	0	1	2	1	2711.5130	-0.0061	0.010
2	1	1	1	1	←	1	1	0	0	1	2866.1620	-0.0003	0.010
2	1	1	3	2	←	1	1	0	0	1	2866.3240	0.0017	0.010
2	1	1	2	1	←	1	1	0	2	1	2866.6716	-0.0097	0.010
2	1	1	3	3	←	1	1	0	2	3	2867.1626	-0.0014	0.010
2	1	1	1	2	←	1	1	0	2	1	2867.6995	-0.0023	0.010
2	1	1	3	4	←	1	1	0	2	3	2868.0565	0.0009	0.010
2	1	1	2	3	←	1	1	0	2	2	2868.2022	0.0029	0.010
2	1	1	2	2	←	1	1	0	1	1	2868.4268	0.0060	0.010
2	1	1	2	2	←	1	1	0	1	2	2868.5957	0.0037	0.010
2	1	1	3	3	←	1	1	0	1	2	2868.8823	0.0001	0.010
2	1	1	2	1	←	1	1	0	1	0	2869.5195	-0.0004	0.010
2	1	1	1	1	←	1	1	0	1	1	2869.8534	0.0142	0.010
2	1	1	3	2	←	1	1	0	1	1	2870.0018	0.0027	0.010
2	1	1	3	2	←	1	1	0	1	2	2870.1733	0.0029	0.010
3	1	3	4	3	←	2	1	2	2	3	3845.0678	-0.0040	0.010
3	1	3	2	2	←	2	1	2	2	2	3845.3038	0.0009	0.010
3	1	3	2	3	←	2	1	2	3	3	3846.0859	-0.0030	0.010
3	1	3	2	1	←	2	1	2	1	1	3846.6507	-0.0020	0.010
3	1	3	4	5	←	2	1	2	3	4	3847.2425	0.0068	0.010
3	1	3	3	4	←	2	1	2	3	3	3847.4877	-0.0019	0.010
3	1	3	3	3	←	2	1	2	2	2	3847.7658	-0.0005	0.010
3	1	3	2	2	←	2	1	2	1	1	3847.9207	-0.0014	0.010
3	1	3	2	2	←	2	1	2	3	2	3848.2198	-0.0012	0.010
3	1	3	3	3	←	2	1	2	2	3	3848.3217	-0.0007	0.010
3	1	3	4	4	←	2	1	2	3	4	3849.0507	0.0030	0.010
3	1	3	3	2	←	2	1	2	1	2	3849.2287	0.0012	0.010
3	0	3	4	3	←	2	0	2	2	3	4046.1101	-0.0105	0.010
3	0	3	2	2	←	2	0	2	2	2	4046.2509	0.0089	0.010
3	0	3	2	3	←	2	0	2	3	3	4046.6212	-0.0031	0.010
3	0	3	2	1	←	2	0	2	1	1	4046.9222	0.0079	0.010
3	0	3	2	2	←	2	0	2	2	3	4046.5349	0.0022	0.010
3	0	3	4	5	←	2	0	2	3	4	4047.2189	-0.0066	0.010
3	0	3	3	3	←	2	0	2	2	2	4047.5161	0.0004	0.010
3	0	3	2	2	←	2	0	2	1	1	4047.5861	0.0047	0.010
3	0	3	2	2	←	2	0	2	3	2	4047.7342	0.0000	0.010
3	0	3	3	3	←	2	0	2	2	3	4047.8125	0.0060	0.010

3	0	3	3	4	←	2	0	2	3	4	4048.1660	0.0051	0.010
3	0	3	3	2	←	2	0	2	1	2	4048.2558	-0.0010	0.010
3	2	1	4	3	←	2	2	0	3	2	4106.3471	-0.0106	0.010
3	2	1	2	3	←	2	2	0	1	2	4106.4769	-0.0155	0.010
3	2	1	4	5	←	2	2	0	3	4	4106.6612	-0.0018	0.010
3	2	1	4	4	←	2	2	0	2	3	4107.2876	-0.0127	0.010
3	1	2	2	2	←	2	1	1	1	2	4296.5992	0.0097	0.010
3	1	2	4	4	←	2	1	1	3	4	4296.7135	-0.0030	0.010
3	1	2	3	2	←	2	1	1	3	2	4296.9123	-0.0022	0.010
3	1	2	2	1	←	2	1	1	1	0	4297.0091	-0.0059	0.010
3	1	2	3	2	←	2	1	1	1	1	4297.0787	0.0042	0.010
3	1	2	4	3	←	2	1	1	3	2	4297.1874	0.0015	0.010
3	1	2	2	3	←	2	1	1	1	2	4297.2970	0.0026	0.010
3	1	2	4	5	←	2	1	1	3	4	4297.3803	-0.0041	0.010
3	1	2	3	4	←	2	1	1	2	3	4297.4518	0.0045	0.010
3	1	2	4	4	←	2	1	1	3	3	4297.6094	0.0014	0.010
4	1	4	3	4	←	3	1	3	3	4	5120.2135	0.0000	0.010
4	1	4	3	2	←	3	1	3	2	2	5120.5064	0.0051	0.010
4	1	4	5	6	←	3	1	3	4	5	5121.5773	0.0103	0.010
4	1	4	4	5	←	3	1	3	3	4	5121.7348	0.0058	0.010
4	1	4	4	4	←	3	1	3	3	3	5121.8603	0.0007	0.010
4	1	4	4	3	←	3	1	3	2	2	5121.9349	-0.0045	0.010
4	1	4	4	4	←	3	1	3	4	4	5122.7769	-0.0006	0.010
4	1	4	5	5	←	3	1	3	4	5	5123.4630	0.0036	0.010
4	1	4	3	3	←	3	1	3	2	3	5123.5833	-0.0005	0.010
4	0	4	5	4	←	3	0	3	3	4	5361.2037	0.0017	0.010
4	0	4	3	3	←	3	0	3	3	3	5361.3239	0.0004	0.010
4	0	4	3	4	←	3	0	3	4	4	5361.6352	-0.0054	0.010
4	0	4	3	2	←	3	0	3	2	2	5361.7664	-0.0020	0.010
4	0	4	5	6	←	3	0	3	4	5	5362.3675	-0.0026	0.010
4	0	4	4	5	←	3	0	3	4	4	5362.5175	0.0005	0.010
4	0	4	3	3	←	3	0	3	2	2	5362.5904	-0.0068	0.010
4	0	4	4	4	←	3	0	3	3	3	5362.6742	-0.0014	0.010
4	0	4	3	3	←	3	0	3	4	3	5362.9975	-0.0116	0.010
4	0	4	4	4	←	3	0	3	3	4	5363.1581	-0.0016	0.010
4	0	4	5	5	←	3	0	3	4	5	5363.4474	0.0051	0.010
4	2	3	3	2	←	3	2	2	2	1	5430.0276	-0.0025	0.010
4	2	3	5	6	←	3	2	2	4	5	5430.1575	-0.0041	0.010
4	2	3	3	3	←	3	2	2	2	2	5430.2719	0.0019	0.010
4	2	3	5	5	←	3	2	2	3	4	5430.3657	0.0006	0.010
4	2	3	4	5	←	3	2	2	4	4	5430.4615	-0.0076	0.010
4	2	3	4	4	←	3	2	2	3	3	5430.6608	0.0022	0.010
4	2	2	5	6	←	3	2	1	4	5	5503.8583	-0.0148	0.010
4	2	2	4	5	←	3	2	1	3	4	5503.9818	0.0020	0.010
4	2	2	4	4	←	3	2	1	3	3	5504.1051	-0.0079	0.010
4	1	3	5	5	←	3	1	2	4	5	5720.0392	0.0095	0.010

4	1	3	4	3	←	3	1	2	3	2	5720.5132	0.0043	0.010
4	1	3	5	6	←	3	1	2	4	5	5720.5847	0.0028	0.010
5	1	5	6	5	←	4	1	4	5	5	6387.2693	0.0061	0.010
5	1	5	5	4	←	4	1	4	4	4	6387.3622	0.0025	0.010
5	1	5	4	5	←	4	1	4	4	5	6388.0175	-0.0068	0.010
5	1	5	4	3	←	4	1	4	4	3	6388.1969	0.0024	0.010
5	1	5	6	7	←	4	1	4	5	6	6389.5015	-0.0016	0.010
5	1	5	5	5	←	4	1	4	4	4	6389.7177	0.0085	0.010
5	0	5	5	4	←	4	0	4	4	4	6649.6952	0.0032	0.010
5	0	5	4	5	←	4	0	4	4	5	6649.9669	-0.0080	0.010
5	0	5	4	3	←	4	0	4	3	3	6650.0419	-0.0050	0.010
5	0	5	6	7	←	4	0	4	5	6	6650.8427	-0.0048	0.010
5	0	5	5	6	←	4	0	4	4	5	6651.0045	-0.0021	0.010
5	0	5	5	5	←	4	0	4	4	4	6651.1788	-0.0054	0.010
5	2	4	6	7	←	4	2	3	5	6	6778.4347	-0.0033	0.010
5	2	4	5	5	←	4	2	3	4	4	6778.7388	0.0009	0.010
5	2	3	4	4	←	4	2	2	4	4	6922.6526	0.0030	0.010
5	1	4	4	3	←	4	1	3	3	2	7135.0298	0.0080	0.010
6	1	6	7	8	←	5	1	5	6	7	7650.2607	0.0047	0.010
6	1	6	6	6	←	5	1	5	5	5	7650.4293	0.0053	0.010
6	1	6	7	7	←	5	1	5	6	7	7652.2649	0.0017	0.010
6	0	6	7	7	←	5	0	5	6	7	7912.1197	-0.0086	0.010
6	0	6	6	6	←	5	0	5	6	6	7911.8792	-0.0072	0.010
6	0	6	6	5	←	5	0	5	6	5	7911.6704	-0.0131	0.010
6	0	6	6	6	←	5	0	5	5	5	7911.0580	-0.0053	0.010
6	0	6	7	8	←	5	0	5	6	7	7910.7054	-0.0018	0.010
6	0	6	5	5	←	5	0	5	4	4	7910.8810	-0.0019	0.010

Table 13: Line list of hydantoin-$H_2{}^{18}O$- $H_2{}^{16}O$ complex (I). Frequencies are in MHz.

J'	K_a'	K_c'	F_1'	F_2'		J"	K_a"	K_c"	F_1"	F_2"	Obs.	Obs. – Calc.	Exp. Error
a-type transitions													
2	1	2	3	4	←	1	1	1	2	3	2489.0649	0.0051	0.010
2	0	2	3	4	←	1	0	1	2	3	2624.4302	-0.0012	0.010
2	0	2	3	3	←	1	0	1	2	2	2624.5759	-0.0064	0.010
2	1	1	1	2	←	1	1	0	2	1	2772.5795	0.0083	0.010
2	1	1	3	4	←	1	1	0	2	3	2772.9304	0.0055	0.010
2	1	1	2	3	←	1	1	0	2	2	2773.0824	0.0138	0.010
3	1	3	3	4	←	2	1	2	3	3	3730.1012	0.0036	0.010
3	1	3	4	3	←	2	1	2	3	2	3730.0329	-0.0098	0.010
3	1	3	3	3	←	2	1	2	2	2	3730.3797	0.0066	0.010
3	1	3	2	2	←	2	1	2	1	1	3730.5172	-0.0135	0.010
3	0	3	4	5	←	2	0	2	3	4	3920.1165	-0.0019	0.010
3	0	3	3	3	←	2	0	2	2	2	3920.3999	0.0014	0.010
3	1	2	2	3	←	2	1	1	1	2	4155.1140	-0.0045	0.010
3	1	2	4	5	←	2	1	1	3	4	4155.2090	0.0006	0.010

3	1	2	3	4	←	2	1	1	2	3	4155.2816	0.0113	0.010
3	1	2	4	4	←	2	1	1	3	3	4155.4303	-0.0001	0.010
4	1	4	4	5	←	3	1	3	3	4	4966.0586	0.0004	0.010
4	1	4	5	5	←	3	1	3	4	4	4965.9765	0.0005	0.010
4	1	4	5	6	←	3	1	3	4	5	4965.9022	0.0049	0.010
4	0	4	3	4	←	3	0	3	2	3	5196.4425	-0.0100	0.010
4	0	4	4	5	←	3	0	3	4	4	5196.5741	-0.0091	0.010
4	0	4	3	3	←	3	0	3	2	2	5196.6590	-0.0057	0.010
4	0	4	4	4	←	3	0	3	3	3	5196.7369	0.0025	0.010
4	2	3	5	4	←	3	2	2	3	3	5257.0023	-0.0026	0.010
4	2	3	5	6	←	3	2	2	4	5	5257.0589	-0.0123	0.010
4	2	3	3	3	←	3	2	2	2	2	5257.1768	-0.0024	0.010
4	2	3	5	5	←	3	2	2	4	4	5257.2710	-0.0027	0.010
4	2	3	4	5	←	3	2	2	3	4	5257.3686	-0.0093	0.010
4	2	3	4	4	←	3	2	2	3	3	5257.5620	-0.0044	0.010
4	1	3	3	2	←	3	1	2	2	1	5531.8869	-0.0118	0.010
4	1	3	5	4	←	3	1	2	4	3	5531.9691	0.0058	0.010
4	1	3	5	6	←	3	1	2	4	5	5532.0398	0.0044	0.010
5	1	5	6	7	←	4	1	4	5	6	6196.1914	0.0084	0.010
5	0	5	6	7	←	4	0	4	5	6	6448.6655	0.0016	0.010
5	0	5	6	6	←	4	0	4	5	5	6448.8240	0.0016	0.010
5	0	5	5	5	←	4	0	4	4	4	6448.9892	0.0023	0.010
5	2	4	6	7	←	4	2	3	5	6	6563.0775	0.0038	0.010
5	2	4	6	6	←	4	2	3	4	5	6563.2531	0.0132	0.010
5	2	4	5	5	←	4	2	3	4	4	6563.3673	-0.0035	0.010
5	2	3	6	7	←	4	2	2	5	6	6692.3408	-0.0013	0.010
5	1	4	4	3	←	4	1	3	3	2	6901.0903	-0.0024	0.010
5	1	4	6	7	←	4	1	3	5	6	6901.1778	0.0114	0.010
5	1	4	6	6	←	4	1	3	5	5	6901.2576	0.0043	0.010
6	1	6	5	5	←	5	1	5	4	4	7420.0270	0.0086	0.010
6	1	6	6	5	←	5	1	5	5	4	7420.1335	0.0081	0.010
6	0	6	7	8	←	5	0	5	6	7	7674.6229	0.0050	0.010
6	0	6	5	5	←	5	0	5	4	4	7674.7939	0.0064	0.010
6	0	6	6	6	←	5	0	5	5	5	7674.9497	-0.0124	0.010
6	2	5	7	8	←	5	2	4	6	7	7863.5136	-0.0066	0.010
6	2	5	6	7	←	5	2	4	5	6	7863.6174	-0.0003	0.010
6	2	5	6	6	←	5	2	4	5	5	7863.7189	-0.0125	0.010

Table 14: Line list of hydantoin-$H_2{}^{16}O$- $H_2{}^{18}O$ complex (I). Frequencies are in MHz.

J'	K_a'	K_c'	F_1'	F_2'		J"	K_a"	K_c"	F_1"	F_2"	Obs.	Obs. – Calc.	Exp. Error
a-type transitions													
2	1	2	3	4	←	1	1	1	2	3	2510.1595	0.0012	0.010
2	1	2	3	2	←	1	1	1	0	1	2510.5962	0.0005	0.010
2	1	2	3	3	←	1	1	1	2	2	2510.6683	0.0061	0.010
2	1	2	2	3	←	1	1	1	1	2	2510.8661	-0.0087	0.010

2	1	2	2	2	←	1	1	1	1	1	2511.5185	-0.0058	0.010
2	1	1	3	4	←	1	1	0	2	3	2808.1392	0.0048	0.010
2	1	1	2	3	←	1	1	0	2	2	2808.2926	0.0145	0.010
2	1	1	2	2	←	1	1	0	1	1	2808.5046	0.0050	0.010
2	1	1	3	3	←	1	1	0	1	2	2808.9613	0.0002	0.010
3	1	3	2	1	←	2	1	2	1	1	3760.3166	-0.0092	0.010
3	1	3	4	5	←	2	1	2	3	4	3760.9165	0.0072	0.010
3	1	3	3	4	←	2	1	2	3	3	3761.1586	-0.0049	0.010
3	1	3	3	3	←	2	1	2	2	2	3761.4346	-0.0061	0.010
3	1	3	2	2	←	2	1	2	1	1	3761.5942	-0.0016	0.010
3	0	3	4	5	←	2	0	2	3	4	3958.4966	-0.0120	0.010
3	0	3	3	4	←	2	0	2	2	3	3958.6141	0.0050	0.010
3	0	3	3	3	←	2	0	2	2	2	3958.7957	-0.0088	0.010
3	1	2	4	4	←	2	1	1	3	4	4206.7073	-0.0162	0.010
3	1	2	4	3	←	2	1	1	3	2	4207.1921	0.0002	0.010
3	1	2	2	3	←	2	1	1	1	2	4207.2982	-0.0022	0.010
3	1	2	4	5	←	2	1	1	3	4	4207.3907	0.0000	0.010
3	1	2	3	4	←	2	1	1	2	3	4207.4616	0.0076	0.010
3	1	2	4	4	←	2	1	1	3	3	4207.6161	0.0011	0.010
4	1	4	5	6	←	3	1	3	4	5	5006.3118	0.0148	0.010
4	1	4	4	5	←	3	1	3	3	4	5006.4685	0.0089	0.010
4	1	4	4	4	←	3	1	3	3	3	5006.5972	0.0061	0.010
4	1	4	4	3	←	3	1	3	2	2	5006.6766	0.0067	0.010
4	0	4	3	3	←	3	0	3	3	3	5242.3257	0.0017	0.010
4	0	4	5	6	←	3	0	3	4	5	5243.3737	-0.0025	0.010
4	0	4	4	5	←	3	0	3	4	4	5243.5286	0.0025	0.010
4	0	4	3	3	←	3	0	3	2	2	5243.6014	-0.0044	0.010
4	0	4	4	4	←	3	0	3	3	3	5243.6890	0.0000	0.010
4	0	4	5	5	←	3	0	3	4	5	5244.4543	-0.0042	0.010
4	2	3	3	2	←	3	2	2	2	2	5312.4906	-0.0018	0.010
4	2	3	5	6	←	3	2	2	4	5	5312.6156	-0.0090	0.010
4	2	3	5	5	←	3	2	2	3	4	5312.8216	-0.0067	0.010
4	2	2	5	6	←	3	2	1	4	5	5387.9227	-0.0008	0.010
4	2	2	4	5	←	3	2	1	3	4	5388.0225	-0.0045	0.010
4	2	2	4	4	←	3	2	1	3	3	5388.1441	-0.0131	0.010
4	1	3	4	3	←	3	1	2	3	2	5600.2939	0.0026	0.010
5	1	5	6	7	←	4	1	4	5	6	6245.1830	0.0025	0.010
5	1	5	5	5	←	4	1	4	4	4	6245.3920	0.0036	0.010
5	0	5	6	7	←	4	0	4	5	6	6501.1677	-0.0007	0.010
5	0	5	6	6	←	4	0	4	5	5	6501.3355	-0.0035	0.010
5	0	5	5	5	←	4	0	4	4	4	6501.5129	0.0001	0.010
5	2	3	5	6	←	4	2	2	4	5	6778.4529	0.0067	0.010
5	1	4	6	7	←	4	1	3	5	6	6984.4356	0.0150	0.010
6	1	6	7	8	←	5	1	5	6	7	7476.7742	-0.0086	0.010
6	1	6	6	7	←	5	1	5	5	6	7476.8745	-0.0064	0.010
6	1	6	6	6	←	5	1	5	5	5	7476.9658	0.0129	0.010

6	0	6	7	8	←	5	0	5	6	7	7730.1641	-0.0016	0.010
6	0	6	5	5	←	5	0	5	4	4	7730.3452	0.0005	0.010
6	0	6	6	6	←	5	0	5	5	5	7730.5301	0.0020	0.010
6	2	5	7	8	←	5	2	4	6	7	7943.6398	-0.0032	0.010
6	2	5	5	5	←	5	2	4	4	4	7943.7449	-0.0034	0.010
6	2	5	6	6	←	5	2	4	5	5	7943.8649	0.0045	0.010

Table 15: Experimental rotational parameters for hydantoin-$(H_2O)_2$ complex (I). Values in parenthesis are standard errors.

Parameters	Hydantoin-$(H_2{}^{16}O)_2$ (I)	Hydantoin-$H_2{}^{18}O$-$H_2{}^{16}O$ (I)	Hydantoin-$H_2{}^{16}O$-$H_2{}^{18}O$ (I)
A (MHz)	2938.0518(12)	2916.122(54)	2837.940(40)
B (MHz)	754.55686(17)	728.70575(41)	739.27202(42)
C (MHz)	604.47571(17)	586.89834(41)	590.40906(35)
Δ_J (kHz)	0.0621(31)	[0.0621]	[0.0621]
Δ_K (kHz)	4.05(28)	[4.05]	[4.05]
χ_{aa} (MHz)	1.7000(73)	[1.7000]	[1.7000]
X_{bb-cc} (MHz)	5.181(13)	[5.181]	[5.181]
χ_{ab} (MHz)	[0.1539]	[0.1539]	[0.1539]
χ_{aa} (MHz)	1.5713(66)	[1.5713]	[1.5713]
X_{bb-cc} (MHz)	6.500(10)	[6.500]	[6.500]
χ_{ab} (MHz)	[-0.7919]	[-0.7919]	[-0.7919]
Nlines	218	51	56
RMS (kHz)	5.9	7.1	6.8

Table 16: Line list of hydantoin-$(H_2{}^{16}O)_2$ complex (II). Frequencies are in MHz.

J'	K_a'	K_c'	F_1'	F_2'		J"	K_a"	K_c"	F_1"	F_2"	Obs.	Obs. – Calc.	Exp. Error
b-type transitions													
1	1	1	0	1	←	0	0	0	1	2	2777.6810	0.0016	0.010
1	1	1	2	1	←	0	0	0	1	1	2778.4723	0.0015	0.010
1	1	1	2	3	←	0	0	0	1	2	2778.7406	-0.0073	0.010
1	1	1	2	2	←	0	0	0	1	1	2779.0258	-0.0024	0.010
2	1	2	3	4	←	1	0	1	2	3	4096.0183	-0.0009	0.010
2	1	2	1	2	←	1	0	1	0	1	4095.8797	-0.0050	0.010
3	1	3	3	4	←	2	0	2	2	3	5289.5599	0.0070	0.010
3	1	3	2	2	←	2	0	2	2	1	5289.7256	-0.0042	0.010
3	1	3	4	4	←	2	0	2	3	3	5289.8534	-0.0025	0.010
3	1	3	3	3	←	2	0	2	2	2	5290.3975	-0.0003	0.010
4	1	4	4	4	←	3	0	3	3	3	6418.3408	-0.0013	0.010
4	1	4	5	5	←	3	0	3	4	4	6417.8854	0.0050	0.010
4	1	4	3	3	←	3	0	3	2	2	6417.8082	-0.0038	0.010
4	1	4	4	5	←	3	0	3	3	4	6417.6669	0.0096	0.010
2	2	1	3	2	←	1	1	0	2	1	7017.4634	0.0006	0.010
2	2	1	1	0	←	1	1	0	2	1	7017.7202	0.0046	0.010
2	2	1	3	3	←	1	1	0	2	3	7018.3613	-0.0019	0.010

2	2	1	1	2	←	1	1	0	0	1	7018.8867	-0.0069	0.010
2	2	1	3	4	←	1	1	0	2	3	7019.2459	-0.0029	0.010
2	2	1	2	3	←	1	1	0	2	2	7019.4477	-0.0029	0.010
2	2	1	2	2	←	1	1	0	1	1	7019.7113	-0.0064	0.010
2	2	1	3	3	←	1	1	0	1	2	7020.1141	0.0060	0.010
2	2	0	3	3	←	1	1	1	1	2	7352.6490	0.0054	0.010
2	2	0	3	3	←	1	1	1	2	3	7353.5112	0.0070	0.010
2	2	0	2	3	←	1	1	1	2	2	7353.9213	0.0024	0.010
2	2	0	3	4	←	1	1	1	2	3	7354.6467	0.0041	0.010
2	2	0	1	2	←	1	1	1	2	1	7355.1252	0.0024	0.010
2	2	0	1	1	←	1	1	1	0	1	7356.0630	0.0078	0.010
2	2	0	3	2	←	1	1	1	0	1	7356.2416	-0.0019	0.010
5	1	5	5	5	←	4	0	4	4	4	7551.0122	0.0028	0.010
5	1	5	5	6	←	4	0	4	4	5	7550.5361	0.0093	0.010
1	1	1	1	2	←	0	0	0	1	2	2779.5818	-0.0268	0.010
3	0	3	4	3	←	2	1	2	3	2	3704.6005	0.0053	0.010
3	0	3	2	3	←	2	1	2	1	2	3704.4097	0.0033	0.010
3	0	3	3	2	←	2	1	2	1	1	3704.8306	-0.0026	0.010
3	0	3	3	3	←	2	1	2	2	2	3704.1300	-0.0041	0.010
3	0	3	4	4	←	2	1	2	3	3	3704.0532	0.0065	0.010
2	1	2	3	3	←	1	0	1	2	3	4097.7239	0.0071	0.010
3	2	2	3	3	←	3	1	3	3	3	4841.5629	0.0063	0.010
3	2	2	3	4	←	3	1	3	4	4	4842.4005	0.0023	0.010
3	2	2	4	4	←	3	1	3	3	4	4843.4048	0.0083	0.010
3	2	2	3	2	←	3	1	3	3	2	4844.2115	0.0003	0.010
3	2	2	4	5	←	3	1	3	4	5	4844.3757	0.0058	0.010
3	2	2	2	3	←	3	1	3	2	3	4844.6834	0.0077	0.010
3	2	2	4	3	←	3	1	3	4	3	4844.9697	0.0059	0.010
3	1	3	4	3	←	2	0	2	3	3	5287.2991	0.0081	0.010
3	1	3	3	2	←	2	0	2	2	2	5287.7437	-0.0010	0.010
3	1	3	4	5	←	2	0	2	3	4	5289.0218	-0.0007	0.010
3	1	3	3	3	←	2	0	2	3	3	5290.6970	0.0002	0.010
3	1	3	4	4	←	2	0	2	3	4	5290.9973	0.0030	0.010
5	2	4	5	5	←	5	1	5	5	5	6239.1779	-0.0043	0.010
5	2	4	5	6	←	5	1	5	5	6	6240.7655	0.0214	0.010
5	2	4	4	4	←	5	1	5	4	4	6240.2343	0.0041	0.010
5	2	4	6	5	←	5	1	5	6	5	6241.9996	0.0257	0.010
5	2	4	4	3	←	5	1	5	4	3	6242.1900	-0.0054	0.010
4	1	4	4	4	←	3	0	3	4	4	6418.9336	0.0006	0.010
4	1	4	5	4	←	3	0	3	4	4	6415.2370	-0.0038	0.010
4	1	4	4	3	←	3	0	3	3	3	6415.6535	-0.0063	0.010
4	1	4	3	2	←	3	0	3	3	2	6416.2615	-0.0110	0.010
4	3	2	4	4	←	4	2	3	4	4	6731.2815	0.0001	0.010
4	3	2	5	5	←	4	2	3	5	5	6731.6712	-0.0003	0.010
4	3	2	3	3	←	4	2	3	3	3	6731.7629	0.0055	0.010
4	3	2	4	5	←	4	2	3	4	5	6732.1355	-0.0016	0.010

4	3	2	4	3	←	4	2	3	4	3	6732.3881	-0.0007	0.010
4	3	2	4	3	←	4	2	3	5	4	6732.5573	-0.0027	0.010
4	3	2	3	4	←	4	2	3	3	4	6732.6525	-0.0068	0.010
4	3	2	5	4	←	4	2	3	5	4	6732.7659	-0.0012	0.010
4	3	2	3	2	←	4	2	3	3	2	6732.9020	0.0033	0.010
5	3	3	5	5	←	5	2	4	5	5	6951.7820	0.0000	0.010
5	3	3	6	6	←	5	2	4	6	6	6952.1837	-0.0003	0.010
5	3	3	4	4	←	5	2	4	4	4	6952.2552	-0.0013	0.010
5	3	3	5	6	←	5	2	4	5	6	6952.5684	-0.0052	0.010
5	3	3	5	4	←	5	2	4	5	4	6952.7522	-0.0005	0.010
5	3	3	4	5	←	5	2	4	4	5	6953.0728	-0.0034	0.010
5	3	3	6	5	←	5	2	4	6	5	6953.1413	-0.0063	0.010
5	3	3	4	3	←	5	2	4	4	3	6953.2529	0.0047	0.010
2	2	1	2	1	←	1	1	0	2	1	7017.3261	0.0035	0.010
2	2	1	1	1	←	1	1	0	0	1	7017.9285	-0.0027	0.010
2	2	1	2	2	←	1	1	0	2	3	7018.1340	-0.0126	0.010
2	2	1	2	2	←	1	1	0	1	2	7019.8756	-0.0158	0.010
2	2	1	1	2	←	1	1	0	2	2	7019.9296	0.0085	0.010
2	2	1	1	1	←	1	1	0	1	0	7020.7026	-0.0009	0.010
2	2	1	2	1	←	1	1	0	1	1	7021.0856	-0.0136	0.010
2	2	0	2	2	←	1	1	1	1	2	7352.3596	0.0152	0.010
2	2	0	2	2	←	1	1	1	1	1	7352.4402	0.0093	0.010
2	2	0	3	2	←	1	1	1	1	2	7354.3099	-0.0042	0.010
2	2	0	3	2	←	1	1	1	2	1	7355.4532	0.0013	0.010
2	2	0	1	0	←	1	1	1	0	1	7356.5925	0.0013	0.010
5	1	5	5	5	←	4	0	4	5	5	7551.8638	-0.0110	0.010
5	1	5	6	6	←	4	0	4	5	6	7552.4873	0.0000	0.010
6	1	5	6	6	←	5	2	4	5	5	7943.8911	-0.0107	0.010
6	1	5	7	7	←	5	2	4	6	6	7944.1425	0.0037	0.010
6	1	5	6	7	←	5	2	4	5	6	7944.2200	-0.0038	0.010
6	1	5	7	8	←	5	2	4	6	7	7944.4813	0.0074	0.010
3	2	1	4	4	←	3	1	2	3	4	3346.9620	-0.0031	0.010
2	1	2	3	2	←	1	0	1	2	1	4096.4087	0.0039	0.010
2	1	2	2	3	←	1	0	1	1	2	4096.5196	0.0011	0.010
2	1	2	3	3	←	1	0	1	2	2	4096.8202	-0.0035	0.010
4	0	4	3	4	←	3	1	3	2	3	5360.3700	0.0011	0.010
4	0	4	5	4	←	3	1	3	4	3	5360.4636	0.0050	0.010
4	0	4	4	3	←	3	1	3	3	2	5360.5330	-0.0065	0.010
4	0	4	3	2	←	3	1	3	2	1	5360.6109	0.0054	0.010
4	2	3	4	4	←	4	1	4	4	4	5461.8545	-0.0090	0.010
4	2	3	5	5	←	4	1	4	5	5	5462.7330	-0.0074	0.010
4	2	3	3	3	←	4	1	4	3	3	5462.9025	-0.0240	0.010
4	2	3	4	5	←	4	1	4	4	5	5463.5002	-0.0255	0.010
4	2	3	5	6	←	4	1	4	5	6	5464.4711	-0.0024	0.010
5	3	2	5	5	←	5	2	3	5	5	5747.8426	0.0009	0.010
5	1	4	5	5	←	4	2	3	4	4	5871.9506	0.0032	0.010

5	1	4	4	4	←	4	2	3	3	3	5872.3011	-0.0006	0.010
5	1	4	5	4	←	4	2	3	4	3	5872.4106	0.0016	0.010
5	1	4	4	4	←	4	2	3	4	3	5872.6024	-0.0012	0.010
4	3	1	4	5	←	4	2	2	4	5	6131.1940	0.0125	0.010
2	1	2	1	2	←	1	0	1	1	2	4095.4446	0.0094	0.010
a-type transitions													
2	1	2	2	2	←	1	0	1	2	2	4097.3259	-0.0011	0.010
3	2	2	3	3	←	2	2	1	2	2	4816.9987	-0.0030	0.010
3	2	2	3	4	←	2	2	1	3	3	4816.7830	-0.0027	0.010
3	2	2	4	5	←	2	2	1	3	4	4815.8985	-0.0015	0.010
3	2	2	2	3	←	2	2	1	1	2	4815.7592	0.0052	0.010
3	2	2	3	2	←	2	2	1	2	1	4815.6326	0.0108	0.010
3	2	2	4	3	←	2	2	1	3	2	4815.4874	0.0059	0.010
3	1	2	4	3	←	2	1	1	3	2	5215.7589	-0.0141	0.010
3	1	2	2	3	←	2	1	1	1	2	5215.8956	-0.0015	0.010
3	1	2	4	5	←	2	1	1	3	4	5215.9909	0.0000	0.010
3	1	2	4	4	←	2	1	1	3	3	5216.0826	-0.0003	0.010
3	1	2	3	4	←	2	1	1	2	3	5216.3064	0.0009	0.010
4	0	4	5	6	←	3	0	3	4	5	6012.8412	-0.0010	0.010
4	0	4	4	4	←	3	0	3	3	3	6013.4646	-0.0001	0.010
4	2	3	4	3	←	3	2	2	3	2	6384.8233	0.0005	0.010
4	2	3	4	5	←	3	2	2	4	4	6384.9382	-0.0016	0.010
4	2	3	4	4	←	3	2	2	3	3	6385.3407	0.0000	0.010
4	2	2	5	5	←	3	2	1	4	4	6793.0293	-0.0151	0.010
5	0	5	5	5	←	4	0	4	4	4	7324.2354	0.0091	0.010
2	1	1	3	4	←	1	1	0	2	3	3498.6344	0.0063	0.010
2	1	1	3	3	←	1	1	0	2	2	3498.7454	-0.0105	0.010

Table 17: Line list of hydantoin-$H_2{}^{18}O$- $H_2{}^{16}O$ complex (II). Frequencies are in MHz.

J'	K_a'	K_c'	F_1'	F_2'		J"	K_a"	K_c"	F_1"	F_2"	Obs.	Obs. – Calc.	Exp. Error
b-type transitions													
2	1	2	1	2	←	1	0	1	0	1	3994.7706	-0.0040	0.010
2	1	2	3	4	←	1	0	1	2	3	3994.9021	-0.0071	0.010
2	1	2	3	2	←	1	0	1	2	1	3995.2809	-0.0138	0.010
2	1	2	2	1	←	1	0	1	1	0	3995.3305	-0.0056	0.010
2	1	2	2	3	←	1	0	1	1	2	3995.4069	-0.0014	0.010
2	1	2	3	3	←	1	0	1	2	2	3995.7037	-0.0099	0.010
3	1	3	4	5	←	2	0	2	3	4	5163.1449	-0.0033	0.010
4	0	4	4	4	←	3	1	3	3	3	5280.7793	-0.0030	0.010
4	0	4	5	6	←	3	1	3	4	5	5280.8861	0.0025	0.010
4	0	4	3	4	←	3	1	3	2	3	5280.9735	0.0071	0.010
4	0	4	5	4	←	3	1	3	4	3	5281.0539	-0.0016	0.010
4	0	4	4	3	←	3	1	3	3	2	5281.1498	0.0057	0.010
4	0	4	3	2	←	3	1	3	2	1	5281.1898	-0.0089	0.010

4	1	4	5	6	←	3	0	3	4	5	6269.2486	-0.0085	0.010
4	1	4	4	5	←	3	0	3	3	4	6269.7033	-0.0005	0.010
4	1	4	3	3	←	3	0	3	2	2	6269.8455	-0.0093	0.010
4	1	4	5	5	←	3	0	3	4	4	6269.9198	-0.0019	0.010
4	1	4	4	4	←	3	0	3	3	3	6270.3875	0.0089	0.010
5	1	5	6	7	←	4	0	4	5	6	7383.0360	-0.0056	0.010
5	1	5	5	5	←	4	0	4	4	4	7383.8438	0.0073	0.010
4	3	1	5	6	←	4	2	2	5	6	5882.6051	-0.0030	0.010
4	3	1	4	5	←	4	2	2	4	5	5882.6870	0.0129	0.010
5	0	5	6	5	←	4	1	4	5	4	6802.2739	0.0014	0.010
5	0	5	5	4	←	4	1	4	4	3	6802.3611	0.0121	0.010
2	2	1	3	4	←	1	1	0	2	3	6820.3204	0.0041	0.010
2	2	1	2	3	←	1	1	0	2	2	6820.5099	-0.0078	0.010
5	1	5	5	6	←	4	0	4	4	5	7383.3633	-0.0026	0.010
5	1	5	6	6	←	4	0	4	5	5	7383.5142	0.0137	0.010
2	2	0	3	2	←	1	1	1	0	1	7157.0280	-0.0056	0.010
2	2	0	3	4	←	1	1	1	2	3	7155.4356	0.0062	0.010
2	2	0	2	3	←	1	1	1	2	2	7154.7053	0.0031	0.010

Table 18: Line list of hydantoin-$H_2{}^{16}O$- $H_2{}^{18}O$ complex (II). Frequencies are in MHz.

J'	K_a'	K_c'	F_1'	F_2'		J"	K_a"	K_c"	F_1"	F_2"	Obs.	Obs. – Calc.	Exp. Error
b-type transitions													
3	0	3	4	4	←	2	1	2	3	3	3500.2258	-0.0062	0.010
3	0	3	4	5	←	2	1	2	3	4	3500.4887	-0.0103	0.010
3	0	3	2	3	←	2	1	2	1	2	3500.6476	0.0061	0.010
3	0	3	4	3	←	2	1	2	3	2	3500.8335	-0.0019	0.010
2	1	2	1	2	←	1	0	1	0	1	4033.5478	0.0033	0.010
2	1	2	3	4	←	1	0	1	2	3	4033.6806	0.0016	0.010
2	1	2	2	3	←	1	0	1	1	2	4034.1866	0.0085	0.010
4	0	4	3	4	←	3	1	3	2	3	5117.3470	0.0062	0.010
4	0	4	4	5	←	3	1	3	3	4	5117.1871	0.0039	0.010
4	0	4	5	6	←	3	1	3	4	5	5117.2518	0.0036	0.010
3	1	3	4	5	←	2	0	2	3	4	5193.9491	-0.0039	0.010
3	1	3	3	4	←	2	0	2	2	3	5194.4785	-0.0119	0.010
3	1	3	2	2	←	2	0	2	2	1	5194.6681	-0.0069	0.010
3	1	3	4	4	←	2	0	2	3	3	5194.7950	-0.0068	0.010
3	1	3	3	3	←	2	0	2	2	2	5195.3448	-0.0033	0.010
4	1	4	5	6	←	3	0	3	4	5	6287.8079	-0.0125	0.010
4	1	4	4	5	←	3	0	3	3	4	6288.2894	-0.0004	0.010
4	1	4	3	3	←	3	0	3	2	2	6288.4492	-0.0061	0.010
4	1	4	5	5	←	3	0	3	4	4	6288.5276	0.0001	0.010
4	1	4	4	4	←	3	0	3	3	3	6288.9998	-0.0037	0.010
5	1	5	5	6	←	4	0	4	4	5	7378.4532	0.0108	0.010
5	1	5	6	6	←	4	0	4	5	5	7378.6034	0.0055	0.010
5	1	5	5	5	←	4	0	4	4	4	7378.9751	0.0140	0.010

4	2	2	5	6	←	4	1	3	5	6	3328.9888	0.0052	0.010
4	0	4	5	5	←	3	1	3	4	4	5117.0532	0.0041	0.010
4	1	4	5	4	←	3	0	3	4	3	6287.7688	0.0011	0.010
5	0	5	6	7	←	4	1	4	5	6	6648.6713	-0.0057	0.010

Table 19: Experimental rotational parameters for hydantoin-$(H_2O)_2$ complex (II). Values in parenthesis are standard errors.

Parameters	Hydantoin-$(H_2{}^{16}O)_2$ (II)	Hydantoin-$H_2{}^{18}O$-$H_2{}^{16}O$ (II)	Hydantoin-$H_2{}^{16}O$-$H_2{}^{18}O$ (II)
A (MHz)	2120.22255(63)	2058.26175(86)	2117.4477(27)
B (MHz)	946.67424(56)	932.10505(76)	906.6583(11)
C (MHz)	658.71724(43)	645.66749(26)	638.86208(35)
Δ_J (kHz)	0.1959(77)	[0.1959]	[0.1959]
Δ_{JK} (kHz)	-0.689(37)	[-0.689]	[-0.689]
Δ_K (kHz)	2.408(87)	[2.408]	[2.408]
δ_J (kHz)	0.0529(66)	[0.0529]	[0.0529]
χ_{aa} (MHz)	1.2380(73)	[1.2380]	[1.2380]
X_{bb-cc} (MHz)	4.625(14)	[4.625]	[4.625]
χ_{ab} (MHz)	[0.5647]	[0.5647]	[0.5647]
χ_{aa} (MHz)	2.5276(57)	[2.5276]	[2.5276]
X_{bb-cc} (MHz)	6.750(11)	[6.750]	[6.750]
χ_{ab} (MHz)	[0.1878]	[0.1878]	[0.1878]
Nlines	135	31	27
RMS (kHz)	7.5	7.1	6.8

Table 20: The abbreviated results of the fit of the r_0 geometry of 1w-(I) complex of hydantoin with one water molecule to 6 rotational constants from 2 different isotopic species.

Hydantoin+Water [1w-I], r_0 fit

```
!  1/ 1w-I initial geometry from B3LYP-D3(BJ) calculation
!
!  2/ r(OH) and A(HOH) are from the r0 monomer geometry for H2O
!     from De Lucia,Helminger,Gordy, Phys.Rev.A 8,2785(1973)

NUMBER OF ATOMS = 14

  NO  NA  NB  NC       NO.NA     NO.NA.NB   NO.NA.NB.NC        MASS

   1   0   0   0     0.000000     0.000000     0.000000     15.9949150
   2   1   0   0     1.218389     0.000000     0.000000     12.0000000
   3   2   1   0     1.354958   128.436266     0.000000     14.0030740
   4   3   2   1     1.446237   112.785015  -179.067755     12.0000000
   5   4   3   2     1.529280   102.630624    -0.871242     12.0000000
   6   5   4   3     1.378154   105.152812     0.461263     14.0030740
   7   5   4   3     1.204069   127.612635  -179.547787     15.9949150
   8   6   5   4     1.006247   124.503592   179.589261      1.0078250
   9   4   3   2     1.091309   113.108086   117.089595      1.0078250
  10   4   3   2     1.091084   113.134953  -118.918341      1.0078250
  11   3   2   1     1.011369   119.773425    -1.482376      1.0078250
  12   1   2   6     2.794467    94.198645   180.000000     15.9949150
  13  12   3   4     0.965000    68.873842   172.147155      1.0078250
  14  12  13   1     0.965000   104.780000  -145.436201      1.0078250
!
!   Ni=2: 18O1
!
ISOTOPIC SPECIES  2,  changes from parent species:
atom no.,parameter no.,value    12  4       17.9991596

---------------------------------------------------------------------

Converged after:   7 iterations,  ALAMDA=  0.10E-09

FINAL RESULTS OF LEAST SQUARES FIT:

          R(12, 1) =     2.821376 +-  0.000606
       A(12, 1, 2) =    93.722069 +-  0.015205
       A(13,12, 3) =    88.285987 +-  0.359647
    D(13,12, 3, 4) =   164.584926 +-  0.973545
    D(14,12,13, 1) =  -127.128237 +-  0.576734

             Chi-squared =        0.0000020109
         Deviation of fit =        0.001418
```

Ni	Axis	Iobs	Icalc	Io-c	Bobs	Bcalc	Bo-c
1	a	100.47772	100.47833	-0.00061	5029.7618	5029.7314	0.0304
1	b	445.25564	445.25620	-0.00056	1135.0311	1135.0297	0.0014
1	c	541.73688	541.73632	0.00057	932.8865	932.8874	-0.0010
2	a	101.27341	101.27281	0.00061	4990.2437	4990.2736	-0.0299
2	b	466.92162	466.92106	0.00056	1082.3637	1082.3650	-0.0013
2	c	564.19359	564.19416	-0.00057	895.7546	895.7537	0.0009

Correlation coefficients:

		1	2	3	4	5
1:	R(12, 1)	1.000				
2:	A(12, 1, 2)	-0.974	1.000			
3:	A(13,12, 3)	-0.991	0.940	1.000		
4:	D(13,12, 3, 4)	-0.972	0.998	0.936	1.000	
5:	D(14,12,13, 1)	0.986	-0.988	-0.958	-0.992	1.000

Principal coordinates and estimated uncertainties:

ATOM NO.	A	dA	B	dB	C	dC
1	-1.36916	0.00007	-1.39185	0.00015	0.00674	0.00029
2	-0.43300	0.00003	-0.61209	0.00009	-0.00012	0.00021
3	-0.46504	0.00006	0.74249	0.00009	-0.00013	0.00034
4	0.85467	0.00010	1.33395	0.00001	0.01198	0.00017
5	1.77022	0.00002	0.10910	0.00004	-0.00265	0.00009
6	0.92039	0.00005	-0.97582	0.00001	-0.00966	0.00005
7	2.97415	0.00002	0.09155	0.00012	-0.00698	0.00030
8	1.22171	0.00011	-1.93588	0.00001	-0.01369	0.00019
9	1.05046	0.00028	1.92605	0.00008	0.90756	0.00019
10	1.05541	0.00002	1.95220	0.00008	-0.86433	0.00020
11	-1.35405	0.00009	1.22382	0.00015	0.02889	0.00053
12	-3.31170	0.00013	0.65426	0.00068	0.02004	0.00080
13	-3.25219	0.00581	-0.28355	0.00477	0.23959	0.01520
14	-4.05988	0.00621	0.71821	0.01268	-0.58606	0.00557

NOTES: 1/ only the uncertainties for those coordinates which are completely defined by the fitted internals should be trusted
2/ the uncertainties are somewhat limited by the linear approximation coord=(d coord/d parameter)*parameter used for evaluation
3/ only the effect of the internals R, A, and D is propagated

---

Table 21: The abbreviated results of the fit of the r_0 geometry of 1w-(II) complex of hydantoin with one water molecule to 6 rotational constants from 2 different isotopic species.

Hydantoin+Water [1w-II], r_0 fit

```
!  1/ 1w-II initial geometry from B3LYP-D3(BJ) calculation
!
!  2/ r(OH) and A(HOH) are from the r0 monomer geometry for H2O
!     from De Lucia,Helminger,Gordy, Phys.Rev.A 8,2785(1973)

NUMBER OF ATOMS = 14

  NO  NA  NB  NC       NO.NA     NO.NA.NB   NO.NA.NB.NC        MASS

   1   0   0   0     0.000000     0.000000     0.000000     15.9949150
   2   1   0   0     1.217780     0.000000     0.000000     12.0000000
   3   2   1   0     1.396352   125.801349     0.000000     14.0030740
   4   3   2   1     1.375249   112.987377  -179.316029     12.0000000
   5   4   3   2     1.531942   105.512200     0.059467     12.0000000
   6   2   1   3     1.360465   127.667154   179.852520     14.0030740
   7   6   2   1     1.003256   121.120918     3.392790      1.0078250
   8   5   4   3     1.090660   109.691909  -121.154470      1.0078250
   9   5   4   3     1.091057   109.569421   119.469459      1.0078250
  10   4   3   2     1.204124   127.617763  -179.881845     15.9949150
  11   3   2   1     1.015937   120.354216     0.283019      1.0078250
  12   1   2   6     2.789845    95.396689  -180.000000     15.9949150
  13  12   3   2     0.965000    70.255304     3.138293      1.0078250
  14  12  13   1     0.965000   104.780000  -142.670720      1.0078250
!
!   Ni=2: 18O1
!
ISOTOPIC SPECIES  2,  changes from parent species:
atom no.,parameter no.,value    12  4       17.9991596

--------------------------------------------------------------------------

Converged after:   6 iterations,  ALAMDA=  0.10E-08

FINAL RESULTS OF LEAST SQUARES FIT:

          R(12, 1) =     2.811911 +-  0.000874
       A(12, 1, 2) =    95.092369 +-  0.016977
       A(13,12, 3) =    86.780418 +-  0.520878
    D(13,12, 3, 2) =    -5.693901 +-  1.465344
    D(14,12,13, 1) =  -140.175199 +-  1.134192

             Chi-squared =        0.0000102557
          Deviation of fit =        0.003202
```

Ni	Axis	Iobs	Icalc	Io-c	Bobs	Bcalc	Bo-c
1	a	171.62644	171.62507	0.00137	2944.6455	2944.6689	-0.0234
1	b	332.27527	332.27401	0.00126	1520.9649	1520.9706	-0.0058
1	c	500.18088	500.18217	-0.00130	1010.3925	1010.3899	0.0026
2	a	174.18701	174.18837	-0.00136	2901.3587	2901.3360	0.0227
2	b	348.28073	348.28199	-0.00126	1451.0680	1451.0627	0.0053
2	c	518.75164	518.75035	0.00129	974.2215	974.2239	-0.0024

Correlation coefficients:

		1	2	3	4	5
1:	R(12, 1)	1.000				
2:	A(12, 1, 2)	-0.895	1.000			
3:	A(13,12, 3)	-0.945	0.712	1.000		
4:	D(13,12, 3, 2)	-0.899	0.997	0.713	1.000	
5:	D(14,12,13, 1)	0.920	-0.980	-0.743	-0.991	1.000

Principal coordinates and estimated uncertainties:

ATOM NO.	A	dA	B	dB	C	dC
1	-1.55846	0.00009	-1.31380	0.00017	0.00509	0.00050
2	-0.42724	0.00005	-0.86296	0.00008	-0.00336	0.00026
3	-0.08771	0.00006	0.49149	0.00005	-0.00298	0.00035
4	1.27092	0.00008	0.70460	0.00006	0.00119	0.00002
5	1.90442	0.00004	-0.69022	0.00011	0.00543	0.00036
6	0.74365	0.00011	-1.55555	0.00002	-0.01766	0.00016
7	0.75390	0.00018	-2.55770	0.00002	0.02828	0.00031
8	2.54300	0.00028	-0.80650	0.00006	-0.87106	0.00055
9	2.51305	0.00020	-0.81244	0.00029	0.90267	0.00054
10	1.84923	0.00016	1.76076	0.00011	0.00051	0.00004
11	-0.81323	0.00012	1.20264	0.00011	0.00050	0.00065
12	-2.82707	0.00034	1.19556	0.00087	0.02900	0.00120
13	-3.01220	0.00902	0.25324	0.00217	0.12378	0.02330
14	-3.56673	0.01135	1.54124	0.01519	-0.48543	0.00500

NOTES: 1/ only the uncertainties for those coordinates which are completely defined by the fitted internals should be trusted
2/ the uncertainties are somewhat limited by the linear approximation coord=(d coord/d parameter)*parameter used for evaluation
3/ only the effect of the internals R, A, and D is propagated

---

Table 22: The abbreviated results of the fit of the r_0 geometry of 1w-(III) complex of hydantoin with one water molecule to 6 rotational constants from 2 different isotopic species.

Hydantoin+Water [1w-II], r_0 fit

```
 !  1/ 1w-III initial geometry from B3LYP-D3(BJ) calculation
 !
 !  2/ r(OH) and A(HOH) are from the r0 monomer geometry for H2O
 !     from De Lucia,Helminger,Gordy, Phys.Rev.A 8,2785(1973)

 NUMBER OF ATOMS = 14

   NO  NA  NB  NC       NO.NA     NO.NA.NB   NO.NA.NB.NC        MASS

    1   0   0   0     0.000000     0.000000     0.000000     15.9949150
    2   1   0   0     1.215379     0.000000     0.000000     12.0000000
    3   2   1   0     1.362449   127.342160     0.000000     14.0030740
    4   3   2   1     1.409483   113.152140   179.870961     12.0000000
    5   4   3   2     1.368168   105.418670    -0.087847     14.0030740
    6   5   4   3     1.445593   113.169320     0.294298     12.0000000
    7   4   3   2     1.205406   126.076620  -179.991098     15.9949150
    8   6   5   4     1.091449   113.391740  -118.153103      1.0078250
    9   6   5   4     1.091555   113.401870   117.332525      1.0078250
   10   5   4   3     1.002955   120.975340   179.264927      1.0078250
   11   3   2   1     1.015016   122.452880    -0.078186      1.0078250
   12   1   2   3     2.806218    94.094120     0.000000     15.9949150
   13  12   3   4     0.965000    71.092210   180.000000      1.0078250
   14  12  13   1     0.965000   104.780000  -147.400188      1.0078250
 !
 !   Ni=2: 18O1
 !
 ISOTOPIC SPECIES  2,  changes from parent species:
 atom no.,parameter no.,value    12  4       17.9991596

--------------------------------------------------------------------------

Converged after:   6 iterations,  ALAMDA=  0.10E-08

 FINAL RESULTS OF LEAST SQUARES FIT:

          R(12, 1) =     2.831101 +-  0.001003
       A(12, 1, 2) =    93.647709 +-  0.019175
       A(13,12, 3) =    88.604560 +-  0.604915
    D(13,12, 3, 4) =   175.597446 +-  1.651658
    D(14,12,13, 1) =  -142.749905 +-  1.186605

              Chi-squared =        0.0000132486
         Deviation of fit =        0.003640
```

Ni	Axis	Iobs	Icalc	Io-c	Bobs	Bcalc	Bo-c
1	a	170.96654	170.96500	0.00153	2956.0113	2956.0378	-0.0265
1	b	335.23317	335.23172	0.00145	1507.5448	1507.5513	-0.0065
1	c	502.51391	502.51539	-0.00148	1005.7015	1005.6986	0.0030
2	a	173.48099	173.48252	-0.00153	2913.1665	2913.1408	0.0257
2	b	351.45865	351.46009	-0.00145	1437.9473	1437.9414	0.0059
2	c	521.26091	521.25944	0.00147	969.5318	969.5345	-0.0027

Correlation coefficients:

		1	2	3	4	5
1:	R(12, 1)	1.000				
2:	A(12, 1, 2)	-0.897	1.000			
3:	A(13,12, 3)	-0.942	0.709	1.000		
4:	D(13,12, 3, 4)	-0.892	0.997	0.695	1.000	
5:	D(14,12,13, 1)	0.906	-0.979	-0.714	-0.990	1.000

Principal coordinates and estimated uncertainties:

ATOM NO.	A	dA	B	dB	C	dC
1	-1.56884	0.00010	-1.34135	0.00019	0.00427	0.00056
2	-0.45175	0.00006	-0.86253	0.00009	0.00246	0.00030
3	-0.11888	0.00006	0.45861	0.00006	0.00803	0.00039
4	1.27319	0.00008	0.67940	0.00007	0.00091	0.00002
5	1.83899	0.00004	-0.56623	0.00012	-0.01167	0.00035
6	0.86426	0.00013	-1.63376	0.00003	-0.00647	0.00021
7	1.82166	0.00018	1.75279	0.00012	0.00361	0.00004
8	0.91142	0.00045	-2.26792	0.00010	-0.89353	0.00032
9	0.92130	0.00010	-2.26861	0.00016	0.87964	0.00032
10	2.83539	0.00005	-0.68065	0.00021	-0.00771	0.00066
11	-0.81634	0.00014	1.19600	0.00012	0.01570	0.00070
12	-2.84743	0.00039	1.18452	0.00099	0.02228	0.00130
13	-3.07163	0.01014	0.24893	0.00197	0.09726	0.02645
14	-3.57303	0.01283	1.57187	0.01675	-0.48240	0.00442

NOTES: 1/ only the uncertainties for those coordinates which are completely defined by the fitted internals should be trusted
2/ the uncertainties are somewhat limited by the linear approximation coord=(d coord/d parameter)*parameter used for evaluation
3/ only the effect of the internals R, A, and D is propagated

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Table 23: The abbreviated results of the fit of the r_0 geometry of 2w-(I) complex of hydantoin with one water molecule to 9 rotational constants from 3 different isotopic species.

Hydantoin+Water [2w-I], r_0 fit

```
 !  1/ 2w-I initial geometry from B3LYP-D3(BJ) calculation

 NUMBER OF ATOMS = 17

   NO  NA  NB  NC       NO.NA     NO.NA.NB   NO.NA.NB.NC        MASS
    1   0   0   0     0.000000     0.000000     0.000000     15.9949150
    2   1   0   0     3.476383     0.000000     0.000000     12.0000000
    3   2   1   0     1.204420   153.245553     0.000000     15.9949150
    4   1   2   3     1.222840    14.986110   179.297515     12.0000000
    5   2   1   4     1.377969    26.014254   178.722398     14.0030740
    6   4   1   5     1.348284   129.207779   179.971134     14.0030740
    7   6   4   1     1.448085   112.358300  -179.237568     12.0000000
    8   7   6   4     1.091256   112.875844   117.539424      1.0078250
    9   7   6   4     1.091133   112.944174  -118.978112      1.0078250
   10   6   4   1     1.023378   122.498081    -1.277112      1.0078250
   11   5   2   1     1.006173   124.628163   179.593557      1.0078250
   12   1   4   6     2.732030   120.640609     3.900878     15.9949150
   13  12   1   4     0.982921     6.303178   179.423342      1.0078250
   14  12   1   4     0.960622   110.113179   125.171129      1.0078250
   15  12   1   4     2.705814    88.274079    -1.908527     15.9949150
   16  15  12   1     0.984538    10.665595   171.926493      1.0078250
   17  15  12   1     0.960726   111.377557  -126.077151      1.0078250
 !
 !   Ni=2: 18O1
 !
 ISOTOPIC SPECIES  2,  changes from parent species:
 atom no.,parameter no.,value    12  4       17.9991315
 !
 !   Ni=2: 18O2
 !
 ISOTOPIC SPECIES  3,  changes from parent species:
 atom no.,parameter no.,value    15  4       17.9991315

-------------------------------------------------------------------------
Converged after:   7 iterations,  ALAMDA=  0.10E-09

 FINAL RESULTS OF LEAST SQUARES FIT:

          R(12, 1) =     2.776700 +-  0.003217
          R(15,12) =     2.733328 +-  0.002751
       A(12, 1, 4) =   120.908723 +-  0.143085
       A(15,12, 1) =    87.507249 +-  0.060727
    D(12, 1, 4, 6) =     4.235690 +-  0.032704
       A(13,12, 1) =    19.746618 +-  1.309648
       A(16,15,12) =    32.136441 +-  0.969461

             Chi-squared =        0.0000731379
          Deviation of fit =        0.006047
```

Ni	Axis	Iobs	Icalc	Io-c	Bobs	Bcalc	Bo-c
1	a	172.01161	172.01178	-0.00017	2938.0518	2938.0489	0.0029
1	b	669.76929	669.76939	-0.00011	754.5569	754.5567	0.0001
1	c	836.06173	836.06162	0.00011	604.4757	604.4758	-0.0001
2	a	173.30517	173.30158	0.00359	2916.1220	2916.1824	-0.0604
2	b	693.52960	693.52604	0.00357	728.7057	728.7095	-0.0037
2	c	861.10145	861.10502	-0.00358	586.8983	586.8959	0.0024
3	a	178.07953	178.08290	-0.00337	2837.9400	2837.8862	0.0538
3	b	683.61712	683.62054	-0.00341	739.2720	739.2683	0.0037
3	c	855.98112	855.97771	0.00341	590.4091	590.4114	-0.0024

Correlation coefficients:

		1	2	3	4	5	6	7
1:	R(12, 1)	1.000						
2:	R(15,12)	-0.921	1.000					
3:	A(12, 1, 4)	-0.989	0.966	1.000				
4:	A(15,12, 1)	0.958	-0.966	-0.983	1.000			
5:	D(12, 1, 4, 6)	-0.317	0.304	0.328	-0.307	1.000		
6:	A(13,12, 1)	-0.190	-0.131	0.095	-0.030	0.141	1.000	
7:	A(16,15,12)	-0.050	0.028	0.021	-0.086	-0.189	-0.489	1.000

Principal coordinates and estimated uncertainties:

ATOM NO.	A	dA	B	dB	C	dC
1	-0.78568	0.00180	1.55499	0.00248	0.06525	0.00024
2	2.25871	0.00020	-0.12105	0.00116	-0.02289	0.00013
3	3.46176	0.00025	-0.16455	0.00260	-0.06055	0.00044
4	0.09657	0.00079	0.70850	0.00143	0.04523	0.00022
5	1.46557	0.00115	1.00548	0.00022	0.00299	0.00022
6	-0.01128	0.00082	-0.63541	0.00155	0.05719	0.00060
7	1.27839	0.00161	-1.29200	0.00006	0.00628	0.00043
8	1.40804	0.00231	-1.90358	0.00026	-0.88815	0.00056
9	1.47392	0.00240	-1.91391	0.00035	0.88125	0.00055
10	-0.91560	0.00140	-1.11437	0.00264	0.06732	0.00097
11	1.81299	0.00228	1.94970	0.00063	-0.00813	0.00056
12	-3.46353	0.00052	0.82667	0.00224	-0.02835	0.00020
13	-2.65878	0.01285	1.38955	0.01767	0.01254	0.00040
14	-3.90266	0.00099	1.27530	0.00291	-0.75545	0.00025
15	-2.63168	0.00067	-1.77698	0.00101	-0.04067	0.00050
16	-3.37679	0.01052	-1.13941	0.01201	-0.12802	0.00235
17	-3.04905	0.00071	-2.28129	0.00105	0.66250	0.00063

NOTES: 1/ only the uncertainties for those coordinates which are completely defined by the fitted internals should be trusted
2/ the uncertainties are somewhat limited by the linear approximation coord=(d coord/d parameter)*parameter used for evaluation
3/ only the effect of the internals R, A, and D is propagated

---

Table 24: The abbreviated results of the fit of the r_0 geometry of 2w-(II) complex of hydantoin with one water molecule to 9 rotational constants from 3 different isotopic species.

Hydantoin+Water [2w-II], r_0 fit

```
 !  1/ 2w-II initial geometry from B3LYP-D3(BJ) calculation

 NUMBER OF ATOMS = 17

   NO  NA  NB  NC       NO.NA     NO.NA.NB   NO.NA.NB.NC        MASS
    1   0   0   0     0.000000     0.000000     0.000000     15.9949150
    2   1   0   0     3.473833     0.000000     0.000000     12.0000000
    3   2   1   0     1.204572   154.542980     0.000000     15.9949150
    4   1   2   3     1.221576    12.986239  -178.624390     12.0000000
    5   2   1   4     1.376848    27.090810  -176.387575     14.0030740
    6   4   1   5     1.360473   126.352251   179.965412     14.0030740
    7   6   4   1     1.446812   112.542105   178.232893     12.0000000
    8   7   6   4     1.090679   113.168151   119.406894      1.0078250
    9   7   6   4     1.091048   113.192279  -116.185355      1.0078250
   10   6   4   1     1.003212   121.025012     4.177237      1.0078250
   11   5   2   1     1.031426   124.847728  -179.482135      1.0078250
   12   5   2   1     2.797574   130.910252   178.897985     15.9949150
   13  12   5   2     0.960627   123.471104    57.389772      1.0078250
   14  12   5   2     0.983346    98.193470   173.931383      1.0078250
   15  12   5   2     2.708881    86.438109   174.643681     15.9949150
   16  15  12   5     0.960720   123.125693   116.602767      1.0078250
   17  15  12   5     0.981603    91.648344     5.957349      1.0078250
 !
 !   Ni=2: 18O1
 !
 ISOTOPIC SPECIES  2,  changes from parent species:
 atom no.,parameter no.,value    12  4       17.9991315
 !
 !   Ni=3: 18O2
 !
 ISOTOPIC SPECIES  3,  changes from parent species:
 atom no.,parameter no.,value    15  4       17.9991315
-------------------------------------------------------------------------
Converged after:   7 iterations,  ALAMDA=  0.10E-09

 FINAL RESULTS OF LEAST SQUARES FIT:

          R(12, 5) =     2.817088 +-  0.000705
          R(15,12) =     2.738437 +-  0.005040
       A(12, 5, 2) =   131.418705 +-  0.090430
       A(15,12, 5) =    87.534013 +-  0.057525
    D(15,12, 5, 2) =   178.630264 +-  0.280077
       A(14,12, 5) =   117.196080 +-  3.504001
       A(17,15,12) =   107.302876 +-  3.306420

             Chi-squared =        0.0000924803
         Deviation of fit =       0.006800
```

Ni	Axis	Iobs	Icalc	Io-c	Bobs	Bcalc	Bo-c
1	a	238.36130	238.36300	-0.00170	2120.2225	2120.2075	0.0151
1	b	533.84680	533.84864	-0.00184	946.6742	946.6710	0.0033
1	c	767.21692	767.21511	0.00181	658.7172	658.7188	-0.0015
2	a	245.53680	245.53995	-0.00315	2058.2618	2058.2354	0.0264
2	b	542.19104	542.19419	-0.00314	932.1051	932.0996	0.0054
2	c	782.72333	782.72017	0.00317	645.6675	645.6701	-0.0026
3	a	238.67367	238.66955	0.00412	2117.4477	2117.4842	-0.0365
3	b	557.40846	557.40420	0.00426	906.6583	906.6652	-0.0069
3	c	791.06121	791.06546	-0.00425	638.8621	638.8586	0.0034

Correlation coefficients:

		1	2	3	4	5	6	7
1:	R(12, 5)	1.000						
2:	R(15,12)	0.115	1.000					
3:	A(12, 5, 2)	0.000	0.976	1.000				
4:	A(15,12, 5)	-0.286	-0.973	-0.945	1.000			
5:	D(15,12, 5, 2)	0.018	-0.074	-0.022	0.108	1.000		
6:	A(14,12, 5)	-0.121	0.937	0.978	-0.871	-0.027	1.000	
7:	A(17,15,12)	-0.213	-0.959	-0.931	0.925	0.028	-0.926	1.000

Principal coordinates and estimated uncertainties:

ATOM NO.	A	dA	B	dB	C	dC
1	-0.94017	0.00224	-1.60039	0.00277	0.02052	0.00408
2	1.64390	0.00117	0.72121	0.00103	0.00407	0.00117
3	2.10709	0.00280	1.83313	0.00171	0.01287	0.00245
4	0.12845	0.00137	-1.00886	0.00121	0.00090	0.00208
5	0.31303	0.00065	0.36837	0.00094	0.00230	0.00112
6	1.36429	0.00221	-1.57703	0.00063	-0.02716	0.00039
7	2.42677	0.00076	-0.59527	0.00218	-0.00377	0.00179
8	3.06920	0.00162	-0.63717	0.00314	-0.88417	0.00279
9	3.04972	0.00167	-0.65752	0.00313	0.88979	0.00275
10	1.47721	0.00367	-2.57229	0.00079	0.02887	0.00069
11	-0.47355	0.00163	1.03553	0.00209	-0.00174	0.00205
12	-2.02940	0.00097	1.93171	0.00105	-0.06800	0.00410
13	-2.23647	0.00147	2.60548	0.00114	0.58466	0.00411
14	-2.88705	0.02880	1.46094	0.05259	0.03086	0.00749
15	-3.45122	0.00060	-0.40541	0.00527	0.05583	0.00589
16	-4.03446	0.00108	-0.70300	0.00642	-0.64720	0.00761
17	-2.80654	0.04348	-1.14300	0.03289	-0.00664	0.00844

NOTES: 1/ only the uncertainties for those coordinates which are completely defined by the fitted internals should be trusted
2/ the uncertainties are somewhat limited by the linear approximation coord=(d coord/d parameter)*parameter used for evaluation
3/ only the effect of the internals R, A, and D is propagated

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