

Supplementary information for:

Rotational analysis of Naphthol-aromatic ring complexes stabilized by electrostatic and dispersion interactions

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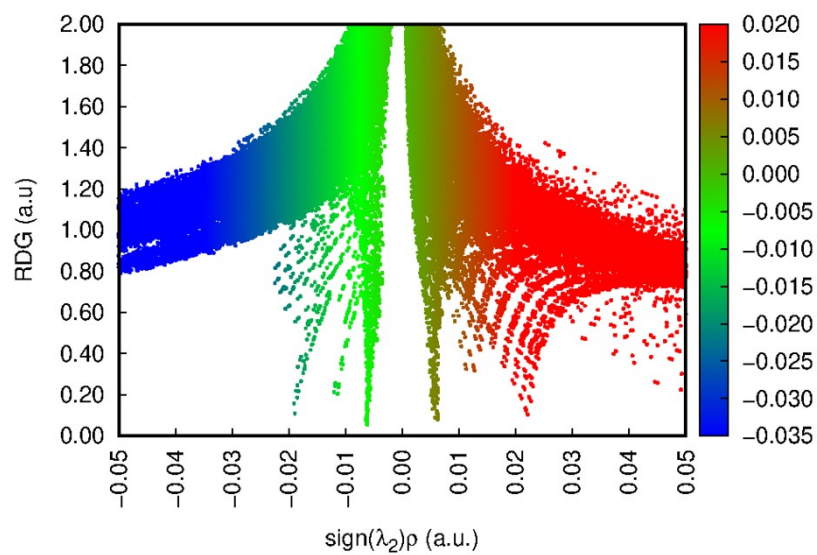
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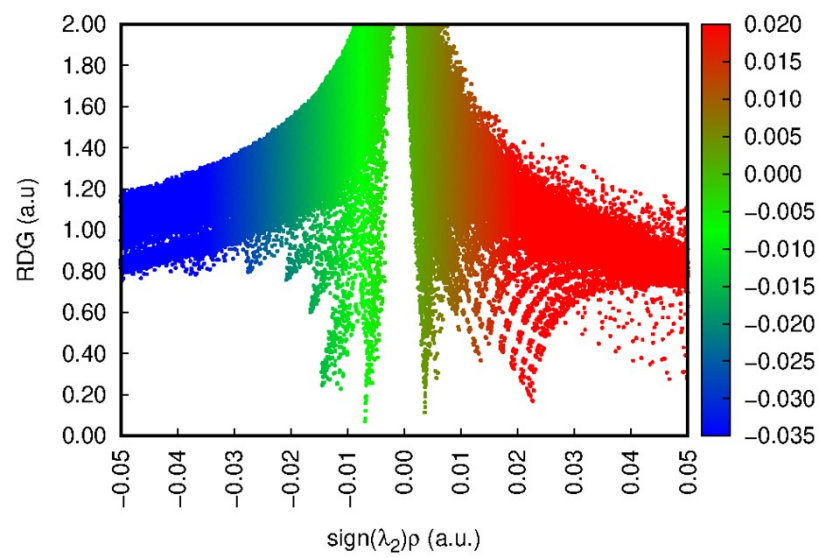
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Figure S1. NCI scatter graphs for the experimentally observed 1NpOH-furan(I), 1NpOH-furan(II), 1NpOH-DMF, and 1NpOH-thiophene complexes.

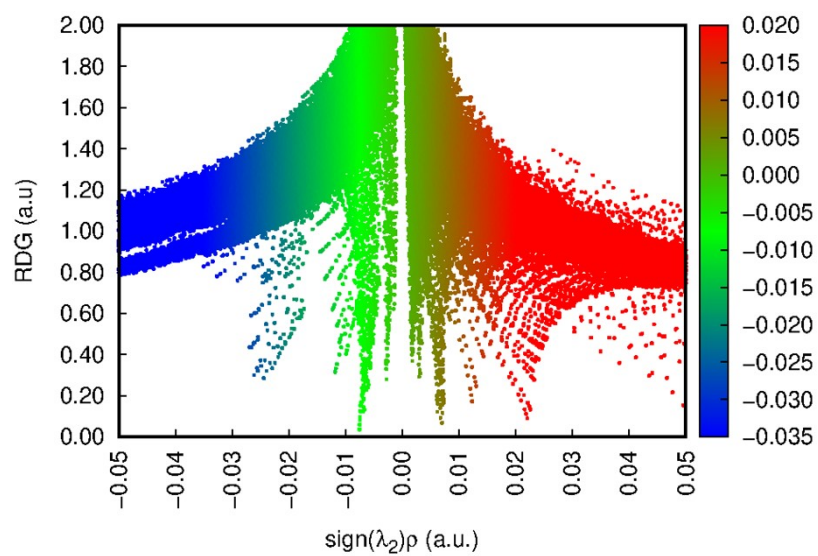
1NpOH-furan(I)



1NpOH-furan(II)



1NpOH-DMF



1NpOH-thiophene

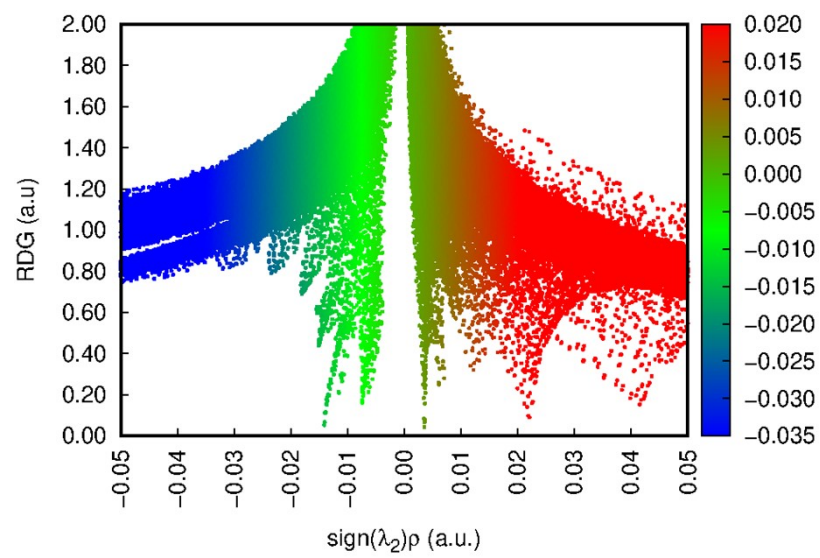
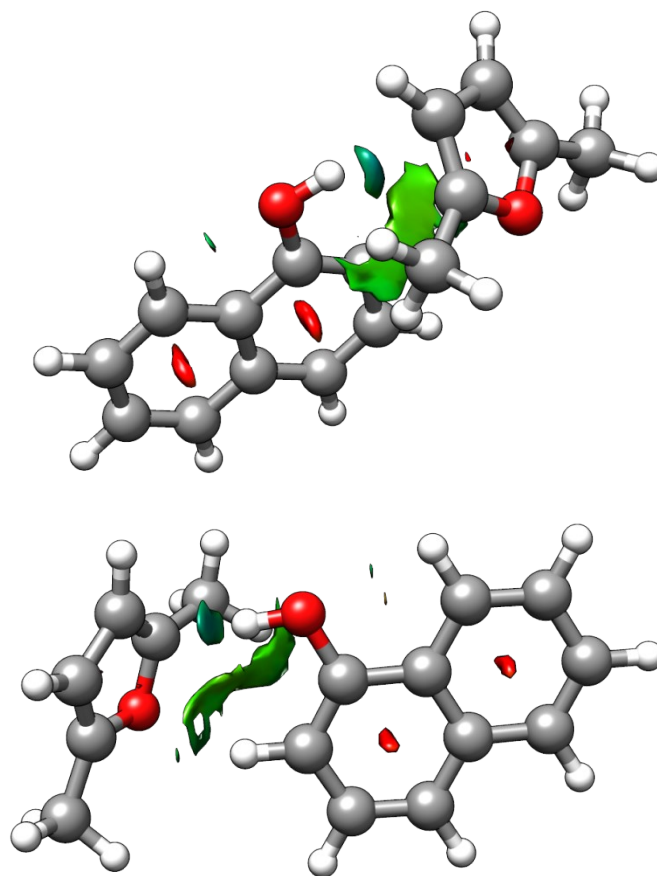


Figure S2. NCI plot and scatter graph for the isomer II of the 1NpOH-DMF complex.



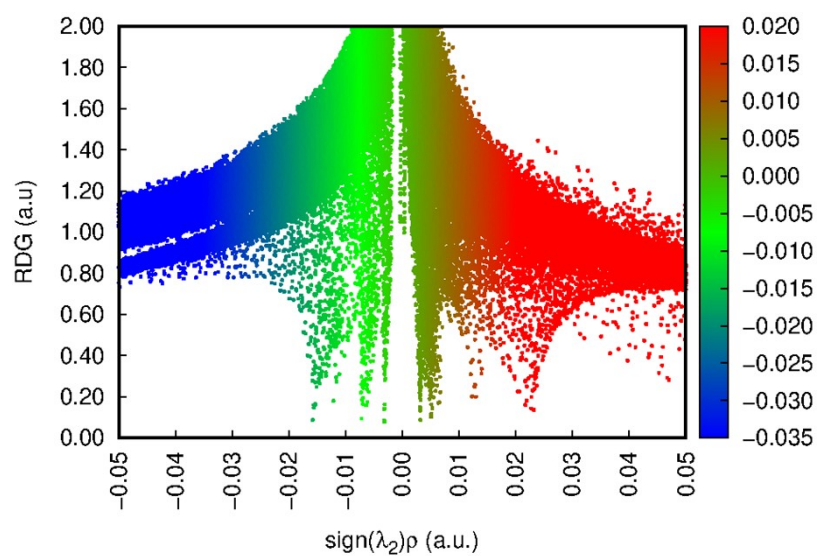


Table S1. Numbering of the isomers compared to that used in ref. 22 in the manuscript.

Our work	Ref. 22
Furan Isomer I	Furan Isomer 1
Furan Isomer II	Furan Isomer 3
DMF Isomer I	DMF Isomer 1
DMF Isomer II	DMF Isomer 2
Thiophene Isomer I	Thiophene Isomer 1
Thiophene Isomer II	Thiophene Isomer 2

Table S2. For the given *a*-type transitions, we provide the intensities and the intensity/ μ_a^2 ratios for 1NpOH-furan (I) and 1NpOH-furan (II) complexes. The labeling of the rotational transitions follows the $J_{K_a K_c}$ scheme. The theoretical μ_a dipole moment components taken are those calculated at the B3LYP-D3/ def2-TZVPP level of theory (1NpOH-furan (I): 3.0 D; 1NpOH-furan (II): 2.2 D).

Transitions	1NpOH-furan (I)		1NpOH-furan (II)	
	Intensity (μV)	I/μ_a^2 ($\mu V/D^2$)	Intensity (μV)	I/μ_a^2 ($\mu V/D^2$)
11₀₁₁-10₀₁₀	6	0.69	1	0.21
12₀₁₂-11₀₁₁	6	0.71	1	0.21
11₁₁₁-10₁₁₀	4	0.46	1	0.26
12₁₁₂-11₁₁₁	10	1.07	1	0.26
11₁₁₀-10₁₉	7	0.82	2	0.33
12₁₁₁-11₁₁₀	13	1.49	3	0.54

Table S3. Normalization of the I/μ_a^2 values obtained in Table S1 with respect to 1NpOH-furan (I).

Transitions	1NpOH-furan (I) / 1NpOH-furan (I)	1NpOH-furan (II) / 1NpOH-furan (I)
11₀₁₁-10₀₁₀	1.00	0.30
12₀₁₂-11₀₁₁	1.00	0.29
11₁₁₁-10₁₁₀	1.00	0.56
12₁₁₂-11₁₁₁	1.00	0.25
11₁₁₀-10₁₉	1.00	0.40
12₁₁₁-11₁₁₀	1.00	0.36
Average	1.00	0.36

Table S4. Observed frequencies and residuals (MHz) for the 1NpOH-furan (I) complex for $J'K'_aK'_c \leftarrow J''K''_aK''_c$ transitions.

$J'K'_aK'_c$	$J''K''_aK''_c$	Obs.	Res.	$J'K'_aK'_c$	$J''K''_aK''_c$	Obs.	Res.	$J'K'_aK'_c$	$J''K''_aK''_c$	Obs.	Res.
5 1 5	4 1 4	2297.9662	0.0014	9 3 7	8 3 6	4275.4473	0.0004	12 3 9	11 3 8	5716.9049	0.0024
5 0 5	4 0 4	2360.6657	-0.0014	9 3 6	8 3 5	4278.2624	-0.0025	12 2 10	11 2 9	5796.8872	-0.0002
5 2 4	4 2 3	2369.9916	0.0023	9 2 7	8 2 6	4318.6656	0.0001	12 1 11	11 1 10	5817.7220	0.0001
5 2 3	4 2 2	2380.5016	-0.0007	10 1 10	9 1 9	4581.5471	0.0014	13 1 13	12 1 12	5941.6233	-0.0074
5 1 4	4 1 3	2439.7650	0.0033	10 0 10	9 0 9	4661.6120	-0.0021	13 0 13	12 0 12	6006.4711	-0.0008
6 1 6	5 1 5	2756.1892	-0.0019	10 2 9	9 2 8	4728.9300	0.0046	13 2 12	12 2 11	6134.5594	-0.0005
6 0 6	5 0 5	2827.1137	-0.0007	10 3 8	9 3 7	4751.7558	-0.0052	13 6 8	12 6 7	6171.1648	-0.0007
6 2 5	5 2 4	2843.0138	0.0025	10 3 7	9 3 6	4756.5650	-0.0058	13 6 7	12 6 6	6171.1648	-0.0008
6 2 4	5 2 3	2861.3038	-0.0007	10 2 8	9 2 7	4809.4938	0.0005	13 5 9	12 5 8	6173.8221	0.0098
6 1 5	5 1 4	2926.1574	0.0006	10 1 9	9 1 8	4860.5655	-0.0032	13 5 8	12 5 7	6173.8221	-0.0027
7 1 7	6 1 6	3213.7268	0.0010	11 1 11	10 1 10	5035.7705	-0.0011	13 4 10	12 4 9	6178.4553	0.0027
7 0 7	6 0 6	3290.6271	-0.0003	11 0 11	10 0 10	5112.3172	0.0016	13 4 9	12 4 8	6179.1261	0.0013
7 2 6	6 2 5	3315.4996	-0.0025	11 2 10	10 2 9	5198.4380	-0.0008	13 3 11	12 3 10	6181.6041	0.0029
7 3 5	6 3 4	3323.6115	0.0163	11 5 7	10 5 6	5222.1138	-0.0016	13 3 10	12 3 9	6199.4020	0.0083
7 3 4	6 3 3	3324.3649	-0.0029	11 5 6	10 5 5	5222.1138	-0.0042	13 2 11	12 2 10	6292.2910	-0.0007
7 2 5	6 2 4	3344.5038	0.0006	11 4 8	10 4 7	5225.0397	0.0040	13 1 12	12 1 11	6292.7864	-0.0013
7 1 6	6 1 5	3411.6461	0.0007	11 4 7	10 4 6	5225.2388	0.0003	14 1 14	13 1 13	6393.3140	-0.0008
8 1 8	7 1 7	3670.4956	-0.0006	11 3 9	10 3 8	5228.2729	-0.0004	14 0 14	13 0 13	6451.0079	-0.0024
8 0 8	7 0 7	3750.9346	0.0040	11 3 8	10 3 7	5236.0407	-0.0012	14 2 13	13 2 12	6601.0289	-0.0014
8 2 7	7 2 6	3787.3657	-0.0091	11 2 9	10 2 8	5302.4113	0.0025	14 7 7	13 7 6	6644.7668	0.0015
8 4 5	7 4 4	3797.4597	0.0054	11 1 10	10 1 9	5340.2153	0.0032	14 7 8	13 7 7	6644.7668	0.0015
8 4 4	7 4 3	3797.4597	-0.0141	12 1 12	11 1 11	5489.1259	-0.0013	14 6 9	13 6 8	6646.7778	-0.0029
8 3 6	7 3 5	3799.3777	-0.0032	12 0 12	11 0 11	5560.4315	0.0047	14 6 8	13 6 7	6646.7778	-0.0033
8 3 5	7 3 4	3800.9382	0.0150	12 2 11	11 2 10	5667.0108	0.0030	14 5 10	13 5 9	6650.0837	0.0177
8 2 6	7 2 5	3830.2746	-0.0068	12 7 6	11 7 5	5694.4253	-0.0120	14 5 9	13 5 8	6650.0837	-0.0073
8 1 7	7 1 6	3896.0275	-0.0006	12 6 7	11 6 6	5695.7372	-0.0011	14 4 11	13 4 10	6655.7210	0.0006
9 1 9	8 1 8	4126.4486	0.0003	12 6 6	11 6 5	5695.7372	-0.0011	14 4 10	13 4 9	6656.8591	0.0006
9 0 9	8 0 8	4207.9082	0.0038	12 5 8	11 5 7	5697.8406	0.0048	14 3 12	13 3 11	6658.2330	0.0014
9 1 8	8 1 7	4379.0836	-0.0006	12 5 7	11 5 6	5697.8406	-0.0010	14 3 11	13 3 10	6683.7678	0.0040
9 2 8	8 2 7	4258.5422	-0.0015	12 4 9	11 4 8	5701.5643	0.0029	14 1 13	13 1 12	6765.0892	-0.0028
9 4 6	8 4 5	4273.0050	-0.0016	12 4 8	11 4 7	5701.9399	-0.0006	14 2 12	13 2 11	6787.9389	-0.0008

9 4 5	8 4 4	4273.0537	0.0001	12 3 10	11 3 9	5704.9175	0.0023	15 1 15	14 1 14	6844.2273	0.0022
Table S4. Continued.											
$J'K'_aK'_c$	$J''K''_aK''_c$	Obs.	Res.	$J'K'_aK'_c$	$J''K''_aK''_c$	Obs.	Res.	$J'K'_aK'_c$	$J''K''_aK''_c$	Obs.	Res.
15 0 15	14 0 14	6894.5698	0.0015	6 1 6	5 0 5	3701.6665	0.0009	8 2 7	7 1 6	6828.0563	0.0022
15 2 14	14 2 13	7066.3630	0.0017	10 0 10	9 1 9	4025.8590	0.0040	16 0 16	15 1 15	7102.6223	-0.0022
15 6 10	14 6 9	7122.5950	-0.0040	7 1 7	6 0 6	4088.2755	-0.0012	7 2 5	6 1 6	7113.6226	0.0012
15 6 9	14 6 8	7122.5950	-0.0048	2 2 0	1 1 1	4393.8823	-0.0012	15 1 15	14 0 14	7129.5425	0.0069
15 4 12	14 4 11	7133.3726	0.0048	8 1 8	7 0 7	4468.1437	-0.0020	3 3 1	2 2 0	7140.3080	0.0036
15 3 13	14 3 12	7134.6938	-0.0002	11 0 11	10 1 10	4556.6178	-0.0070	3 3 0	2 2 1	7140.8363	-0.0026
15 4 11	14 4 10	7135.2263	0.0050	3 2 2	2 1 1	4810.8091	-0.0031	9 2 8	8 1 7	7190.5686	-0.0009
15 3 12	14 3 11	7170.2523	0.0011	9 1 9	8 0 8	4843.6634	0.0000	10 2 9	9 1 8	7540.4009	-0.0098
15 1 14	14 1 13	7234.3215	-0.0039	3 2 1	2 1 2	4898.6104	0.0000	17 0 17	16 1 16	7588.6342	0.0014
15 2 13	14 2 12	7283.1712	0.0006	10 1 10	9 0 9	5217.3062	0.0013	4 3 2	3 2 1	7613.4498	0.0036
16 1 16	15 1 15	7294.4190	0.0032	4 2 3	3 1 2	5242.3790	-0.0013	4 3 1	3 2 2	7616.1264	-0.0038
16 0 16	15 0 15	7337.5926	0.0007	4 2 2	3 1 3	5420.6033	0.0009	8 2 6	7 1 7	7730.1781	0.0011
16 2 15	15 2 14	7530.5016	-0.0025	11 1 11	10 0 10	5591.4615	-0.0007	15 4 11	15 3 12	7875.4156	-0.0109
16 7 9	15 7 8	7595.6699	-0.0034	13 0 13	12 1 12	5598.6229	-0.0018	11 2 10	10 1 9	7878.2790	-0.0019
16 7 10	15 7 9	7595.6699	-0.0034	5 2 4	4 1 3	5659.7320	0.0023	17 1 17	16 0 16	7935.7383	-0.0012
16 6 11	15 6 10	7598.6377	0.0026	7 3 4	7 2 5	5671.2153	-0.0064	13 4 9	13 3 10	7937.3728	0.0112
16 6 10	15 6 9	7598.6377	0.0011	6 3 3	6 2 4	5691.3559	-0.0011	12 4 8	12 3 9	7957.6276	-0.0029
16 5 12	15 5 11	7603.4858	-0.0010	5 3 2	5 2 3	5704.2148	-0.0008	11 4 7	11 3 8	7972.5920	-0.0004
16 5 11	15 5 10	7603.5797	0.0066	6 3 4	6 2 5	5727.5550	-0.0065	12 2 10	12 1 11	2870.5228	0.0004
16 3 14	15 3 13	7610.8639	-0.0042	7 3 5	7 2 6	5735.6531	-0.0014	5 2 3	5 1 4	3238.3897	-0.0055
16 4 13	15 4 12	7611.3871	-0.0016	9 3 7	9 2 8	5764.5645	0.0006	3 2 1	3 1 2	3348.5010	0.0035
16 4 12	15 4 11	7614.3008	-0.0051	10 3 8	10 2 9	5787.4031	0.0035	3 2 2	3 1 3	3516.1620	-0.0023
16 3 13	15 3 12	7659.0640	0.0032	11 3 9	11 2 10	5817.2303	-0.0036	4 2 3	4 1 4	3573.5437	-0.0093
16 1 15	15 1 14	7700.2115	0.0013	12 3 10	12 2 11	5855.1395	-0.0019	5 2 4	5 1 5	3645.5746	-0.0029
17 1 17	16 1 16	7743.9476	-0.0007	5 2 3	4 1 4	5961.9671	-0.0024	6 2 5	6 1 6	3732.3974	-0.0003
16 2 14	15 2 13	7777.3883	-0.0009	12 1 12	11 0 11	5968.2730	-0.0009	2 2 1	1 1 0	4364.9756	0.0062
17 0 17	16 0 16	7780.4230	-0.0008	6 2 5	5 1 4	6062.9793	0.0000	13 2 12	13 1 13	4764.0130	0.0082
17 2 16	16 2 15	7993.4123	-0.0084	13 1 13	12 0 12	6349.4758	-0.0021	11 3 8	11 2 9	5482.1930	0.0192
3 1 3	2 0 2	2481.3159	-0.0013	7 2 6	6 1 5	6452.3233	-0.0012	10 3 7	10 2 8	5548.5508	0.0103
4 1 4	3 0 3	2899.8505	-0.0010	6 2 4	5 1 5	6525.3078	-0.0015	9 3 6	9 2 7	5601.4631	0.0001

8 0 8	7 1 7	2953.2779	-0.0032	15 0 15	14 1 14	6609.2548	-0.0029	8 3 5	8 2 6	5641.8632	-0.0001
5 1 5	4 0 4	3306.1392	-0.0022	14 1 14	13 0 13	6736.3322	0.0113				

Table S5. Observed frequencies and residuals (MHz) for the 1NpOH-furan (II) complex for $J'K'_aK'_c \leftarrow J''K''_aK''_c$ transitions.

$J'K'_aK'_c$	$J''K''_aK''_c$	Obs.	Res.	$J'K'_aK'_c$	$J''K''_aK''_c$	Obs.	Res.
5 1 5	4 1 4	2344.9482	-0.0124	11 1 10	10 1 9	5480.3869	0.0009
5 0 5	4 0 4	2415.4155	-0.0026	12 1 12	11 1 11	5591.2016	-0.0012
6 1 6	5 1 5	2811.9415	-0.0087	12 0 12	11 0 11	5653.7079	-0.0067
6 0 6	5 0 5	2890.1145	-0.0052	12 2 11	11 2 10	5799.2910	-0.0020
6 2 4	5 2 3	2940.9512	0.0050	12 4 9	11 4 8	5850.8351	0.0016
6 1 5	5 1 4	3010.0219	0.0073	12 4 8	11 4 7	5851.7577	-0.0063
7 1 7	6 1 6	3277.9462	-0.0030	12 3 10	11 3 9	5853.7835	0.0014
7 0 7	6 0 6	3360.6456	0.0009	12 3 9	11 3 8	5876.4118	0.0075
7 2 6	6 2 5	3397.3693	-0.0008	12 1 11	11 1 10	5966.0098	-0.0008
7 2 5	6 2 4	3440.2502	0.0036	12 2 10	11 2 9	5979.2264	0.0030
7 1 6	6 1 5	3508.3177	0.0052	13 1 13	12 1 12	6050.5480	-0.0036
8 1 8	7 1 7	3742.8637	-0.0085	13 0 13	12 0 12	6104.5118	-0.0011
8 0 8	7 0 7	3826.7771	-0.0029	13 2 12	12 2 11	6275.6699	0.0067
8 3 5	7 3 4	3900.7113	-0.0046	13 3 11	12 3 10	6342.7908	0.0143
8 2 6	7 2 5	3942.9962	-0.0011	13 3 10	12 3 9	6376.1089	0.0004
8 1 7	7 1 6	4004.8882	0.0035	13 1 12	12 1 11	6447.7483	-0.0011
9 1 9	8 1 8	4206.6588	-0.0070	13 2 11	12 2 10	6490.2766	0.0003
9 2 8	8 2 7	4361.7336	-0.0001	14 1 14	13 1 13	6508.9371	0.0046
9 3 7	8 3 6	4386.5036	-0.0005	14 0 14	13 0 13	6554.4529	-0.0018
9 3 6	8 3 5	4391.8872	-0.0027	14 2 13	13 2 12	6750.4842	-0.0002
9 1 8	8 1 7	4499.3640	-0.0013	14 3 12	13 3 11	6831.4462	0.0028
10 1 10	9 1 9	4669.3057	-0.0024	14 3 11	13 3 10	6878.8128	-0.0068
10 0 10	9 0 9	4746.6082	0.0215	14 1 13	13 1 12	6925.1602	-0.0069
10 2 9	9 2 8	4842.2356	0.0049	15 1 15	14 1 14	6966.4427	0.0070
10 3 7	9 3 6	4884.6689	0.0060	15 3 12	14 3 11	7384.7623	-0.0113
10 1 9	9 1 8	4991.3512	0.0037	15 1 14	14 1 13	7397.9177	-0.0003
11 1 11	10 1 10	5130.8037	-0.0046	16 1 16	15 1 15	7423.1662	0.0078
11 0 11	10 0 10	5201.3452	-0.0007	16 0 16	15 0 15	7453.7833	0.0013
11 2 10	10 2 9	5321.4507	-0.0010	15 2 13	14 2 12	7508.2415	-0.0052

11 3 9	10 3 8	5364.6360	-0.0002	16 1 15	15 1 14	7865.8029	-0.0060
11 3 8	10 3 7	5379.3765	-0.0019				
11 2 9	10 2 8	5467.9872	0.0049				

Table S6. Observed frequencies and residuals (MHz) for the 1NpOH-DMF complex for $J'K'_aK'_c \leftarrow J''K''_aK''_c$ transitions using SPFIT.

$J'K'_aK'_c$	$J''K''_aK''_c$	Obs.	Res.	$J'K'_aK'_c$	$J''K''_aK''_c$	Obs.	Res.	$J'K'_aK'_c$	$J''K''_aK''_c$	Obs.	Res.
5 1 5	4 1 4	2037.7081	0.0032	8 6 3	7 6 2	3293.0227	-0.0079	10 5 5	9 5 4	4116.8861	-0.0124
5 0 5	4 0 4	2057.0620	0.0018	8 5 3	7 5 2	3293.3875	0.0008	10 4 7	9 4 6	4117.4839	-0.0014
5 1 4	4 1 3	2078.6965	0.0014	8 5 4	7 5 3	3293.3875	0.0008	10 4 6	9 4 5	4117.4839	-0.0048
4 1 4	3 0 3	2287.2214	0.0051	8 4 5	7 4 4	3293.7697	0.0016	10 3 8	9 3 7	4118.2626	0.0016
6 1 6	5 1 5	2445.0410	-0.0039	8 4 4	7 4 3	3293.7697	0.0009	10 3 7	9 3 6	4118.5928	-0.0005
6 0 6	5 0 5	2467.6582	-0.0001	8 2 6	7 2 5	3298.8017	-0.0130	10 2 8	9 2 7	4127.0276	-0.0022
6 2 5	5 2 4	2469.8417	0.0067	8 1 7	7 1 6	3324.8896	0.0041	10 1 9	9 1 8	4154.8752	0.0017
6 5 1	5 5 0	2469.9770	0.0140	7 1 7	6 0 6	3451.4361	0.0027	9 1 9	8 0 8	4211.9087	0.0020
6 5 2	5 5 1	2469.9770	0.0140	9 1 9	8 1 8	3666.3766	0.0034	11 1 11	10 1 10	4479.8896	0.0022
6 4 2	5 4 1	2470.2020	0.0046	9 0 9	8 0 8	3696.5705	0.0017	11 0 11	10 0 10	4512.8887	0.0029
6 4 3	5 4 2	2470.2020	0.0047	9 2 8	8 2 7	3703.8955	0.0003	11 2 10	10 2 9	4526.0508	-0.0019
6 3 4	5 3 3	2470.4882	0.0165	9 6 3	8 6 2	3704.7030	-0.0019	11 7 4	10 7 3	4527.5254	-0.0064
6 3 3	5 3 2	2470.4882	-0.0070	9 6 4	8 6 3	3704.7030	-0.0019	11 7 5	10 7 4	4527.5254	-0.0064
6 2 4	5 2 3	2472.4184	-0.0039	9 5 4	8 5 3	3705.1289	-0.0013	11 6 5	10 6 4	4528.1043	0.0011
6 1 5	5 1 4	2494.2233	0.0031	9 5 5	8 5 4	3705.1289	-0.0013	11 6 6	10 6 5	4528.1043	0.0011
5 1 5	4 0 4	2678.8337	0.0060	9 4 6	8 4 5	3705.6080	0.0017	11 5 7	10 5 6	4528.6894	-0.0050
7 1 7	6 1 6	2852.2799	0.0007	9 4 5	8 4 4	3705.6080	0.0002	11 5 6	10 5 5	4528.6894	-0.0050
7 0 7	6 0 6	2877.8185	0.0002	9 3 7	8 3 6	3706.2339	0.0021	11 4 8	10 4 7	4529.4120	0.0020
7 2 6	6 2 5	2881.2851	0.0036	9 3 6	8 3 5	3706.4251	-0.0008	11 4 7	10 4 6	4529.4120	-0.0047
7 5 2	6 5 1	2881.6670	0.0017	9 2 7	8 2 6	3712.6759	0.0006	11 3 9	10 3 8	4530.3503	0.0040
7 5 3	6 5 2	2881.6670	0.0017	9 1 8	8 1 7	3739.9800	0.0027	11 3 8	10 3 7	4530.8884	0.0027
7 4 4	6 4 3	2881.9672	0.0005	8 1 8	7 0 7	3833.0139	0.0057	11 2 9	10 2 8	4541.9044	0.0025
7 4 3	6 4 2	2881.9672	0.0003	10 1 10	9 1 9	4073.1998	-0.0081	11 1 10	10 1 9	4569.5526	0.0070
7 3 5	6 3 4	2882.3656	0.0259	10 0 10	9 0 9	4105.0563	0.0047	10 1 10	9 0 9	4588.5471	0.0012
7 3 4	6 3 3	2882.3656	-0.0270	10 2 9	9 2 8	4115.0356	-0.0015	12 1 12	11 1 11	4886.4087	0.0058
7 2 5	6 2 4	2885.4166	0.0042	10 8 2	9 8 1	4115.3636	-0.0053	12 0 12	11 0 11	4920.0537	0.0039
7 1 6	6 1 5	2909.6314	0.0065	10 8 3	9 8 2	4115.3636	-0.0053	12 2 11	11 2 10	4936.9218	-0.0076
6 1 6	5 0 5	3066.8157	0.0032	10 7 3	9 7 2	4115.8939	-0.0019	12 9 3	11 9 2	4937.8082	-0.0028

8 1 8	7 1 7	3259.3935	0.0005	10 7 4	9 7 3	4115.8939	-0.0019	12 9 4	11 9 3	4937.8082	-0.0028
8 0 8	7 0 7	3287.4770	0.0023	10 6 4	9 6 3	4116.3942	-0.0009	12 8 4	11 8 3	4938.5196	0.0034
8 2 7	7 2 6	3292.6415	0.0025	10 6 5	9 6 4	4116.3942	-0.0009	12 8 5	11 8 4	4938.5196	0.0034
8 6 2	7 6 1	3293.0227	-0.0079	10 5 6	9 5 5	4116.8861	-0.0124	12 7 5	11 7 4	4939.1850	0.0039

Table S6. Continued.

$J'K'_aK'_c$	$J''K''_aK''_c$	Obs.	Res.	$J'K'_aK'_c$	$J''K''_aK''_c$	Obs.	Res.	$J'K'_aK'_c$	$J''K''_aK''_c$	Obs.	Res.
12 7 6	11 7 5	4939.1850	0.0039	14 1 14	13 1 13	5698.9255	0.0069	15 5 10	14 5 9	6176.2097	0.0000
12 6 6	11 6 5	4939.8328	0.0019	13 1 13	12 0 12	5709.5884	-0.0088	15 4 12	14 4 11	6177.6714	0.0278
12 6 7	11 6 6	4939.8328	0.0019	14 0 14	13 0 13	5732.3714	0.0026	15 4 11	14 4 10	6177.6714	-0.0355
12 5 8	11 5 7	4940.5219	0.0013	14 2 13	13 2 12	5758.2073	-0.0103	15 3 13	14 3 12	6179.1667	-0.0214
12 5 7	11 5 6	4940.5219	0.0012	14 9 5	13 9 4	5760.8504	0.0003	15 3 12	14 3 11	6181.7155	-0.0400
12 4 9	11 4 8	4941.3880	0.0038	14 9 6	13 9 5	5760.8504	0.0003	15 2 13	14 2 12	6206.4637	0.0069
12 4 8	11 4 7	4941.3880	-0.0090	14 8 6	13 8 5	5761.7096	0.0060	15 1 14	14 1 13	6225.3424	0.0027
12 3 10	11 3 9	4942.4887	0.0028	14 8 7	13 8 6	5761.7096	0.0060	15 1 15	14 0 14	6454.5010	-0.0178
12 3 9	11 3 8	4943.3233	-0.0004	14 7 7	13 7 6	5762.5281	0.0039	16 1 16	15 1 15	6510.7385	0.0140
12 2 10	11 2 9	4957.3000	0.0001	14 7 8	13 7 7	5762.5281	0.0039	16 0 16	15 0 15	6542.2000	0.0008
11 1 11	10 0 10	4963.3823	0.0007	14 6 8	13 6 7	5763.3575	0.0052	16 2 15	15 2 14	6578.7912	-0.0165
12 1 11	11 1 10	4983.9656	0.0029	14 6 9	13 6 8	5763.3575	0.0052	16 9 7	15 9 6	6583.9211	-0.0007
13 1 13	12 1 12	5292.7498	0.0015	14 5 10	13 5 9	5764.2754	0.0003	16 9 8	15 9 7	6583.9211	-0.0007
13 0 13	12 0 12	5326.5442	0.0050	14 5 9	13 5 8	5764.2754	-0.0001	16 8 8	15 8 7	6584.9336	-0.0041
12 1 12	11 0 11	5336.8940	-0.0047	14 4 11	13 4 10	5765.5108	0.0134	16 8 9	15 8 8	6584.9336	-0.0041
13 2 12	12 2 11	5347.6469	-0.0081	14 4 10	13 4 9	5765.5108	-0.0253	16 7 9	15 7 8	6585.9242	-0.0107
13 9 4	12 9 3	5349.3137	-0.0130	14 3 12	13 3 11	5766.9357	0.0225	16 7 10	15 7 9	6585.9242	-0.0107
13 9 5	12 9 4	5349.3137	-0.0130	14 3 11	13 3 10	5768.7054	-0.0264	16 6 10	15 6 9	6586.9632	-0.0104
13 8 5	12 8 4	5350.0983	-0.0061	14 2 12	13 2 11	5789.6192	0.0033	16 6 11	15 6 10	6586.9632	-0.0104
13 8 6	12 8 5	5350.0983	-0.0061	14 1 13	13 1 12	5811.8978	0.0012	16 5 12	15 5 11	6588.1759	-0.0081
13 7 6	12 7 5	5350.8408	-0.0040	15 1 15	14 1 14	6104.9219	0.0109	16 5 11	15 5 10	6588.1759	-0.0096
13 7 7	12 7 6	5350.8408	-0.0040	15 0 15	14 0 14	6137.5787	0.0069	16 3 14	15 3 13	6591.5077	0.0149
13 6 7	12 6 6	5351.5773	-0.0026	15 2 14	14 2 13	6168.5889	-0.0167	16 3 13	15 3 12	6595.0072	-0.0248
13 6 8	12 6 7	5351.5773	-0.0026	15 9 6	14 9 5	6172.3840	0.0024	16 2 14	15 2 13	6623.6706	-0.0005
13 5 9	12 5 8	5352.3833	0.0034	15 9 7	14 9 6	6172.3840	0.0024	16 1 15	15 1 14	6638.3756	-0.0050
13 5 8	12 5 7	5352.3833	0.0032	15 8 7	14 8 6	6173.3169	0.0025	17 1 17	16 1 16	6916.3746	0.0147
13 4 10	12 4 9	5353.4260	0.0140	15 8 8	14 8 7	6173.3169	0.0025	17 0 17	16 0 16	6946.3195	0.0041
13 4 9	12 4 8	5353.4260	-0.0088	15 7 8	14 7 7	6174.2212	0.0007	17 2 16	16 2 15	6988.7985	-0.0143

13 3 11	12 3 10	5354.6848	0.0081	15 7 9	14 7 8	6174.2212	0.0007	17 5 13	16 5 12	7000.2053	0.0017
13 3 10	12 3 9	5355.9422	0.0116	15 6 9	14 6 8	6175.1531	0.0035	17 5 12	16 5 11	7000.2053	-0.0008
13 2 11	12 2 10	5373.2173	0.0030	15 6 10	14 6 9	6175.1531	0.0035	17 4 14	16 4 13	7002.1682	0.0372
13 1 12	12 1 11	5398.0959	0.0044	15 5 11	14 5 10	6176.2097	0.0008	17 4 13	16 4 12	7002.2950	0.0100

Table S6. Continued.

$J'K'_aK'_c$	$J''K''_aK''_c$	Obs.	Res.	$J'K'_aK'_c$	$J''K''_aK''_c$	Obs.	Res.
17 3 15	16 3 14	7003.8367	0.0203	19 4 16	18 4 15	7826.8972	0.0035
17 3 14	16 3 13	7008.5731	-0.0205	19 4 15	18 4 14	7827.2426	0.0113
17 2 15	16 2 14	7041.1820	0.0033	19 3 17	18 3 16	7828.4753	0.0056
17 1 16	16 1 15	7050.9858	0.0092	19 3 16	18 3 15	7836.6891	-0.0206
18 1 18	17 1 17	7321.8480	0.0287	19 1 18	18 1 17	7874.6534	-0.0020
18 0 18	17 0 17	7350.0036	0.0090	19 2 17	18 2 16	7876.7076	0.0032
18 2 17	17 2 16	7398.5827	-0.0281				
18 6 13	17 6 12	7410.7103	0.0007				
18 6 12	17 6 11	7410.7103	0.0006				
18 5 14	17 5 13	7412.2720	0.0019				
18 5 13	17 5 12	7412.2720	-0.0023				
18 4 15	17 4 14	7414.4750	-0.0020				
18 4 14	17 4 13	7414.7075	-0.0002				
18 3 16	17 3 15	7416.1472	0.0006				
18 3 15	17 3 14	7422.4597	-0.0148				
18 2 16	17 2 15	7458.8998	0.0113				
18 1 17	17 1 16	7463.0848	0.0015				
19 1 19	18 1 18	7727.1251	0.0186				
19 0 19	18 0 18	7753.3033	-0.0119				
19 2 18	18 2 17	7808.1613	-0.0304				
19 10 9	18 10 8	7817.2793	0.0040				
19 10 10	18 10 9	7817.2793	0.0040				
19 9 10	18 9 9	7818.6099	0.0088				
19 9 11	18 9 10	7818.6099	0.0088				
19 8 11	18 8 10	7819.9001	0.0082				
19 8 12	18 8 11	7819.9001	0.0082				
19 7 12	18 7 11	7821.2070	0.0075				
19 7 13	18 7 12	7821.2070	0.0075				

19 6 14	18 6 13	7822.6286	0.0034
19 6 13	18 6 12	7822.6286	0.0033
19 5 15	18 5 14	7824.3848	-0.0013
19 5 14	18 5 13	7824.3848	-0.0084

Table S7. Observed frequencies and residuals (MHz) for the 1NpOH-DMF complex for $J'K'_aK'_c \leftarrow J''K''_aK''_c$ transitions using XIAM.

The angles δ and ε were fixed to those calculated at the B3LYP-D3/def2-TZVPP level of theory, because they could not be determined.

$J'K'_aK'_c$	$J''K''_aK''_c$	State	Obs.	Res.	$J'K'_aK'_c$	$J''K''_aK''_c$	State	Obs.	Res.
5 1 5	4 1 4	AA	2037.7081	0.0036	8 4 4	7 4 3	AA	3293.7697	0.0002
5 0 5	4 0 4	AA	2057.0620	0.0009	8 2 6	7 2 5	AA	3298.8017	-0.0151
5 1 4	4 1 3	AA	2078.6965	-0.0006	8 1 7	7 1 6	AA	3324.8896	0.0014
4 1 4	3 0 3	AA	2287.2214	-0.0024	7 1 7	6 0 6	AA	3451.4361	-0.0010
6 1 6	5 1 5	AA	2445.0410	-0.0037	9 1 9	8 1 8	AA	3666.3766	0.0032
6 0 6	5 0 5	AA	2467.6582	-0.0014	9 0 9	8 0 8	AA	3696.5705	-0.0008
6 2 5	5 2 4	AA	2469.8417	0.0066	9 2 8	8 2 7	AA	3703.8955	0.0016
6 5 1	5 5 0	AA	2469.9770	0.0136	9 6 3	8 6 2	AA	3704.7030	-0.0022
6 5 2	5 5 1	AA	2469.9770	0.0136	9 6 4	8 6 3	AA	3704.7030	-0.0022
6 4 2	5 4 1	AA	2470.2020	0.0040	9 5 4	8 5 3	AA	3705.1289	-0.0020
6 4 3	5 4 2	AA	2470.2020	0.0041	9 5 5	8 5 4	AA	3705.1289	-0.0020
6 2 4	5 2 3	AA	2472.4184	-0.0053	9 4 6	8 4 5	AA	3705.6080	0.0010
6 1 5	5 1 4	AA	2494.2233	0.0008	9 4 5	8 4 4	AA	3705.6080	-0.0006
5 1 5	4 0 4	AA	2678.8337	-0.0005	9 3 7	8 3 6	AA	3706.2340	0.0013
7 1 7	6 1 6	AA	2852.2799	0.0009	9 3 6	8 3 5	AA	3706.4251	-0.0017
7 0 7	6 0 6	AA	2877.8185	-0.0014	9 2 7	8 2 6	AA	3712.6759	-0.0019
7 2 6	6 2 5	AA	2881.2851	0.0038	9 1 8	8 1 7	AA	3739.9800	0.0000
7 5 2	6 5 1	AA	2881.6670	0.0013	8 1 8	7 0 7	AA	3833.0139	0.0037
7 5 3	6 5 2	AA	2881.6670	0.0013	10 1 10	9 1 9	AA	4073.1998	-0.0087
7 4 4	6 4 3	AA	2881.9672	-0.0001	10 0 10	9 0 9	AA	4105.0563	0.0017
7 4 3	6 4 2	AA	2881.9672	-0.0004	10 2 9	9 2 8	AA	4115.0357	0.0004
7 2 5	6 2 4	AA	2885.4166	0.0026	10 8 2	9 8 1	AA	4115.3636	-0.0045
7 1 6	6 1 5	AA	2909.6314	0.0040	10 8 3	9 8 2	AA	4115.3636	-0.0045
6 1 6	5 0 5	AA	3066.8157	-0.0020	10 7 3	9 7 2	AA	4115.8939	-0.0018
8 1 8	7 1 7	AA	3259.3935	0.0006	10 7 4	9 7 3	AA	4115.8939	-0.0018
8 0 8	7 0 7	AA	3287.4770	0.0004	10 6 4	9 6 3	AA	4116.3942	-0.0012

8 2 7	7 2 6	AA	3292.6415	0.0031
8 6 2	7 6 1	AA	3293.0227	-0.0081
8 6 3	7 6 2	AA	3293.0227	-0.0081
8 5 3	7 5 2	AA	3293.3875	0.0003
8 5 4	7 5 3	AA	3293.3875	0.0003
8 4 5	7 4 4	AA	3293.7697	0.0009

10 6 5	9 6 4	AA	4116.3942	-0.0012
10 5 6	9 5 5	AA	4116.8861	-0.0131
10 5 5	9 5 4	AA	4116.8861	-0.0131
10 4 7	9 4 6	AA	4117.4839	-0.0022
10 4 6	9 4 5	AA	4117.4839	-0.0057
10 2 8	9 2 7	AA	4127.0276	-0.0052

Table S7. Continued.

$J' K'_a K'_c$	$J'' K''_a K''_c$	State	Obs.	Res.
10 1 9	9 1 8	AA	4154.8752	-0.0011
9 1 9	8 0 8	AA	4211.9087	0.0018
11 1 11	10 1 10	AA	4479.8896	0.0012
11 0 11	10 0 10	AA	4512.8887	-0.0009
11 2 10	10 2 9	AA	4526.0508	0.0010
11 7 4	10 7 3	AA	4527.5254	-0.0064
11 7 5	10 7 4	AA	4527.5254	-0.0064
11 6 5	10 6 4	AA	4528.1043	0.0007
11 6 6	10 6 5	AA	4528.1043	0.0007
11 5 7	10 5 6	AA	4528.6894	-0.0057
11 5 6	10 5 5	AA	4528.6894	-0.0057
11 4 8	10 4 7	AA	4529.4120	0.0013
11 4 7	10 4 6	AA	4529.4120	-0.0056
11 2 9	10 2 8	AA	4541.9044	-0.0011
11 1 10	10 1 9	AA	4569.5527	0.0043
10 1 10	9 0 9	AA	4588.5471	0.0029
12 1 12	11 1 11	AA	4886.4087	0.0041
12 0 12	11 0 11	AA	4920.0537	-0.0007
12 2 11	11 2 10	AA	4936.9218	-0.0035
12 9 3	11 9 2	AA	4937.8082	-0.0012
12 9 4	11 9 3	AA	4937.8082	-0.0012
12 8 4	11 8 3	AA	4938.5196	0.0041
12 8 5	11 8 4	AA	4938.5196	0.0041
12 7 5	11 7 4	AA	4939.1850	0.0039
12 7 6	11 7 5	AA	4939.1850	0.0039
12 6 6	11 6 5	AA	4939.8328	0.0014
12 6 7	11 6 6	AA	4939.8328	0.0014

$J' K'_a K'_c$	$J'' K''_a K''_c$	State	Obs.	Res.
11 1 11	10 0 10	AA	4963.3823	0.0044
12 1 11	11 1 10	AA	4983.9656	0.0003
13 1 13	12 1 12	AA	5292.7498	-0.0009
13 0 13	12 0 12	AA	5326.5442	-0.0007
12 1 12	11 0 11	AA	5336.8940	0.0010
13 2 12	12 2 11	AA	5347.6469	-0.0026
13 9 4	12 9 3	AA	5349.3137	-0.0117
13 9 5	12 9 4	AA	5349.3137	-0.0117
13 8 5	12 8 4	AA	5350.0983	-0.0057
13 8 6	12 8 5	AA	5350.0983	-0.0057
13 7 6	12 7 5	AA	5350.8408	-0.0042
13 7 7	12 7 6	AA	5350.8408	-0.0042
13 6 7	12 6 6	AA	5351.5773	-0.0032
13 6 8	12 6 7	AA	5351.5773	-0.0032
13 5 9	12 5 8	AA	5352.3833	0.0028
13 5 8	12 5 7	AA	5352.3833	0.0026
13 4 10	12 4 9	AA	5353.4260	0.0133
13 4 9	12 4 8	AA	5353.4260	-0.0095
13 2 11	12 2 10	AA	5373.2173	-0.0019
13 1 12	12 1 11	AA	5398.0959	0.0018
14 1 14	13 1 13	AA	5698.9255	0.0035
13 1 13	12 0 12	AA	5709.5884	-0.0008
14 0 14	13 0 13	AA	5732.3714	-0.0043
14 2 13	13 2 12	AA	5758.2073	-0.0032
14 9 5	13 9 4	AA	5760.8504	0.0014
14 9 6	13 9 5	AA	5760.8504	0.0014
14 8 6	13 8 5	AA	5761.7096	0.0062

12 5 8	11 5 7	AA	4940.5219	0.0007
12 5 7	11 5 6	AA	4940.5219	0.0006
12 4 9	11 4 8	AA	4941.3880	0.0031
12 4 8	11 4 7	AA	4941.3880	-0.0097
12 2 10	11 2 9	AA	4957.3000	-0.0041

14 8 7	13 8 6	AA	5761.7096	0.0062
14 7 7	13 7 6	AA	5762.5281	0.0035
14 7 8	13 7 7	AA	5762.5281	0.0035
14 6 8	13 6 7	AA	5763.3575	0.0046
14 6 9	13 6 8	AA	5763.3575	0.0046

Table S7. Continued.

$J'K'_aK'_c$	$J''K''_aK''_c$	State	Obs.	Res.
14 5 10	13 5 9	AA	5764.2754	-0.0004
14 5 9	13 5 8	AA	5764.2754	-0.0008
14 4 11	13 4 10	AA	5765.5108	0.0129
14 4 10	13 4 9	AA	5765.5108	-0.0258
14 2 12	13 2 11	AA	5789.6192	-0.0024
14 1 13	13 1 12	AA	5811.8978	-0.0011
15 1 15	14 1 14	AA	6104.9219	0.0063
15 0 15	14 0 14	AA	6137.5787	-0.0015
15 2 14	14 2 13	AA	6168.5889	-0.0076
15 9 6	14 9 5	AA	6172.3840	0.0029
15 9 7	14 9 6	AA	6172.3840	0.0029
15 8 7	14 8 6	AA	6173.3169	0.0023
15 8 8	14 8 7	AA	6173.3169	0.0023
15 7 8	14 7 7	AA	6174.2212	0.0001
15 7 9	14 7 8	AA	6174.2212	0.0001
15 6 9	14 6 8	AA	6175.1531	0.0029
15 6 10	14 6 9	AA	6175.1531	0.0029
15 5 11	14 5 10	AA	6176.2097	0.0002
15 5 10	14 5 9	AA	6176.2097	-0.0006
15 4 12	14 4 11	AA	6177.6714	0.0274
15 4 11	14 4 10	AA	6177.6714	-0.0358
15 2 13	14 2 12	AA	6206.4637	0.0002
15 1 14	14 1 13	AA	6225.3424	0.0005
15 1 15	14 0 14	AA	6454.5010	-0.0051
16 1 16	15 1 15	AA	6510.7385	0.0079
16 0 16	15 0 15	AA	6542.2000	-0.0091
16 2 15	15 2 14	AA	6578.7912	-0.0053

$J'K'_aK'_c$	$J''K''_aK''_c$	State	Obs.	Res.
16 7 10	15 7 9	AA	6585.9242	-0.0116
16 6 10	15 6 9	AA	6586.9632	-0.0112
16 6 11	15 6 10	AA	6586.9632	-0.0112
16 5 12	15 5 11	AA	6588.1759	-0.0088
16 5 11	15 5 10	AA	6588.1759	-0.0102
16 2 14	15 2 13	AA	6623.6706	-0.0084
16 1 15	15 1 14	AA	6638.3756	-0.0070
17 1 17	16 1 16	AA	6916.3746	0.0070
17 0 17	16 0 16	AA	6946.3195	-0.0076
17 2 16	16 2 15	AA	6988.7985	-0.0007
17 5 13	16 5 12	AA	7000.2053	0.0012
17 5 12	16 5 11	AA	7000.2053	-0.0014
17 4 14	16 4 13	AA	7002.1682	0.0372
17 4 13	16 4 12	AA	7002.2950	0.0103
17 2 15	16 2 14	AA	7041.1820	-0.0059
17 1 16	16 1 15	AA	7050.9858	0.0074
18 1 18	17 1 17	AA	7321.8480	0.0189
18 0 18	17 0 17	AA	7350.0036	-0.0046
18 2 17	17 2 16	AA	7398.5827	-0.0117
18 6 13	17 6 12	AA	7410.7103	-0.0003
18 6 12	17 6 11	AA	7410.7103	-0.0004
18 5 14	17 5 13	AA	7412.2720	0.0016
18 5 13	17 5 12	AA	7412.2720	-0.0027
18 4 15	17 4 14	AA	7414.4750	-0.0018
18 4 14	17 4 13	AA	7414.7075	0.0005
18 2 16	17 2 15	AA	7458.8998	0.0006
18 1 17	17 1 16	AA	7463.0848	-0.0001

16 9 7	15 9 6	AA	6583.9211	-0.0008
16 9 8	15 9 7	AA	6583.9211	-0.0008
16 8 8	15 8 7	AA	6584.9336	-0.0048
16 8 9	15 8 8	AA	6584.9336	-0.0048
16 7 9	15 7 8	AA	6585.9242	-0.0116

19 1 19	18 1 18	AA	7727.1251	0.0063
19 0 19	18 0 18	AA	7753.3033	-0.0278
19 2 18	18 2 17	AA	7808.1613	-0.0111
19 10 9	18 10 8	AA	7817.2793	0.0018
19 10 10	18 10 9	AA	7817.2793	0.0018

Table S7. Continued.

$J'K'_aK'_c$	$J''K''_aK''_c$	State	Obs.	Res.
19 9 10	18 9 9	AA	7818.6099	0.0063
19 9 11	18 9 10	AA	7818.6099	0.0063
19 8 11	18 8 10	AA	7819.9001	0.0059
19 8 12	18 8 11	AA	7819.9001	0.0059
19 7 12	18 7 11	AA	7821.2070	0.0057
19 7 13	18 7 12	AA	7821.2070	0.0057
19 6 14	18 6 13	AA	7822.6286	0.0023
19 6 13	18 6 12	AA	7822.6286	0.0022
19 5 15	18 5 14	AA	7824.3848	-0.0016
19 5 14	18 5 13	AA	7824.3848	-0.0086
19 4 16	18 4 15	AA	7826.8972	0.0042
19 4 15	18 4 14	AA	7827.2426	0.0127
19 3 17	18 3 16	AA	7828.4753	0.0085
19 3 16	18 3 15	AA	7836.6891	-0.0170
19 1 18	18 1 17	AA	7874.6534	-0.0035
19 2 17	18 2 16	AA	7876.7076	-0.0094
9 3 7	8 3 6	AA	3706.2332	0.0005
9 3 7	8 3 6	EA	3706.2332	0.0073
9 K 3	8 K 3	EE+	3706.3185	0.0134
9 K 3	8 K 3	EE-	3706.3185	0.0134
9 K 3	8 K 3	AE	3706.3185	0.0061
9 3 6	8 3 5	AA	3706.4246	-0.0022
9 3 6	8 3 5	EA	3706.4246	0.0046
9 K -3	8 K -3	EE+	3706.3185	-0.0289
9 K -3	8 K -3	EE-	3706.3185	-0.0289
9 K -3	8 K -3	AE	3706.3185	-0.0150
11 3 9	10 3 8	AA	4530.3497	0.0028

$J'K'_aK'_c$	$J''K''_aK''_c$	State	Obs.	Res.
11 3 8	10 3 7	EA	4530.8881	0.0098
11 K -3	10 K -3	EE+	4530.7747	-0.0004
11 K -3	10 K -3	EE-	4530.7747	-0.0004
11 K -3	10 K -3	AE	4530.6947	-0.0095
12 3 10	11 3 9	AA	4942.4883	0.0018
12 3 10	11 3 9	EA	4942.4883	0.0108
12 K 3	11 K 3	EE+	4942.5717	0.0002
12 K 3	11 K 3	EE-	4942.5717	0.0002
12 K 3	11 K 3	AE	4942.6738	0.0036
12 3 9	11 3 8	AA	4943.3227	-0.0016
12 3 9	11 3 8	EA	4943.3227	0.0072
12 K -3	11 K -3	EE+	4943.2292	-0.0012
12 K -3	11 K -3	EE-	4943.2292	-0.0012
12 K -3	11 K -3	AE	4943.1221	-0.0007
13 3 11	12 3 10	AA	5354.6838	0.0068
13 3 11	12 3 10	EA	5354.6838	0.0165
13 K 3	12 K 3	EE+	5354.7388	0.0038
13 K 3	12 K 3	EE-	5354.7388	0.0038
13 3 10	12 3 9	AA	5355.9420	0.0111
13 3 10	12 3 9	EA	5355.9420	0.0206
13 K -3	12 K -3	EE+	5355.8680	0.0047
13 K -3	12 K -3	EE-	5355.8680	0.0047
13 K -3	12 K -3	AE	5355.7452	-0.0009
6 3 4	5 3 3	AA	2470.4882	0.0158
6 3 3	5 3 2	AA	2470.4882	-0.0077
10 3 8	9 3 7	AA	4118.2622	0.0004
10 3 8	9 3 7	EA	4118.2622	0.0079

11 3 9	10 3 8	EA	4530.3497	0.0111	10 K 3	9 K 3	EE+	4118.3527	-0.0066
11 K 3	10 K 3	EE+	4530.4488	-0.0013	10 K 3	9 K 3	EE-	4118.3527	-0.0066
11 K 3	10 K 3	EE-	4530.4488	-0.0013	10 3 7	9 3 6	AA	4118.5929	-0.0013
11 K 3	10 K 3	AE	4530.5011	-0.0117	10 3 7	9 3 6	EA	4118.5929	0.0062
11 3 8	10 3 7	AA	4530.8881	0.0017	10 K -3	9 K -3	EE+	4118.4853	-0.0039

Table S7. Continued.

$J'K_a'K_c'$	$J''K_a''K_c''$	State	Obs.	Res.
10 K -3	9 K -3	EE-	4118.4853	-0.0039
14 3 12	13 3 11	AA	5766.9355	0.0223
14 3 12	13 3 11	EA	5766.9355	0.0327
14 K 3	13 K 3	EE+	5766.9355	-0.0132
14 K 3	13 K 3	EE-	5766.9355	-0.0132
14 K 3	13 K 3	AE	5767.0377	-0.0007
14 3 11	13 3 10	AA	5768.7054	-0.0265
14 3 11	13 3 10	EA	5768.7054	-0.0164
14 K -3	13 K -3	EE+	5768.7054	0.0193
14 K -3	13 K -3	EE-	5768.7054	0.0193
14 K -3	13 K -3	AE	5768.5804	-0.0059
15 3 13	14 3 12	AA	6179.1670	-0.0208
15 3 13	14 3 12	EA	6179.1670	-0.0097
15 K 3	14 K 3	EE+	6179.2255	0.0173
15 K 3	14 K 3	EE-	6179.2255	0.0173
15 3 12	14 3 11	AA	6181.7711	0.0160
15 3 12	14 3 11	EA	6181.7711	0.0266
15 K -3	14 K -3	EE+	6181.7155	-0.0084
15 K -3	14 K -3	EE-	6181.7155	-0.0084
15 K -3	14 K -3	AE	6181.6445	-0.0052

Table S8. Observed frequencies and residuals (MHz) for the 1NpOH- thiophene complex for $J'K'_aK'_c \leftarrow J''K''_aK''_c$ transitions.

$J'K'_aK'_c$	$J''K''_aK''_c$	Obs.	Res.	$J'K'_aK'_c$	$J''K''_aK''_c$	Obs.	Res.	$J'K'_aK'_c$	$J''K''_aK''_c$	Obs.	Res.
5 0 5	4 0 4	2088.2667	0.0000	10 1 9	9 1 8	4285.4078	0.0012	14 3 12	13 3 11	5882.9116	0.0095
5 2 4	4 2 3	2095.0485	0.0000	11 1 11	10 1 10	4471.1560	0.0033	14 1 13	13 1 12	5971.1889	0.0000
5 2 3	4 2 2	2102.6955	0.0018	11 0 11	10 0 10	4534.2504	0.0001	14 2 12	13 2 11	5980.2717	0.0086
5 1 4	4 1 3	2149.5245	0.0019	11 2 10	10 2 9	4597.8277	-0.0017	15 1 15	14 1 14	6080.0440	0.0003
6 1 6	5 1 5	2445.7241	-0.0011	11 5 7	10 5 6	4615.0665	-0.0013	15 0 15	14 0 14	6123.7939	0.0007
6 1 5	5 1 4	2578.3028	0.0007	11 5 6	10 5 5	4615.0665	-0.0028	15 2 14	14 2 13	6253.4368	-0.0080
7 1 7	6 1 6	2852.0097	0.0013	11 4 8	10 4 7	4617.1921	0.0036	15 4 12	14 4 11	6302.3106	0.0022
7 2 6	6 2 5	2931.2622	-0.0046	11 4 7	10 4 6	4617.3110	-0.0056	15 4 11	14 4 10	6303.4851	0.0018
7 2 5	6 2 4	2952.3947	-0.0029	11 3 9	10 3 8	4619.7033	0.0048	15 3 13	14 3 12	6303.9046	0.0003
7 1 6	6 1 5	3006.4279	-0.0012	11 3 8	10 3 7	4624.9703	-0.0048	15 1 14	14 1 13	6387.7103	0.0038
8 1 8	7 1 7	3257.7297	0.0004	11 2 9	10 2 8	4674.4047	0.0032	15 2 13	14 2 12	6416.0345	-0.0187
8 0 8	7 0 7	3322.1080	-0.0056	11 1 10	10 1 9	4709.3504	-0.0041	16 1 16	15 1 15	6480.7780	-0.0011
8 2 7	7 2 6	3348.7358	0.0010	12 1 12	11 1 11	4874.3259	0.0012	16 0 16	15 0 15	6518.8283	-0.0008
8 3 6	7 3 5	3357.4967	-0.0042	12 0 12	11 0 11	4933.8220	0.0009	16 2 15	15 2 14	6665.2641	-0.0017
8 3 5	7 3 4	3358.5478	0.0012	12 2 11	11 2 10	5012.8911	-0.0032	16 4 13	15 4 12	6724.2991	-0.0001
8 2 6	7 2 5	3380.0524	0.0007	12 4 9	11 4 8	5038.0502	-0.0014	16 3 14	15 3 13	6724.7399	0.0011
8 1 7	7 1 6	3433.7634	0.0010	12 4 8	11 4 7	5038.2992	0.0076	16 4 12	15 4 11	6726.1485	-0.0013
9 1 9	8 1 8	3662.8468	0.0022	12 3 10	11 3 9	5040.7246	-0.0017	16 3 13	15 3 12	6757.7968	-0.0050
9 0 9	8 0 8	3728.6016	0.0016	12 3 9	11 3 8	5048.8746	-0.0032	16 1 15	15 1 14	6801.7899	-0.0180
9 2 8	8 2 7	3765.6898	-0.0018	12 2 10	11 2 9	5108.9501	0.0036	16 2 14	15 2 13	6851.3113	0.0038
9 5 4	8 5 3	3775.0223	-0.0033	12 1 11	11 1 10	5131.7828	-0.0003	17 1 17	16 1 16	6880.9918	-0.0028
9 5 5	8 5 4	3775.0223	-0.0031	13 1 13	12 1 12	5276.8510	0.0018	17 0 17	16 0 16	6913.5924	0.0024
9 4 6	8 4 5	3776.2480	0.0310	13 0 13	12 0 12	5331.6676	0.0002	17 2 16	16 2 15	7076.1991	0.0185
9 4 5	8 4 4	3776.2480	0.0014	13 2 12	12 2 11	5427.2143	-0.0031	17 3 14	16 3 13	7189.1875	0.0014
9 3 7	8 3 6	3778.0463	-0.0009	13 3 10	12 3 9	5473.9318	-0.0021	17 1 16	16 1 15	7213.3151	0.0057
9 3 6	8 3 5	3779.9589	0.0002	13 2 11	12 2 10	5544.4011	0.0046	18 1 18	17 1 17	7280.7291	-0.0070
9 2 7	8 2 6	3809.6765	-0.0005	13 1 12	12 1 11	5552.4695	-0.0017	17 2 15	16 2 14	7285.6326	0.0106
9 1 8	8 1 7	3860.1438	-0.0020	14 1 14	13 1 13	5678.7480	0.0021	18 0 18	17 0 17	7308.2993	0.0079
10 1 10	9 1 9	4067.3234	-0.0013	14 0 14	13 0 13	5728.1901	-0.0014	18 2 17	17 2 16	7486.1608	-0.0042
10 0 10	9 0 9	4132.5971	-0.0011	14 2 13	13 2 12	5840.7399	-0.0091	18 3 16	17 3 15	7565.5391	-0.0033
10 2 9	9 2 8	4182.0755	-0.0006	14 4 11	13 4 10	5880.6075	0.0035	18 4 15	17 4 14	7569.0896	-0.0113

10 2 8	9 2 7	4241.1995	0.0013	14 4 10	13 4 9	5881.3250	0.0001	18 4 14	17 4 13	7573.3210	0.0076
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Table S8. Continued.

$J' K'_a K'_c$	$J'' K''_a K''_c$	Obs.	Res.
18 1 17	17 1 16	7622.0850	0.0046
18 3 15	17 3 14	7622.4423	-0.0104
19 1 19	18 1 18	7680.0540	0.0030
19 0 19	18 0 18	7703.0815	0.0020
18 2 16	17 2 15	7718.6655	0.0102
19 2 18	18 2 17	7895.1949	-0.0089