Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Effect of Aromatic Ring Fluorination on CH···π Interactions: Rotational Spectrum and Structure of the Fluorobenzene···Acetylene Weakly Bound Dimer

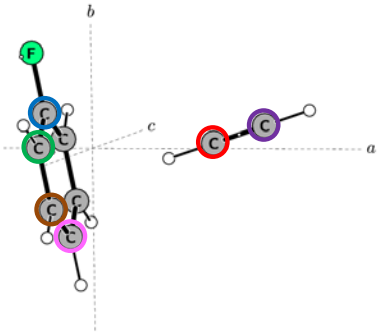
Supporting Information

Table of contents:

Table S1 Principal axis coordinates (Å) for the ab initio (MP2/6-311++G(2d,2p)) optimized structure of fluorobenzene···acetylene (FBZ···HCCH). Atoms for Structure I are color coded and follow the same numbering scheme as in Figure 1 of the main paper.

Structure I

F1	-1.373770	2.045041	0.000000
C2	-1.060908	0.729995	0.000000
C3	-0.904780	0.080669	-1.216735
C4	-0.904780	0.080669	1.216735
C5	-0.580785	-1.277375	-1.208461
C6	-0.580785	-1.277375	1.208461
C7	-0.418057	-1.958161	0.000000
H8	-1.031166	0.631247	-2.136711
H9	-1.031166	0.631247	2.136711
H10	-0.452376	-1.797879	-2.146369
H11	-0.452376	-1.797879	2.146369
H12	-0.164505	-3.007931	0.000000
C15	3.754205	0.570304	0.000000
H16	4.762842	0.898804	0.000000
C17	2.600296	0.197686	0.000000
H18	1.590083	-0.131273	0.000000



Structure II

C1	-4.271737	-0.836573	0.000000
H2	-4.941879	-1.658911	0.000000
C3	-3.511653	0.107994	0.000000
H4	-2.835263	0.927133	0.000000
C5	0.425736	0.675456	0.000000
C6	0.088649	-0.669964	0.000000
C7	1.738423	1.121606	0.000000
C8	1.123375	-1.606985	0.000000
H9	-0.949381	-0.966874	0.000000
C10	2.760092	0.170510	0.000000
H11	1.944432	2.181323	0.000000
C12	2.456188	-1.191897	0.000000
H13	0.882645	-2.660197	0.000000
H14	3.789637	0.497903	0.000000
H15	3.250744	-1.923416	0.000000
F16	-0.571561	1.599580	0.000000

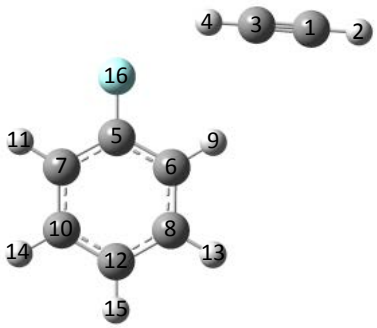


Table S2 Parent isotopic rotational transition frequencies (MHz) for the fluorobenzene···acetylene complex. $\Delta\nu$ is the difference between the observed frequencies (ν_{obs}) and the frequencies calculated (ν_{calc}) using the spectroscopic parameters in Table 2 of the main paper.

Parent species			
JK_aK_c'	JK_aK_c''	ν_{obs}	$\Delta\nu$
2 2 0	1 1 1	6532.6831	0.0013
5 2 3	4 3 2	6588.2239	-0.0010
8 5 3	8 4 4	7014.1337	0.0076
7 5 2	7 4 3	7152.1744	0.0003
8 5 4	8 4 5	7176.0831	0.0038
7 5 3	7 4 4	7210.5095	-0.0002
6 2 5	5 3 2	7217.5152	0.0045
4 0 4	3 1 3	7218.8502	-0.0001
6 5 1	6 4 2	7229.0778	0.0011
6 5 2	6 4 3	7245.8355	-0.0031
5 5 0	5 4 1	7270.4381	0.0021
5 5 1	5 4 2	7273.9098	0.0028
3 3 0	3 0 3	7544.5121	0.0000
4 1 4	3 0 3	7807.8144	-0.0010
4 3 1	4 0 4	7935.2373	-0.0037
3 2 2	2 1 1	8072.3037	-0.0004
7 3 5	6 4 2	8237.6647	0.0065
7 2 6	6 3 3	8625.1357	0.0016
5 1 4	4 2 3	8629.0904	0.0018
8 6 2	8 5 3	8818.2807	-0.0043
8 6 3	8 5 4	8827.2419	0.0042
3 2 1	2 1 2	8842.3297	0.0012
7 6 1	7 5 2	8865.3798	0.0001
7 6 2	7 5 3	8867.5231	0.0034
6 6 0	6 5 1	8895.4951	-0.0023
6 6 1	6 5 2	8895.8688	0.0055
7 3 4	6 4 3	8936.9738	0.0024
6 2 4	5 3 3	9037.0389	0.0000
5 0 5	4 1 4	9136.3099	-0.0021
5 1 5	4 0 4	9469.1026	-0.0019
8 2 7	7 3 4	9716.8252	0.0038
4 2 3	3 1 2	9744.0313	0.0003
3 3 1	2 2 0	9988.3694	0.0010
3 3 0	2 2 1	10028.5204	0.0023

JK_aK_c'	JK_aK_c''	ν_{obs}	$\Delta\nu$
8 3 6	7 4 3	10088.7861	-0.0037
8 7 1	8 6 2	10492.2042	-0.0015
8 7 2	8 6 3	10492.4403	-0.0044
6 1 5	5 2 4	10886.4381	-0.0008
6 0 6	5 1 5	10993.9282	-0.0012
6 1 6	5 0 5	11165.3018	-0.0024
5 2 4	4 1 3	11325.1975	-0.0001
4 2 2	3 1 3	11412.3972	0.0007
8 3 5	7 4 4	11430.1382	0.0039
7 2 5	6 3 4	11544.1634	0.0005
4 3 2	3 2 1	11886.0554	0.0006
4 3 1	3 2 2	12087.3453	0.0006
7 0 7	6 1 6	12812.0147	-0.0029
6 2 5	5 1 4	12844.3966	0.0005
7 1 7	6 0 6	12894.6626	-0.0022
7 1 6	6 2 5	13053.6120	0.0006
3 3 1	2 0 2	13325.6602	0.0053
4 4 1	3 3 0	13613.0258	0.0001
4 4 0	3 3 1	13617.5686	0.0010
5 3 3	4 2 2	13668.3021	0.0005
5 3 2	4 2 3	14255.9746	0.0006
5 2 3	4 1 4	14277.2050	0.0021
7 2 6	6 1 5	14347.7105	0.0012
8 0 8	7 1 7	14607.5923	-0.0046
8 1 8	7 0 7	14645.6755	-0.0013
8 1 7	7 2 6	15106.4501	-0.0064
6 3 4	5 2 3	15313.0336	0.0004
4 3 2	3 0 3	15496.7923	-0.0009
5 4 2	4 3 1	15579.8488	-0.0053
5 4 1	4 3 2	15611.8259	-0.0016
8 2 7	7 1 6	15885.3685	0.0004
9 0 9	8 1 8	16391.4513	0.0085
6 3 3	5 2 4	16609.0110	-0.0030
7 3 5	6 2 4	16829.8839	-0.0043
5 5 1	4 4 0	17221.0857	-0.0049
5 5 0	4 4 1	17221.5213	0.0022
6 2 4	5 1 5	17429.7815	-0.0005
9 2 8	8 1 7	17487.2496	-0.0040
6 4 3	5 3 2	17502.7012	0.0040
6 4 2	5 3 3	17629.2705	0.0015
5 3 3	4 0 4	17861.8463	-0.0014

Tables S3(a) - (f) Rotational transition frequencies (MHz) for the ^{13}C singly isotopically substituted species of FBZ···HCCH. Atom numbering scheme is the same as Figure 3 of the main paper.

Table S3(a) Isotopic transition frequencies (MHz) for $^{13}C_2$ species

$^{13}C_2$

JK_aK_c'	JK_aK_c''	ν_{obs}	$\Delta\nu$
4 0 4	3 1 3	7199.0160	-0.0010
4 1 4	3 0 3	7786.4770	0.0010
3 2 1	2 1 2	8824.4455	-0.0013
5 0 5	4 1 4	9111.0900	0.0001
5 1 5	4 0 4	9442.8027	-0.0011
4 2 3	3 1 2	9720.6849	0.0010
3 3 1	2 2 0	9968.2176	-0.0021
3 3 0	2 2 1	10008.4350	0.0000
5 2 4	4 1 3	11296.7367	0.0012
4 2 2	3 1 3	11389.8088	0.0010
4 3 2	3 2 1	11860.7285	0.0013
4 3 1	3 2 2	12062.3381	0.0014
7 0 7	6 1 6	12776.1794	-0.0006
7 1 7	6 0 6	12858.4446	0.0008
4 4 1	3 3 0	13585.8651	0.0026
4 4 0	3 3 1	13590.4160	-0.0020
5 3 3	4 2 2	13637.6882	-0.0024
5 3 2	4 2 3	14226.2356	-0.0004
5 4 2	4 3 1	15547.6028	0.0000

Table S3(b) Isotopic transition frequencies (MHz) for $^{13}C_{3,4}$ species

$^{13}C_{3,4}$			
JK_aK_c'	JK_aK_c''	ν_{obs}	$\Delta\nu$
4 0 4	3 1 3	7200.3714	-0.0001
4 1 4	3 0 3	7792.5947	0.0000
3 2 2	2 1 1	8040.0821	-0.0027
5 1 4	4 2 3	8594.3924	-0.0037
3 2 1	2 1 2	8792.4991	0.0027
5 0 5	4 1 4	9115.1296	0.0006
5 1 5	4 0 4	9452.0117	0.0016
4 2 3	3 1 2	9711.3800	0.0007
3 3 1	2 2 0	9938.2302	-0.0011
3 3 0	2 2 1	9977.0180	-0.0005
6 1 5	5 2 4	10844.0539	0.0017
6 0 6	5 1 5	10970.7423	-0.0008
6 1 6	5 0 5	11145.4524	0.0006
5 2 4	4 1 3	11293.6796	-0.0030
4 3 2	3 2 1	11831.7686	-0.0011
4 3 1	3 2 2	12026.3045	-0.0002
7 0 7	6 1 6	12786.9084	0.0020
6 2 5	5 1 4	12814.4085	0.0009
7 1 7	6 0 6	12871.7608	0.0015
4 4 1	3 3 0	13543.3605	0.0035
4 4 0	3 3 1	13547.6868	-0.0014
5 3 2	4 2 3	14181.4893	0.0017
7 2 6	6 1 5	14318.0068	0.0006
8 1 8	7 0 7	14619.7800	-0.0029
5 4 1	4 3 2	15534.4939	-0.0017

Table S3(c) Isotopic transition frequencies (MHz) for $^{13}C_{5,6}$ species

$^{13}C_{5,6}$			
JK_aK_c'	JK_aK_c''	ν_{obs}	$\Delta\nu$
4 0 4	3 1 3	7199.7779	0.0035
4 1 4	3 0 3	7769.3074	-0.0005
3 2 2	2 1 1	8005.1427	-0.0014
5 1 4	4 2 3	8628.3654	-0.0065
3 2 1	2 1 2	8773.0049	0.0009
5 0 5	4 1 4	9107.3590	0.0027
5 1 5	4 0 4	9426.8533	0.0006
4 2 3	3 1 2	9671.2762	-0.0003
3 3 1	2 2 0	9888.0669	-0.0012
3 3 0	2 2 1	9928.5925	-0.0003
6 1 5	5 2 4	10871.8040	0.0022
6 0 6	5 1 5	10955.9979	-0.0028
6 1 6	5 0 5	11119.2807	0.0002
5 2 4	4 1 3	11247.6548	0.0000
4 2 2	3 1 3	11335.3097	0.0024
4 3 2	3 2 1	11777.9322	0.0014
4 3 1	3 2 2	11981.0145	-0.0024
6 2 5	5 1 4	12763.3723	0.0028
7 1 6	6 2 5	13023.6144	0.0008
4 4 1	3 3 0	13474.2642	0.0000
4 4 0	3 3 1	13478.9115	-0.0006
5 3 3	4 2 2	13552.1232	-0.0012
5 3 2	4 2 3	14144.4750	0.0000
7 2 6	6 1 5	14264.9950	-0.0011
6 3 4	5 2 3	15189.4161	-0.0014
5 4 2	4 3 1	15433.5573	0.0019
5 4 1	4 3 2	15466.2692	0.0001

Table S3(d) Isotopic transition frequencies (MHz) for $^{13}C_7$ species

$^{13}C_7$

JK_aK_c'	JK_aK_c''	ν_{obs}	$\Delta\nu$
4 0 4	3 1 3	7196.5727	0.0006
3 2 2	2 1 1	7982.1539	0.0063
3 2 1	2 1 2	8782.9817	0.0001
5 1 5	4 0 4	9392.1533	-0.0029
4 2 3	3 1 2	9638.4597	0.0010
3 3 1	2 2 0	9864.4736	-0.0016
3 3 0	2 2 1	9908.2449	-0.0012
6 0 6	5 1 5	10932.3664	-0.0011
6 1 6	5 0 5	11081.3627	0.0016
5 2 4	4 1 3	11202.8773	-0.0017
4 3 1	3 2 2	11968.3602	-0.0016
6 2 5	5 1 4	12707.5450	-0.0002
7 0 7	6 1 6	12733.1746	0.0016
7 1 7	6 0 6	12802.9066	-0.0008
4 4 1	3 3 0	13442.9771	0.0018
4 4 0	3 3 1	13448.1975	-0.0021
5 3 3	4 2 2	13511.9073	-0.0004
5 3 2	4 2 3	14149.0084	0.0000
5 4 2	4 3 1	15401.6657	0.0039
5 4 1	4 3 2	15438.4048	-0.0022

Table S3(e) Isotopic transition frequencies (MHz) for the $^{13}C_{15}$ species

$^{13}C_{15}$

JK_aK_c'	JK_aK_c''	ν_{obs}	$\Delta\nu$
4 0 4	3 1 3	6989.6589	-0.0020
4 1 4	3 0 3	7651.2336	0.0031
3 2 2	2 1 1	7999.2953	0.0043
3 2 1	2 1 2	8716.2351	-0.0016
5 0 5	4 1 4	8872.1064	0.0030
4 2 3	3 1 2	9631.0767	0.0022
3 3 1	2 2 0	9954.4320	-0.0004
3 3 0	2 2 1	9989.0731	-0.0030
6 1 6	5 0 5	10905.3672	-0.0076
5 2 4	4 1 3	11175.4844	-0.0018
4 3 2	3 2 1	11805.6919	-0.0007
4 3 1	3 2 2	11979.7921	0.0023
6 2 5	5 1 4	12655.9539	-0.0004
7 0 7	6 1 6	12475.5980	0.0032
7 1 6	6 2 5	12589.7056	-0.0007
4 4 1	3 3 0	13573.5708	0.0011
4 4 0	3 3 1	13577.1649	-0.0002
5 3 3	4 2 2	13552.9987	-0.0031
5 3 2	4 2 3	14064.1724	0.0012
7 2 6	6 1 5	14111.6381	0.0018

Table S3(f) Isotopic transition frequencies (MHz) for $^{13}C_{17}$ species

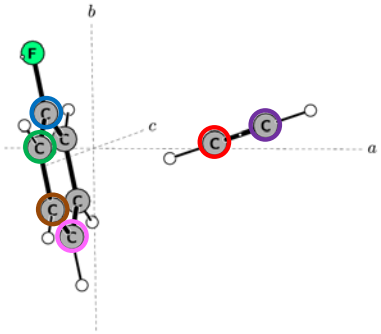
$^{13}C_{17}$

JK_aK_c'	JK_aK_c''	ν_{obs}	$\Delta\nu$
4 0 4	3 1 3	7105.9665	-0.0012
4 1 4	3 0 3	7731.3314	-0.0070
3 2 2	2 1 1	8037.5220	-0.0045
3 2 1	2 1 2	8780.1970	0.0050
5 0 5	4 1 4	9006.5434	0.0070
5 1 5	4 0 4	9367.8939	-0.0021
4 2 3	3 1 2	9689.7849	-0.0002
3 3 1	2 2 0	9973.3873	0.0008
3 3 0	2 2 1	10010.6475	0.0002
6 0 6	5 1 5	10847.2304	0.0033
6 1 6	5 0 5	11037.7666	0.0035
4 2 2	3 1 3	11297.6640	-0.0057
4 3 2	3 2 1	11848.4037	0.0002
4 3 1	3 2 2	12035.4476	0.0005
7 0 7	6 1 6	12647.0305	-0.0073
7 1 7	6 0 6	12741.1328	0.0025
4 4 1	3 3 0	13595.9456	0.0005
4 4 0	3 3 1	13599.9815	0.0012
5 3 3	4 2 2	13613.8756	0.0029
5 3 2	4 2 3	14161.5757	0.0032
5 4 2	4 3 1	15536.1135	-0.0043

Table S4 Principal axis coordinates (Å) resulting from the inertial fits in which combinations of the moments of inertia for all 7 isotopologues are fitted; structural parameters for the dimer derived from these coordinates are listed in Table 4 of the main paper. Color codes in coordinates below refer to picture to right; atom numbering is given in Figure 3 of the main paper. X13 and X14 are centers of mass of the fluorobenzene and acetylene molecules, respectively.

Fitting I_a, I_b, I_c

	a	*b*	*c*	mass (u)
F1	-1.397371	-2.048065	0.000030	18.9984032
C2	**-1.082226**	**-0.725698**	**0.000006**	**12.0000000**
C3	**-0.928414**	**-0.080307**	**1.217346**	**12.0000000**
C4	-0.928429	-0.080347	-1.217357	12.0000000
C5	**-0.606665**	**1.269770**	**1.211266**	**12.0000000**
C6	-0.606680	1.269730	-1.211326	12.0000000
C7	**-0.444097**	**1.951925**	**0.000020**	**12.0000000**
H8	-1.061416	-0.638402	2.136247	1.0078250
H9	-1.061443	-0.638472	-2.136238	1.0078250
H10	-0.480888	1.797528	2.146028	1.0078250
H11	-0.480915	1.797457	-2.146107	1.0078250
H12	-0.193400	3.003865	0.000096	1.0078250
X13	-0.885173	0.101145	0.000007	0.0000001
X14	3.267636	-0.373412	-0.000002	0.0000001
C15	**3.844903**	**-0.549409**	**-0.000003**	**12.0000000**
H16	4.856914	-0.857950	-0.000006	1.0078250
C17	**2.690368**	**-0.197415**	**0.000000**	**12.0000000**
H18	1.678357	0.111126	0.000002	1.0078250



Fitting I_a, I_b

	a	*b*	*c*	mass (u)
F1	-1.428081	-2.031602	0.000030	18.9984032
C2	**-1.092102**	**-0.714375**	**0.000006**	**12.0000000**
C3	**-0.928121**	**-0.071492**	**1.217346**	**12.0000000**
C4	-0.928137	-0.071531	-1.217357	12.0000000
C5	**-0.585101**	**1.273338**	**1.211266**	**12.0000000**
C6	-0.585118	1.273299	-1.211325	12.0000000
C7	**-0.411786**	**1.952843**	**0.000020**	**12.0000000**
H8	-1.069917	-0.627418	2.136247	1.0078250
H9	-1.069945	-0.627488	-2.136238	1.0078250
H10	-0.451010	1.799045	2.146028	1.0078250
H11	-0.451038	1.798975	-2.146107	1.0078250
H12	-0.144516	3.000694	0.000096	1.0078250
X13	-0.882022	0.109255	0.000007	0.0000001
X14	3.256001	-0.403350	-0.000002	0.0000001
C15	**3.837887**	**-0.563416**	**-0.000003**	**12.0000000**
H16	4.857996	-0.844028	-0.000006	1.0078250
C17	**2.674116**	**-0.243284**	**0.000000**	**12.0000000**
H18	1.654007	0.037328	0.000002	1.0078250

Fitting I_a, I_c

	a	b	c	mass (u)
F1	-1.430826	-2.032485	0.000030	18.9984032
C2	**-1.095234**	**-0.715160**	**0.000006**	**12.0000000**
C3	**-0.931443**	**-0.072228**	**1.217346**	**12.0000000**
C4	-0.931459	-0.072268	-1.217357	12.0000000
C5	**-0.588818**	**1.272702**	**1.211266**	**12.0000000**
C6	-0.588834	1.272663	-1.211325	12.0000000
C7	**-0.415703**	**1.952258**	**0.000020**	**12.0000000**
H8	-1.073075	-0.628196	2.136247	1.0078250
H9	-1.073103	-0.628266	-2.136238	1.0078250
H10	-0.454881	1.798448	2.146028	1.0078250
H11	-0.454909	1.798378	-2.146107	1.0078250
H12	-0.148740	3.000187	0.000096	1.0078250
X13	-0.885397	0.108532	0.000007	0.0000001
X14	3.268459	-0.400681	-0.000002	0.0000001
C15	**3.849399**	**-0.564147**	**-0.000003**	**12.0000000**
H16	4.867849	-0.850720	-0.000006	1.0078250
C17	**2.687519**	**-0.237214**	**0.000000**	**12.0000000**
H18	1.669070	0.049359	0.000002	1.0078250

Fitting I_b, I_c

	a	b	c	mass (u)
F1	-1.321658	-2.082653	0.000030	18.9984032
C2	**-1.054876**	**-0.749688**	**0.000006**	**12.0000000**
C3	**-0.924668**	**-0.099123**	**1.217346**	**12.0000000**
C4	-0.924682	-0.099163	-1.217357	12.0000000
C5	**-0.652296**	**1.261775**	**1.211266**	**12.0000000**
C6	-0.652310	1.261735	-1.211326	12.0000000
C7	**-0.514677**	**1.949398**	**0.000020**	**12.0000000**
H8	-1.037259	-0.661691	2.136247	1.0078250
H9	-1.037284	-0.661763	-2.136238	1.0078250
H10	-0.545821	1.793763	2.146028	1.0078250
H11	-0.545845	1.793691	-2.146107	1.0078250
H12	-0.302452	3.009769	0.000095	1.0078250
X13	-0.888064	0.083783	0.000007	0.0000001
X14	3.278307	-0.309320	-0.000002	0.0000001
C15	**3.850648**	**-0.500730**	**-0.000003**	**12.0000000**
H16	4.854024	-0.836292	-0.000006	1.0078250
C17	**2.705966**	**-0.117911**	**0.000000**	**12.0000000**
H18	1.702591	0.217651	0.000003	1.0078250

Table S5 Output of the dipole moment determination for fluorobenzene···acetylene using the QSTARK program.

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|   QSTARK - Fully diagonalizing fit of Stark shifts in a rotor               |
|            with zero or one quadrupolar nuclei                              |
|_____________________________________________________________________________|
 version 10.X.2007                                              Zbigniew KISIEL
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FBZ-acetylene dipole moment fit
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Calculation for J and F exceeding the value in data by at least 2
The fit will be made to TRANSITION FREQUENCIES

   25 Lines read in
   20 Lines fitted    --->    0 field free and   20 at non-zero field
    2 Constants fitted
   50 energy levels
    6 distinct voltages

TRANSITIONS (F and MF in units of 1/2):
   J K  K  <- J K  K     F MF<- F MF     Field        Obs         Obs-Calc       Calc            Field    Field**2
     -1 +1      -1 +1                   (V/cm)       (MHz)       (MHz)          (MHz)           (V/cm)  ((V/cm)**2)

 1.   2  2  1   1  1  0    4  0   2  0      0.0     6297.59980      0.00173--    6297.5981       0.0000       0.00
 2.   2  2  1   1  1  0    4  0   2  0     69.7     6297.69610     -0.00593      6297.7020      69.6950    4857.39
 3.   2  2  1   1  1  0    4  0   2  0    102.2     6297.81420     -0.00728      6297.8215     102.1680   10438.30
 4.   2  2  0   1  1  1    4  0   2  0      0.0     6532.68600      0.00416--    6532.6818       0.0000       0.00
 5.   2  2  0   1  1  1    4  0   2  0     37.1     6532.63680      0.00689      6532.6299      37.1200    1377.89
 6.   2  2  0   1  1  1    4  0   2  0     69.7     6532.50760      0.00882      6532.4988      69.6950    4857.39
 7.   2  2  0   1  1  1    4  2   2  2     37.1     6532.72510     -0.00376      6532.7289      37.1200    1377.89
 8.   2  2  0   1  1  1    4  2   2  2     69.7     6532.84210     -0.00547      6532.8476      69.6950    4857.39
 9.   2  2  0   1  1  1    4  2   2  2    102.2     6533.04410      0.00615      6533.0379     102.1680   10438.30
10.   4  1  4   3  0  3    8  2   6  2      0.0     7807.81470     -0.00029--    7807.8150       0.0000       0.00
11.   4  1  4   3  0  3    8  2   6  2    102.2     7807.93330      0.00836      7807.9249     102.1680   10438.30
12.   4  1  4   3  0  3    8  2   6  2    115.1     7807.95970      0.00505      7807.9546     115.1480   13259.06
13.   3  2  2   2  1  1    6  0   4  0      0.0     8072.30460      0.00045--    8072.3042       0.0000       0.00
14.   3  2  2   2  1  1    6  0   4  0     69.7     8072.35120      0.00171      8072.3495      69.6950    4857.39
15.   3  2  2   2  1  1    6  0   4  0    102.2     8072.40220      0.00062      8072.4016     102.1680   10438.30
16.   3  2  2   2  1  1    6  0   4  0    134.6     8072.47690      0.00362      8072.4733     134.6140   18120.93
17.   3  2  2   2  1  1    6  2   4  2     69.7     8072.22210      0.00104      8072.2211      69.6950    4857.39
18.   3  2  2   2  1  1    6  2   4  2    102.2     8072.12120     -0.00444      8072.1256     102.1680   10438.30
19.   3  2  2   2  1  1    6  2   4  2    134.6     8071.99460      0.00025      8071.9943     134.6140   18120.93
20.   3  3  1   2  2  0    6  0   4  0      0.0     9988.36990      0.00143--    9988.3685       0.0000       0.00
21.   3  3  1   2  2  0    6  0   4  0     69.7     9988.34960     -0.00831      9988.3579      69.6950    4857.39
22.   3  3  1   2  2  0    6  0   4  0    102.2     9988.34040     -0.00539      9988.3458     102.1680   10438.30
23.   3  3  1   2  2  0    6  2   4  2     69.7     9988.30260      0.00157      9988.3010      69.6950    4857.39
24.   3  3  1   2  2  0    6  2   4  2    102.2     9988.22780      0.00387      9988.2239     102.1680   10438.30
25.   3  3  1   2  2  0    6  2   4  2    134.6     9988.11620     -0.00224      9988.1184     134.6140   18120.93
   Standard deviation =       0.005521

   ITERATION NO =10 CONSTANTS, deviations and changes:
       Mu.a     =         0.033485437 +-      0.000916931          0.000000000
       Mu.b     =         1.501606822 +-      0.006353066          0.000000000

   FINAL RESULTS OF LEAST SQUARES FITTING PROCEDURE
   ================================================
   FITTED CONSTANTS:
   A     /MHz        1803.408791999999948 1:Xab /MHz           0.
   B     /MHz        1086.626393000000007 1:XJ.a/kHz           0.
   C     /MHz         887.513133000000038 1:XK.a/kHz           0.
   DJ    /kHz           2.863779999999999 1:XJbc/kHz           0.
   DJK   /kHz           7.752399999999999 1:Ma  /MHz           0.
   DK    /kHz          -6.989200000000000 1:Mb-c/MHz           0.
   dJ    /kHz           0.86134           1:Tr  /MHz           0.
   dK    /kHz           6.236499999999999 1:Xd  /kHz           0.
   HJ    / Hz           0.
   HJK   / Hz           0.
   HKJ   / Hz           0.
   HK    / Hz           0.
   hJ    / Hz           0.
   hJK   / Hz           0.                Mu.a  /D              0.03348(91)
   hK    / Hz           0.                Mu.b  /D              1.5016(63)
   LKKJ  /mHz           0.                Mu.c  /D              0.
   1:Xa  /MHz           0.                 d    /cm             1.
   1:Xb-c/MHz           0.                 k    /cm             0.

   CORRELATION COEFFICIENTS:
            Mu.a     Mu.b
   Mu.a     1.0000
   Mu.b    -0.3463   1.0000
```