

Supplementary data

Spectroscopic Fits of Transitions of C₂H₂ --- CuCl and C₂H₄ --- CuCl

The results of the spectroscopic fits (the .log files output by the program) performed in PGOPHER [Ref. 18] are provided below. The original .log files are available from the corresponding author on request. An explanation of the program which was written and is maintained by Colin Western of Bristol University is given at: <http://pgopher.chm.bris.ac.uk/> where it is also freely available for download.

The terms fitted are:

A_0 , B_0 , C_0 , Δ_{JK} , Δ_J , d_J , δ_J , $\chi_{aa}(\text{Cu})$, $\chi_{bb}-\chi_{cc}(\text{Cu})$, $C_{aa}(\text{Cu})$, $C_{bb}(\text{Cu})$ and $C_{cc}(\text{Cu})$, $\chi_{aa}(\text{Cl})$, and $\chi_{bb}-\chi_{cc}(\text{Cl})$

which are represented in these files as:

A, B, C, DJK, DJ, deltaJ, Copper CHlzz, Copper CHlxxmyy, Copper Caa, Copper Cbb, Copper Ccc, Chlorine CHlzz, Chlorine CHlxxmyy.

The units of all quoted parameters are MHz. The $\sigma_{r.m.s}$ listed in the tables of the value is listed by each file as the "predicted new error". Data is presented in the format applied by PGOPHER when the user selects a "Detailed" output log.

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- 4) ¹²C₂H₂ --- ⁶³Cu³⁷Cl
- 5) ¹²C₂D₂ --- ⁶³Cu³⁵Cl
- 6) ¹³C₂H₂ --- ⁶³Cu³⁵Cl
- 7) ¹²C₂H₄ --- ⁶³Cu³⁵Cl
- 8) ¹²C₂H₄ --- ⁶⁵Cu³⁵Cl
- 9) ¹²C₂H₄ --- ⁶³Cu³⁷Cl
- 10) ¹²C₂H₄ --- ⁶⁵Cu³⁷Cl
- 11) ¹³C₂H₄ --- ⁶³Cu³⁵Cl
- 12) ¹³C₂H₄ --- ⁶⁵Cu³⁵Cl

Format of the .log files

First, information is presented about the program options selected when the program was run. This can be interpreted to understand the model Hamiltonian used. Parameters that are floated during the fit are indicated by "Float" written next to the parameter. Values are given for parameters fixed during the fit. The list of measured lines is presented together with predictions of transition frequencies made using the model Hamiltonian. Individual lines are labelled as shown below;

J'S' #	J"S' #"	Observed	Calculated	Obs-Calc	StdDev	.00013	0 : qR1,1(1)2.5,4,1.5,3	v=0 2 1 2 2.5 4 - v=0 1 1 1.5 3 :	1:<LineList>
4 B2 2	3 B1 2	8040.7985	8040.7990	-0.0005	1				

"Observed" = Observed frequency of transition.

"Calculated" = Frequency of transition calculated from the model Hamiltonian.

"obs-calc" = is the difference between the observed and calculated frequencies.

"StDev" = User-selected weighting assigned to the individual line measurement for the purposes of fitting. All measured transitions were equally weighted with a nominal value of "1" during this work. A prediction of the relative intensity of the transition is provided in the column to the right of the weights. Quantum numbers for rotational transitions are indicated at the end of each line in format as follows;

	J	K_1'	K_{+1}'	F_1'	F_2'	←	J	K_1'	K_{+1}'	F_1'	F_2'
v=0	2	1	2	2.5	4	- v=0	1	1	1	1.5	3

where $F_1 = J + I(\text{Cu})$ and $F_2 = F_1 + I(\text{Cl})$

A summary of the fitted values of parameters and the associated uncertainties (given in parentheses) is provided at the end of each line list. The fitted values of parameters are also given in Tables 1-4 of the paper.

Gpopher 8.0.102 08 Dec 2013 16:55 32 bit (Delphi 18.5/18)

Mixture: Cavity 12C2 H2 --- 63Cu 35Cl.pgo

Units MHz
PrintLevel Detail
Precision 4
BasisOrder boDefault
QuantumNumberFormat J
FitCycles 1
FitDetails False
AutoReplot True
AllowComplex False
NoLineList False
ShowEstUnc False
ShowDerivatives False
SVDlimit 5
SVDThresh 1E-15
ScaleChanges 1
Species: C2H2_CuCl
Jmax 30
Concentration 1
AsymmetricMolecule: C2H2_63-35
nNuclei 2
JAdjustSym False
BlockMatrix True
PointGroup C2v
Representation Ir
SReduction False
eeWt 1
eoWt 1
oeWt 1
ooWt 1
C2zAxis a
C2xAxis c
PseudoC2v False
FakeSym False
PhaseAdjust False
Abundance 1
AsymmetricManifold: Ground
Initial True
EigenSearch True
LimitSearch True

AutoQConverge True
UsePopParams False
AsymmetricTop: v=0
Symmetry A1
Kmin all
Kmax all
A 34613.7340489415 Float
B 2103.9851432661 Float
C 1981.20500591417 Float
DJK 0.0312373534767369 Float
DJ 0.000296811524034439 Float
deltaJ 1.61294705662282E-5 Float
AsymmetricTopNucleus: Copper
Spin 1.5
AsNext False
CHlzz 65.3136541638263 Float
CHlxxmyy -65.8480942010567 Float
Caa 0.0308604436387406 Float
Cbb 0.00906828525696892 Float
Ccc 0.00708182308405192 Float
AsymmetricTopNucleus: Chlorine
Spin 1.5
AsNext False
CHlzz -21.7549482425027 Float
CHlxxmyy -6.41012293807684 Float
<N ,K |A|N,K> = K^2
<N ,K-2|B|N,K> = sqrt((N*(N+1)+(-K+1)*(K-2))*(N*(N+1)-K*(K-1)))/4
<N ,K |B|N,K> = (N*(N+1)-K^2)/2
<N ,K+2|B|N,K> = sqrt((N*(N+1)+(-K-1)*(K+2))*(N*(N+1)-K*(K+1)))/4
<N ,K-2|C|N,K> = (-sqrt((N*(N+1)+(-K+1)*(K-2))*(N*(N+1)-K*(K-1)))/4
<N ,K |C|N,K> = (N*(N+1)-K^2)/2
<N ,K+2|C|N,K> = (-sqrt((N*(N+1)+(-K-1)*(K+2))*(N*(N+1)-K*(K+1)))/4
<N ,K |DJK|N,K> = -N*(N+1)*K^2
<N ,K |DJ|N,K> = -N^2*(N+1)^2
<N ,K-2|deltaJ|N,K> = -N*(N+1)*sqrt((N*(N+1)+(-K+1)*(K-2))*(N*(N+1)-K*(K-1)))
<N ,K+2|deltaJ|N,K> = -N*(N+1)*sqrt((N*(N+1)+(-K-1)*(K+2))*(N*(N+1)-K*(K+1)))
TransitionMoments: <Ground|mu|Ground>
CartesianTransitionMoment: <v=0|a|v=0>
Axis a
Strength 1
Symbolic Matrix Elements not available for <v=0|a|v=0>

Residuals before fit for C2H2_63-35 for the Ground manifold

J"S" #"	J"S" #"	Observed	Calculated	Obs-Calc	StdDev	
4 B2 2	3 B1 2	8040.7985	8040.7990	-0.0005 1	.00013	0 : qR1,1(1)2.5,4,1.5,3 : v=0 2 1 2 2.5 4 - v=0 1 1 1 1.5 3 : 1:<LineList>
5 B2 1	4 B1 1	8045.6056	8045.6059	-0.0003 1	.00026	0 : qR1,1(1)3.5,5,2.5,4 : v=0 2 1 2 3.5 5 - v=0 1 1 1 2.5 4 : 2:<LineList>
3 A1 4	2 A2 3	8164.8770	8164.8766	0.0004 1	.00061	0 : qR0,1(1)2.5,3,0.5,2 : v=0 2 0 2 2.5 3 - v=0 1 0 1 0.5 2 : 4:<LineList>
3 A1 2	2 A2 2	8166.7884	8166.7890	-0.0006 1	.00069	0 : qR0,1(1)1.5,3,2.5,2 : v=0 2 0 2 1.5 3 - v=0 1 0 1 2.5 2 : 5:<LineList>
4 A1 1	3 A2 1	8168.3070	8168.3073	-0.0003 1	.00115	0 : qR0,1(1)2.5,4,1.5,3 : v=0 2 0 2 2.5 4 - v=0 1 0 1 1.5 3 : 6:<LineList>
2 A1 3	1 A2 2	8168.9447	8168.9447	-0.0000 1	.00051	0 : qR0,1(1)1.5,2,0.5,1 : v=0 2 0 2 1.5 2 - v=0 1 0 1 0.5 1 : 7:<LineList>
5 A1 1	4 A2 1	8169.1164	8169.1160	0.0004 1	.00165	0 : qR0,1(1)3.5,5,2.5,4 : v=0 2 0 2 3.5 5 - v=0 1 0 1 2.5 4 : 8:<LineList>
4 A1 2	3 A2 2	8169.8800	8169.8803	-0.0003 1	.00101	0 : qR0,1(1)3.5,4,2.5,3 : v=0 2 0 2 3.5 4 - v=0 1 0 1 2.5 3 : 9:<LineList>
3 A1 3	2 A2 1	8187.4527	8187.4530	-0.0003 1	.0003	0 : qR0,1(1)3.5,3,1.5,2 : v=0 2 0 2 3.5 3 - v=0 1 0 1 1.5 2 : 10:<LineList>
4 B1 2	3 B2 2	8284.5062	8284.5074	-0.0012 1	.00013	0 : qR1,0(1)2.5,4,1.5,3 : v=0 2 1 1 2.5 4 - v=0 1 1 0 1.5 3 : 11:<LineList>
5 B1 1	4 B2 1	8289.6228	8289.6226	0.0002 1	.00027	0 : qR1,0(1)3.5,5,2.5,4 : v=0 2 1 1 3.5 5 - v=0 1 1 0 2.5 4 : 12:<LineList>
4 B1 3	3 B2 1	8305.6720	8305.6725	-0.0005 1	.00014	0 : qR1,0(1)3.5,4,2.5,3 : v=0 2 1 1 3.5 4 - v=0 1 1 0 2.5 3 : 13:<LineList>
4 B1 3	3 B2 1	8305.6720	8305.6725	-0.0005 1	.00014	0 : qR1,0(1)3.5,4,2.5,3 : v=0 2 1 1 3.5 4 - v=0 1 1 0 2.5 3 : 14:<LineList>
5 B1 2	4 B2 2	12069.1533	12069.1519	0.0014 1	.00027	0 : qR1,2(2)3.5,5,2.5,4 : v=0 3 1 3 3.5 5 - v=0 2 1 2 2.5 4 : 15:<LineList>
6 B1 1	5 B2 1	12070.2442	12070.2439	0.0003 1	.00038	0 : qR1,2(2)4.5,6,3.5,5 : v=0 3 1 3 4.5 6 - v=0 2 1 2 3.5 5 : 16:<LineList>
4 B1 6	3 B2 5	12072.8801	12072.8797	0.0004 1	.00022	0 : qR1,2(2)4.5,4,3.5,3 : v=0 3 1 3 4.5 4 - v=0 2 1 2 3.5 3 : 17:<LineList>
5 B1 3	4 B2 3	12074.0371	12074.0372	-0.0001 1	.00028	0 : qR1,2(2)4.5,5,3.5,4 : v=0 3 1 3 4.5 5 - v=0 2 1 2 3.5 4 : 19:<LineList>
3 A2 6	2 A1 5	12252.2504	12252.2513	-0.0009 1	.00064	0 : qR0,2(2)2.5,3,0.5,2 : v=0 3 0 3 2.5 3 - v=0 2 0 2 0.5 2 : 20:<LineList>
4 A2 4	3 A1 4	12252.6160	12252.6163	-0.0003 1	.00111	0 : qR0,2(2)4.5,4,2.5,3 : v=0 3 0 3 4.5 4 - v=0 2 0 2 2.5 3 : 21:<LineList>
5 A2 1	4 A1 1	12253.3457	12253.3462	-0.0005 1	.0015	0 : qR0,2(2)3.5,5,2.5,4 : v=0 3 0 3 3.5 5 - v=0 2 0 2 2.5 4 : 22:<LineList>
4 A2 2	3 A1 2	12253.3584	12253.3574	0.0010 1	.00117	0 : qR0,2(2)2.5,4,1.5,3 : v=0 3 0 3 2.5 4 - v=0 2 0 2 1.5 3 : 23:<LineList>
6 A2 1	5 A1 1	12253.6640	12253.6643	-0.0003 1	.00194	0 : qR0,2(2)4.5,6,3.5,5 : v=0 3 0 3 4.5 6 - v=0 2 0 2 3.5 5 : 24:<LineList>
3 A2 4	2 A1 3	12253.7148	12253.7148	-0.0000 1	.00092	0 : qR0,2(2)1.5,3,1.5,2 : v=0 3 0 3 1.5 3 - v=0 2 0 2 1.5 2 : 25:<LineList>
5 A2 2	4 A1 2	12253.9215	12253.9220	-0.0005 1	.00144	0 : qR0,2(2)4.5,5,3.5,4 : v=0 3 0 3 4.5 5 - v=0 2 0 2 3.5 4 : 26:<LineList>
3 A2 5	2 A1 4	12255.6306	12255.6303	0.0003 1	.00074	0 : qR0,2(2)3.5,3,3.5,2 : v=0 3 0 3 3.5 3 - v=0 2 0 2 3.5 2 : 27:<LineList>
2 A2 5	1 A1 3	12256.5943	12256.5930	0.0013 1	.00037	0 : qR0,2(2)2.5,2,2.5,1 : v=0 3 0 3 2.5 2 - v=0 2 0 2 2.5 1 : 28:<LineList>
4 A2 3	3 A1 3	12257.5941	12257.5934	0.0007 1	.00087	0 : qR0,2(2)3.5,4,3.5,3 : v=0 3 0 3 3.5 4 - v=0 2 0 2 3.5 3 : 29:<LineList>
5 B2 2	4 B1 2	12436.3625	12436.3623	0.0002 1	.0003	0 : qR1,1(2)3.5,5,2.5,4 : v=0 3 1 2 3.5 5 - v=0 2 1 1 2.5 4 : 30:<LineList>
4 B2 4	3 B1 3	12436.6908	12436.6910	-0.0002 1	.00024	0 : qR1,1(2)2.5,4,1.5,3 : v=0 3 1 2 2.5 4 - v=0 2 1 1 1.5 3 : 31:<LineList>
6 B2 1	5 B1 1	12437.7227	12437.7236	-0.0009 1	.00038	0 : qR1,1(2)4.5,6,3.5,5 : v=0 3 1 2 4.5 6 - v=0 2 1 1 3.5 5 : 32:<LineList>
3 B2 7	2 B1 5	12437.9883	12437.9891	-0.0008 1	.00019	0 : qR1,1(2)1.5,3,0.5,2 : v=0 3 1 2 1.5 3 - v=0 2 1 1 0.5 2 : 33:<LineList>
4 B2 6	3 B1 5	12440.4420	12440.4407	0.0013 1	.0002	0 : qR1,1(2)3.5,4,2.5,3 : v=0 3 1 2 3.5 4 - v=0 2 1 1 2.5 3 : 34:<LineList>
3 B2 9	2 B1 7	12440.8313	12440.8308	0.0005 1	.00013	0 : qR1,1(2)2.5,3,2.5,2 : v=0 3 1 2 2.5 3 - v=0 2 1 1 2.5 2 : 35:<LineList>
5 B2 3	4 B1 3	12441.7940	12441.7931	0.0009 1	.00027	0 : qR1,1(2)4.5,5,3.5,4 : v=0 3 1 2 4.5 5 - v=0 2 1 1 3.5 4 : 36:<LineList>
4 B2 5	3 B1 4	12443.7614	12443.7608	0.0006 1	.00019	0 : qR1,1(2)4.5,4,3.5,3 : v=0 3 1 2 4.5 4 - v=0 2 1 1 3.5 3 : 37:<LineList>
3 B2 10	2 B1 8	16092.9035	16092.9038	-0.0003 1	.00011	0 : qR1,3(3)4.5,3,3.5,2 : v=0 4 1 4 4.5 3 - v=0 3 1 3 3.5 2 : 38:<LineList>
6 B2 2	5 B1 2	16093.2459	16093.2471	-0.0012 1	.00026	0 : qR1,3(3)4.5,6,3.5,5 : v=0 4 1 4 4.5 6 - v=0 3 1 3 3.5 5 : 39:<LineList>
5 B2 4	4 B1 4	16093.3291	16093.3295	-0.0004 1	.00021	0 : qR1,3(3)3.5,5,2.5,4 : v=0 4 1 4 3.5 5 - v=0 3 1 3 2.5 4 : 40:<LineList>
7 B2 1	6 B1 1	16093.8362	16093.8339	0.0023 1	.00032	0 : qR1,3(3)5.5,7,4.5,6 : v=0 4 1 4 5.5 7 - v=0 3 1 3 4.5 6 : 41:<LineList>
4 B2 8	3 B1 8	16094.1072	16094.1065	0.0007 1	.00017	0 : qR1,3(3)5.5,4,4.5,3 : v=0 4 1 4 5.5 4 - v=0 3 1 3 4.5 3 : 42:<LineList>

4 B2 9	3 B1 7	16094.2159	16094.2171	-0.0012 1	.00018	0 : qR1,3(3)3.5,4,2.5,3 : v=0 4 1 4 3.5 4 - v=0 3 1 3 2.5 3 : 43:<LineList>
3 B2 11	2 B1 9	16094.4447	16094.4448	-0.0001 1	.00011	0 : qR1,3(3)3.5,3,2.5,2 : v=0 4 1 4 3.5 3 - v=0 3 1 3 2.5 2 : 44:<LineList>
5 B2 5	4 B1 5	16094.6350	16094.6344	0.0006 1	.00016	0 : qR1,3(3)4.5,5,3.5,4 : v=0 4 1 4 4.5 5 - v=0 3 1 3 3.5 4 : 45:<LineList>
5 B2 6	4 B1 6	16095.1747	16095.1746	0.0001 1	.00022	0 : qR1,3(3)5.5,5,4.5,4 : v=0 4 1 4 5.5 5 - v=0 3 1 3 4.5 4 : 46:<LineList>
6 B2 3	5 B1 3	16095.4833	16095.4839	-0.0006 1	.00026	0 : qR1,3(3)5.5,6,4.5,5 : v=0 4 1 4 5.5 6 - v=0 3 1 3 4.5 5 : 47:<LineList>
4 A1 6	3 A2 6	16336.0256	16336.0267	-0.0011 1	.00073	0 : qR0,3(3)3.5,4,2.5,3 : v=0 4 0 4 3.5 4 - v=0 3 0 3 2.5 3 : 48:<LineList>
5 A1 2	4 A2 2	16336.5599	16336.5605	-0.0006 1	.00107	0 : qR0,3(3)3.5,5,2.5,4 : v=0 4 0 4 3.5 5 - v=0 3 0 3 2.5 4 : 49:<LineList>
5 A1 4	4 A2 4	16336.6037	16336.6040	-0.0003 1	.00105	0 : qR0,3(3)5.5,5,4.5,4 : v=0 4 0 4 5.5 5 - v=0 3 0 3 4.5 4 : 50:<LineList>
6 A1 1	5 A2 1	16336.7638	16336.7632	0.0006 1	.00129	0 : qR0,3(3)4.5,6,3.5,5 : v=0 4 0 4 4.5 6 - v=0 3 0 3 3.5 5 : 51:<LineList>
7 A1 1	6 A2 1	16336.9244	16336.9244	0.0000 1	.00157	0 : qR0,3(3)5.5,7,4.5,6 : v=0 4 0 4 5.5 7 - v=0 3 0 3 4.5 6 : 52:<LineList>
7 A1 1	6 A2 1	16336.9245	16336.9244	0.0001 1	.00157	0 : qR0,3(3)5.5,7,4.5,6 : v=0 4 0 4 5.5 7 - v=0 3 0 3 4.5 6 : 53:<LineList>
4 A1 5	3 A2 5	16337.9666	16337.9670	-0.0004 1	.00078	0 : qR0,3(3)4.5,4,3.5,3 : v=0 4 0 4 4.5 4 - v=0 3 0 3 3.5 3 : 54:<LineList>
5 A1 3	4 A2 3	16338.7212	16338.7198	0.0014 1	.00089	0 : qR0,3(3)4.5,5,3.5,4 : v=0 4 0 4 4.5 5 - v=0 3 0 3 3.5 4 : 55:<LineList>
6 B1 2	5 B2 2	16583.7787	16583.7795	-0.0008 1	.00026	0 : qR1,2(3)4.5,6,3.5,5 : v=0 4 1 3 4.5 6 - v=0 3 1 2 3.5 5 : 56:<LineList>
7 B1 1	6 B2 1	16584.3966	16584.3977	-0.0011 1	.00031	0 : qR1,2(3)5.5,7,4.5,6 : v=0 4 1 3 5.5 7 - v=0 3 1 2 4.5 6 : 57:<LineList>
4 B1 8	3 B2 7	16584.4174	16584.4153	0.0021 1	.00018	0 : qR1,2(3)2.5,4,1.5,3 : v=0 4 1 3 2.5 4 - v=0 3 1 2 1.5 3 : 58:<LineList>
4 B1 8	3 B2 7	16584.4174	16584.4153	0.0021 1	.00018	0 : qR1,2(3)2.5,4,1.5,3 : v=0 4 1 3 2.5 4 - v=0 3 1 2 1.5 3 : 59:<LineList>
6 B1 3	5 B2 3	16586.0786	16586.0813	-0.0027 1	.00025	0 : qR1,2(3)5.5,6,4.5,5 : v=0 4 1 3 5.5 6 - v=0 3 1 2 4.5 5 : 60:<LineList>
4 B1 2	3 B2 2	8284.5086	8284.5074	0.0012 1	.00013	0 : qR1,0(1)2.5,4,1.5,3 : v=0 2 1 1 2.5 4 - v=0 1 1 0 1.5 3 : 61:<LineList>
3 B2 4	2 B1 2	8044.1462	8044.1457	0.0005 1	6.6e-5	0 : qR1,1(1)1.5,3,2.5,2 : v=0 2 1 2 1.5 3 - v=0 1 1 1 2.5 2 : 62:<LineList>
2 B1 9	1 B2 5	12070.7406	12070.7422	-0.0016 1	4.6e-5	0 : qR1,2(2)2.5,2,1.5,1 : v=0 3 1 3 2.5 2 - v=0 2 1 2 1.5 1 : 63:<LineList>
3 B1 7	2 B2 5	12070.9608	12070.9610	-0.0002 1	8.7e-5	0 : qR1,2(2)2.5,3,1.5,2 : v=0 3 1 3 2.5 3 - v=0 2 1 2 1.5 2 : 64:<LineList>
5 B2 2	5 B1 1	12434.7616	12434.7622	-0.0006 1	2.3e-5	0 : qR1,1(2)3.5,5,3.5,5 : v=0 3 1 2 3.5 5 - v=0 2 1 1 3.5 5 : 65:<LineList>

63 Observations, 13 Parameters
Initial Average Error: 0.00101226071742208
Predicted New Error: 0.00101226043491747
Parameters:

# Old	New	Std Dev	Change/Std Sens	Summary	Name
1 34613.7340489415	34613.7165537651	15.617108	-0.0011 .180203	34614(16)	v=0 A
2 2103.9851432661	2103.98514460921	.00029136	0.0046 2.33e-6	2103.985145(291)	v=0 B
3 1981.20500591417	1981.20500474469	.00024933	-0.0047 2.18e-6	1981.205005(249)	v=0 C
4 .0312373534767369	.0312375275672653	.00013625	0.0013 1.53e-6	0.03124(14)	v=0 DJK
5 .000296811524034439	.000296805701041005	4.9651e-6	-0.0012 4.59e-8	2.9681(497)e-4	v=0 DJ
6 1.61294705662282e-5	1.61485646486935e-5	3.8156e-6	0.0050 5.72e-8	1.61(38)e-5	v=0 deltaJ
7 65.3136541638263	65.3136495710219	.00379727	-0.0012 .000162	65.3136(38)	Copper CHlzz
8 -65.8480942010567	-65.8480445299882	.01794902	0.0028 .000524	-65.848(18)	Copper CHlxxmyy
9 .0308604436387406	.0308591519021819	.0013605	-0.0009 6.8e-5	0.0309(14)	Copper Caa
10 .00906828525696892	.00906594377952444	.00073265	-0.0032 1.11e-5	9.07(73)e-3	Copper Cbb
11 .00708182308405192	.00708351020797891	.00049975	0.0034 1.1e-5	7.08(50)e-3	Copper Ccc
12 -21.7549482425027	-21.7549509726099	.00280498	-0.0010 .000136	-21.7550(28)	Chlorine CHlzz
13 -6.41012293807684	-6.41012176571873	.00872062	0.0001 .000467	-6.4101(87)	Chlorine CHlxxmyy

Correlation Matrix

1	2	3	4	5	6	7	8	9	10	11	12	13
1 1.000												
2 -0.436	1.000											
3 0.041	-0.721	1.000										
4 -0.949	0.457	-0.046	1.000									
5 0.832	-0.257	0.240	-0.805	1.000								
6 -0.181	0.851	-0.873	0.222	-0.174	1.000							
7 0.027	-0.379	0.095	-0.012	-0.175	-0.190	1.000						
8 -0.306	0.564	-0.478	0.317	-0.313	0.398	-0.119	1.000					
9 0.213	-0.313	0.352	-0.233	0.289	-0.349	-0.161	-0.284	1.000				
10 0.293	-0.720	0.553	-0.258	0.238	-0.451	0.377	-0.753	0.268	1.000			
11 -0.291	0.596	-0.601	0.266	-0.341	0.436	-0.075	0.732	-0.232	-0.852	1.000		
12 0.017	-0.222	0.073	-0.049	-0.094	-0.156	0.229	-0.387	-0.090	0.147	-0.105	1.000	
13 0.035	0.005	-0.054	-0.054	0.020	0.048	0.006	-0.327	-0.101	0.097	-0.072	0.211	1.000

Gpogher 8.0.102 08 Dec 2013 16:55 32 bit (Delphi 18.5/18)

Mixture: Cavity 12C2H2 --- 65Cu 35Cl.pgo

Units MHz
PrintLevel Detail
Precision 4
BasisOrder boDefault
QuantumNumberFormat J
FitCycles 1
FitDetails False
AutoReplot True
AllowComplex False
NoLineList False
ShowEstUnc False
ShowDerivatives False
SVDlimit 5
SVDThresh 1E-15
ScaleChanges 1
Species: C2H2_CuCl
Jmax 30
Concentration 1
AsymmetricMolecule: C2H2_65-35
nNuclei 2
Jmax 30
JAdjustSym False
BlockMatrix True
PointGroup C2v
Representation Ir
SReduction False
eeWt 1
eoWt 1

oeWt 1
ooWt 1
C2zAxis a
C2xAxis c
PseudoC2v False
FakeSym False
PhaseAdjust False
Abundance 1
AsymmetricManifold: Ground
Jmin 0
Jmax 30
Initial True
EigenSearch True
LimitSearch True
AutoQConverge True
UsePopParams False
AsymmetricTop: v=0
Symmetry A1
Kmin all
Kmax all
A 34540.907584005 Float
B 2103.43216000134 Float
C 1980.71468032904 Float
DJK 0.03173 Float
DJ 0.0002557 Float
deltaJ 1.61E-5
AsymmetricTopNucleus: Cu
Spin 1.5
AsNext False
CHlzz 60.38 Float
CHlxxmyy -60.96 Float

Caa 0.0309
Cbb 0.00907
Ccc 0.00708
AsymmetricTopNucleus: Cl
Spin 1.5
AsNext False
CHlzz -21.75 Float
CHlxxmyy -6.16 Float
 $\langle N, K | A | N, K \rangle = K^2$
 $\langle N, K-2 | B | N, K \rangle = \sqrt{(N*(N+1)+(-K+1)*(K-2))}*(N*(N+1)-K*(K-1))/4$
 $\langle N, K | B | N, K \rangle = (N*(N+1)-K^2)/2$
 $\langle N, K+2 | B | N, K \rangle = \sqrt{(N*(N+1)+(-K-1)*(K+2))}*(N*(N+1)-K*(K+1))/4$
 $\langle N, K-2 | C | N, K \rangle = (-\sqrt{(N*(N+1)+(-K+1)*(K-2))}*(N*(N+1)-K*(K-1)))/4$
 $\langle N, K | C | N, K \rangle = (N*(N+1)-K^2)/2$
 $\langle N, K+2 | C | N, K \rangle = (-\sqrt{(N*(N+1)+(-K-1)*(K+2))}*(N*(N+1)-K*(K+1)))/4$
 $\langle N, K | DJK | N, K \rangle = -N*(N+1)*K^2$
 $\langle N, K | DJ | N, K \rangle = -N^2*(N+1)^2$
 $\langle N, K-2 | \text{delta}J | N, K \rangle = -N*(N+1)*\sqrt{(N*(N+1)+(-K+1)*(K-2))}*(N*(N+1)-K*(K-1))$
 $\langle N, K+2 | \text{delta}J | N, K \rangle = -N*(N+1)*\sqrt{(N*(N+1)+(-K-1)*(K+2))}*(N*(N+1)-K*(K+1))$
TransitionMoments: <Ground| mu |Ground>
CartesianTransitionMoment: <v=0| a |v=0>
Axis a
Strength 1
Symbolic Matrix Elements not available for <v=0| a |v=0>

Residuals before fit for C2H2_65-35 for the Ground manifold

J'S' #'	J'S' #'	Observed	Calculated	Obs-Calc	StdDev	
5 B2 1	4 B1 1	8043.8243	8043.8248	-0.0005 1	4.4e-5	0 : qR1,1(1)3.5,5,2.5,4 : C2H2_65-35 v=0 2 1 2 3.5 5 - v=0 1 1 1 2.5 4 : 1:<LineList>
5 B1 2	4 B2 2	12066.2063	12066.2077	-0.0014 1	.00027	0 : qR1,2(2)3.5,5,2.5,4 : C2H2_65-35 v=0 3 1 3 3.5 5 - v=0 2 1 2 2.5 4 : 2:<LineList>
6 B1 1	5 B2 1	12067.3104	12067.3100	0.0004 1	.00039	0 : qR1,2(2)4.5,6,3.5,5 : C2H2_65-35 v=0 3 1 3 4.5 6 - v=0 2 1 2 3.5 5 : 3:<LineList>
4 A2 4	3 A1 4	12249.5915	12249.5908	0.0007 1	.0011	0 : qR0,2(2)4.5,4,2.5,3 : C2H2_65-35 v=0 3 0 3 4.5 4 - v=0 2 0 2 2.5 3 : 4:<LineList>
5 A2 1	4 A1 1	12250.2821	12250.2818	0.0003 1	.00149	0 : qR0,2(2)3.5,5,2.5,4 : C2H2_65-35 v=0 3 0 3 3.5 5 - v=0 2 0 2 2.5 4 : 5:<LineList>
4 A2 2	3 A1 2	12250.3132	12250.3146	-0.0014 1	.00116	0 : qR0,2(2)2.5,4,1.5,3 : C2H2_65-35 v=0 3 0 3 2.5 4 - v=0 2 0 2 1.5 3 : 6:<LineList>
6 A2 1	5 A1 1	12250.5963	12250.5942	0.0021 1	.00192	0 : qR0,2(2)4.5,6,3.5,5 : C2H2_65-35 v=0 3 0 3 4.5 6 - v=0 2 0 2 3.5 5 : 7:<LineList>
5 A2 2	4 A1 2	12250.8483	12250.8500	-0.0017 1	.00143	0 : qR0,2(2)4.5,5,3.5,4 : C2H2_65-35 v=0 3 0 3 4.5 5 - v=0 2 0 2 3.5 4 : 8:<LineList>
5 B2 2	4 B1 2	12433.3009	12433.2984	0.0025 1	.0003	0 : qR1,1(2)3.5,5,2.5,4 : C2H2_65-35 v=0 3 1 2 3.5 5 - v=0 2 1 1 2.5 4 : 9:<LineList>
4 B2 4	3 B1 3	12433.6313	12433.6304	0.0009 1	.00024	0 : qR1,1(2)2.5,4,1.5,3 : C2H2_65-35 v=0 3 1 2 2.5 4 - v=0 2 1 1 1.5 3 : 10:<LineList>
4 B2 4	3 B1 3	12433.6313	12433.6304	0.0009 1	.00024	0 : qR1,1(2)2.5,4,1.5,3 : C2H2_65-35 v=0 3 1 2 2.5 4 - v=0 2 1 1 1.5 3 : 11:<LineList>
6 B2 1	5 B1 1	12434.6627	12434.6626	0.0001 1	.00039	0 : qR1,1(2)4.5,6,3.5,5 : C2H2_65-35 v=0 3 1 2 4.5 6 - v=0 2 1 1 3.5 5 : 12:<LineList>
3 B2 7	2 B1 5	12434.9256	12434.9254	0.0002 1	.00019	0 : qR1,1(2)1.5,3,0.5,2 : C2H2_65-35 v=0 3 1 2 1.5 3 - v=0 2 1 1 0.5 2 : 13:<LineList>
6 B2 2	5 B1 2	16089.2571	16089.2609	-0.0038 1	.00026	0 : qR1,3(3)4.5,6,3.5,5 : C2H2_65-35 v=0 4 1 4 4.5 6 - v=0 3 1 3 3.5 5 : 14:<LineList>
5 B2 4	4 B1 4	16089.3605	16089.3643	-0.0038 1	.00021	0 : qR1,3(3)3.5,5,3.5,4 : C2H2_65-35 v=0 4 1 4 3.5 5 - v=0 3 1 3 3.5 4 : 15:<LineList>
4 B2 10	3 B1 9	16089.8428	16089.8391	0.0037 1	.00015	0 : qR1,3(3)2.5,4,1.5,3 : C2H2_65-35 v=0 4 1 4 2.5 4 - v=0 3 1 3 1.5 3 : 16:<LineList>
7 B2 1	6 B1 1	16089.8571	16089.8444	0.0127 1	.00032	0 : qR1,3(3)5.5,7,4.5,6 : C2H2_65-35 v=0 4 1 4 5.5 7 - v=0 3 1 3 4.5 6 : 17:<LineList>
5 B2 5	4 B1 5	16090.4828	16090.4872	-0.0044 1	.00017	0 : qR1,3(3)4.5,5,2.5,4 : C2H2_65-35 v=0 4 1 4 4.5 5 - v=0 3 1 3 2.5 4 : 19:<LineList>
5 B2 6	4 B1 6	16091.0838	16091.0865	-0.0027 1	.00022	0 : qR1,3(3)5.5,5,4.5,4 : C2H2_65-35 v=0 4 1 4 5.5 5 - v=0 3 1 3 4.5 4 : 20:<LineList>
6 B2 3	5 B1 3	16091.3692	16091.3697	-0.0005 1	.00026	0 : qR1,3(3)5.5,6,4.5,5 : C2H2_65-35 v=0 4 1 4 5.5 6 - v=0 3 1 3 4.5 5 : 21:<LineList>
4 A1 4	3 A2 4	16332.7179	16332.7196	-0.0017 1	.0009	0 : qR0,3(3)2.5,4,1.5,3 : C2H2_65-35 v=0 4 0 4 2.5 4 - v=0 3 0 3 1.5 3 : 22:<LineList>
7 A1 1	6 A2 1	16332.7945	16332.7928	0.0017 1	.00159	0 : qR0,3(3)5.5,7,4.5,6 : C2H2_65-35 v=0 4 0 4 5.5 7 - v=0 3 0 3 4.5 6 : 23:<LineList>
6 B1 2	5 B2 2	16579.5770	16579.5778	-0.0008 1	.00026	0 : qR1,2(3)4.5,6,3.5,5 : C2H2_65-35 v=0 4 1 3 4.5 6 - v=0 3 1 2 3.5 5 : 24:<LineList>
7 B1 1	6 B2 1	16580.1928	16580.1963	-0.0035 1	.00032	0 : qR1,2(3)5.5,7,4.5,6 : C2H2_65-35 v=0 4 1 3 5.5 7 - v=0 3 1 2 4.5 6 : 25:<LineList>
4 B1 8	3 B2 7	16580.2157	16580.2148	0.0009 1	.00018	0 : qR1,2(3)2.5,4,1.5,3 : C2H2_65-35 v=0 4 1 3 2.5 4 - v=0 3 1 2 1.5 3 : 26:<LineList>
6 B1 3	5 B2 3	16581.7599	16581.7583	0.0016 1	.00025	0 : qR1,2(3)5.5,6,4.5,5 : C2H2_65-35 v=0 4 1 3 5.5 6 - v=0 3 1 2 4.5 5 : 27:<LineList>
5 B1 1	4 B2 1	8287.8235	8287.8256	-0.0021 1	.00027	0 : qR1,0(1)3.5,5,2.5,4 : C2H2_65-35 v=0 2 1 1 3.5 5 - v=0 1 1 0 2.5 4 : 28:<LineList>

27 Observations, 9 Parameters

Initial Average Error: 0.00393024274957085

Predicted New Error: 0.00392680282421331

Parameters:

# Old	New	Std Dev	Change/Std Sens	Summary	Name
1 34540.907584005	34542.7616300943	127.74074	0.0145 1.17846	34543(128)	v=0 A
2 2103.43216000134	2103.43216548914	.0009403	0.0058 1.19e-5	2103.43217(94)	v=0 B
3 1980.71468032904	1980.71468339371	.00082474	0.0037 1.12e-5	1980.71468(82)	v=0 C
4 .03173	.031713475070171	.00113229	-0.0146 7.21e-6	0.03171(113)	v=0 DJK
5 .0002557	.000256545413306987	4.2419e-5	0.0199 2.27e-7	2.565(424)e-4	v=0 DJ
6 60.38	60.3782312962619	.07652172	-0.0231 .001627	60.378(77)	Cu CHlzz
7 -60.96	-60.9622877710731	.17737871	-0.0129 .005243	-60.96(18)	Cu CHlxxmyy
8 -21.75	-21.7467227969902	.03382109	0.0969 .001633	-21.747(34)	Cl CHlzz
9 -6.16	-6.14542958487309	.14021194	0.1039 .005378	-6.15(14)	Cl CHlxxmyy

Correlation Matrix

1	2	3	4	5	6	7	8	9
1 1.000								
2 -0.363	1.000							
3 -0.478	0.707	1.000						
4 -0.968	0.311	0.449	1.000					
5 0.805	0.187	0.060	-0.838	1.000				
6 0.426	0.534	0.242	-0.494	0.745	1.000			
7 -0.223	-0.428	0.027	0.263	-0.392	-0.553	1.000		
8 -0.120	-0.158	-0.051	0.166	-0.222	-0.443	0.259	1.000	
9 0.053	0.066	-0.104	-0.046	0.060	-0.018	-0.582	-0.106	1.000

¹²C₆H₂ --- ⁶³Cu⁺Cl (Page 1 of 1)

Pgopher 8.0.102 08 Dec 2013 16:55 32 bit (Delphi 18.5/18)

Mixture: Cavity 12C2 H2 --- 63Cu 37Cl.pgo

Units MHz
PrintLevel Detail
Precision 4
BasisOrder boDefault
QuantumNumberFormat J
FitCycles 1
FitDetails False
AutoReplot True
AllowComplex False
NoLineList False
ShowEstUnc False
ShowDerivatives False
SVDlimit 5
SVDThresh 1E-15
ScaleChanges 1
Species: C2H2_CuCl
Jmax 30
Concentration 1
AsymmetricMolecule: C2H2_63-37
nNuclei 2
JAdjustSym False
BlockMatrix True
PointGroup C2v
Representation Ir
SReduction False
eeWt 1
eoWt 1

oeWt 1
ooWt 1
C2zAxis a
C2xAxis c
PseudoC2v False
FakeSym False
PhaseAdjust False
Abundance 1
AsymmetricManifold: Ground
Initial True
EigenSearch True
LimitSearch True
AutoQConverge True
UsePopParams False
AsymmetricTop: v=0
Symmetry A1
Kmin all
Kmax all
A 34629.8978197417 Float
B 2044.60911079035 Float
C 1928.45975254769 Float
DJK 0.03003
DJ 0.0002817
deltaJ 1.49E-5
AsymmetricTopNucleus: Cl
Spin 1.5
AsNext False
CHlzz -17.188321388508 Float
CHlxxmyy -5.18325437891298 Float
AsymmetricTopNucleus: Cu

Spin 1.5
AsNext False
CHlzz 65.34629980313 Float
CHlxxmyy -65.8366587357878 Float
Caa 0.0309
Cbb 0.00907
Ccc 0.00708
<N ,K |A|N,K> = K^2
<N ,K-2|B|N,K> = sqrt((N*(N+1)+(-K+1)*(K-2))*(N*(N+1)-K*(K-1)))/4
<N ,K |B|N,K> = (N*(N+1)-K^2)/2
<N ,K+2|B|N,K> = sqrt((N*(N+1)+(-K-1)*(K+2))*(N*(N+1)-K*(K+1)))/4
<N ,K-2|C|N,K> = (-sqrt((N*(N+1)+(-K+1)*(K-2))*(N*(N+1)-K*(K-1)))/4
<N ,K |C|N,K> = (N*(N+1)-K^2)/2
<N ,K+2|C|N,K> = (-sqrt((N*(N+1)+(-K-1)*(K+2))*(N*(N+1)-K*(K+1)))/4
<N ,K |DJK|N,K> = -N*(N+1)*K^2
<N ,K |DJ|N,K> = -N^2*(N+1)^2
<N ,K-2|deltaJ|N,K> = -N*(N+1)*sqrt((N*(N+1)+(-K+1)*(K-2))*(N*(N+1)-K*(K-1)))
<N ,K+2|deltaJ|N,K> = -N*(N+1)*sqrt((N*(N+1)+(-K-1)*(K+2))*(N*(N+1)-K*(K+1)))
TransitionMoments: <Ground|mu|Ground>
CartesianTransitionMoment: <v=0|a|v=0>
Axis a
Strength 1
Symbolic Matrix Elements not available for <v=0|a|v=0>

Residuals before fit for C2H2_63-37 for the Ground manifold

J"S"	#"	J"S"	#"	Observed	Calculated	Obs-Calc	StdDev
6 B1 1	5 B2 1	11743.7281	11743.7273	0.0008	1 .00036	0 : qR1,2(2)4.5,6,3,5,5 : v=0 3 1 3 4.5 6 - v=0 2 1 2 3.5 5 : 1:<LineList>	
4 B1 6	3 B2 5	11746.4239	11746.4232	0.0007	1 .00021	0 : qR1,2(2)4.5,4,3,5,3 : v=0 3 1 3 4.5 4 - v=0 2 1 2 3.5 3 : 2:<LineList>	
5 B1 3	4 B2 3	11747.5489	11747.5497	-0.0008	1 .00026	0 : qR1,2(2)4.5,5,3,5,4 : v=0 3 1 3 4.5 5 - v=0 2 1 2 3.5 4 : 3:<LineList>	
6 A2 1	5 A1 1	11917.3955	11917.3947	0.0008	1 .0019	0 : qR0,2(2)4.5,6,3,5,5 : v=0 3 0 3 4.5 6 - v=0 2 0 2 3.5 5 : 4:<LineList>	
5 A2 2	4 A1 2	11917.6012	11917.6008	0.0004	1 .0014	0 : qR0,2(2)4.5,5,3,5,4 : v=0 3 0 3 4.5 5 - v=0 2 0 2 3.5 4 : 5:<LineList>	
4 A2 3	3 A1 3	11921.4721	11921.4721	0.0000	1 .00089	0 : qR0,2(2)4.5,4,3,5,3 : v=0 3 0 3 4.5 4 - v=0 2 0 2 3.5 3 : 6:<LineList>	
5 B2 2	4 B1 2	12090.2581	12090.2577	0.0004	1 .00028	0 : qR1,1(2)3.5,5,2,5,4 : v=0 3 1 2 3.5 5 - v=0 2 1 1 2.5 4 : 7:<LineList>	
6 B2 1	5 B1 1	12091.3289	12091.3300	-0.0011	1 .00036	0 : qR1,1(2)4.5,6,3,5,5 : v=0 3 1 2 4.5 6 - v=0 2 1 1 3.5 5 : 8:<LineList>	
5 B2 3	4 B1 3	12095.3986	12095.3977	0.0009	1 .00026	0 : qR1,1(2)4.5,5,3,5,4 : v=0 3 1 2 4.5 5 - v=0 2 1 1 3.5 4 : 9:<LineList>	
7 B2 1	6 B1 1	15658.6251	15658.6244	0.0007	1 .0003	0 : qR1,3(3)5.7,4,5,6 : v=0 4 1 4 5.5 7 - v=0 3 1 3 4.5 6 : 10:<LineList>	
4 B2 4	3 B1 3	12090.5108	12090.5106	0.0002	1 .00022	0 : qR1,1(2)2.5,4,1.5,3 : v=0 3 1 2 2.5 4 - v=0 2 1 1 1.5 3 : 11:<LineList>	
6 B2 3	5 B1 3	15660.2719	15660.2742	-0.0023	1 .00025	0 : qR1,3(3)5.5,6,4,5,5 : v=0 4 1 4 5.5 6 - v=0 3 1 3 4.5 5 : 12:<LineList>	
6 B2 2	5 B1 2	15658.1559	15658.1538	0.0021	1 .00025	0 : qR1,3(3)4.5,6,3,5,5 : v=0 4 1 4 4.5 6 - v=0 3 1 3 3.5 5 : 13:<LineList>	
5 B2 4	4 B1 4	15658.1759	15658.1781	-0.0022	1 .00021	0 : qR1,3(3)3.5,5,2,5,4 : v=0 4 1 4 3.5 5 - v=0 3 1 3 2.5 4 : 14:<LineList>	
6 B1 2	5 B2 2	16122.1886	16122.1869	0.0017	1 .00025	0 : qR1,2(3)4.5,6,3,5,5 : v=0 4 1 3 4.5 6 - v=0 3 1 2 3.5 5 : 15:<LineList>	
5 B1 4	4 B2 4	16122.1886	16122.1912	-0.0026	1 .00021	0 : qR1,2(3)3.5,5,2,5,4 : v=0 4 1 3 3.5 5 - v=0 3 1 2 2.5 4 : 16:<LineList>	
7 B1 1	6 B2 1	16122.6748	16122.6758	-0.0010	1 .00031	0 : qR1,2(3)5.5,7,4,5,6 : v=0 4 1 3 5.5 7 - v=0 3 1 2 4.5 6 : 17:<LineList>	
4 B1 8	3 B2 7	16122.6893	16122.6871	0.0022	1 .00017	0 : qR1,2(3)2.5,4,1.5,3 : v=0 4 1 3 2.5 4 - v=0 3 1 2 1.5 3 : 18:<LineList>	
5 B1 6	4 B2 6	16123.7120	16123.7105	0.0015	1 .0002	0 : qR1,2(3)4.5,5,3,5,4 : v=0 4 1 3 4.5 5 - v=0 3 1 2 3.5 4 : 19:<LineList>	
4 B1 10	3 B2 9	16123.7120	16123.7134	-0.0014	1 .00015	0 : qR1,2(3)3.5,4,2.5,3 : v=0 4 1 3 3.5 4 - v=0 3 1 2 2.5 3 : 20:<LineList>	
4 A2 2	3 A1 2	11917.0951	11917.0960	-0.0009	1 .00116	0 : qR0,2(2)2.5,4,1.5,3 : v=0 3 0 3 2.5 4 - v=0 2 0 2 1.5 3 : 21:<LineList>	
6 B1 3	5 B2 3	16124.3471	16124.3460	0.0011	1 .00025	0 : qR1,2(3)5.5,6,4,5,5 : v=0 4 1 3 5.5 6 - v=0 3 1 2 4.5 5 : 22:<LineList>	
4 B1 10	4 B2 6	16124.3471	16124.3499	-0.0028	1 2e-5	0 : qR1,2(3)3.5,4,3,5,4 : v=0 4 1 3 3.5 4 - v=0 3 1 2 3.5 4 : 23:<LineList>	
5 B2 6	4 B1 6	15659.9532	15659.9521	0.0011	1 .00022	0 : qR1,3(3)5.5,5,4,5,4 : v=0 4 1 4 5.5 5 - v=0 3 1 3 4.5 4 : 24:<LineList>	
5 B1 5	4 B2 5	16126.1415	16126.1406	0.0009	1 .00019	0 : qR1,2(3)5.5,5,4,5,4 : v=0 4 1 3 5.5 5 - v=0 3 1 2 4.5 4 : 25:<LineList>	

25 Observations, 7 Parameters

Initial Average Error: 0.00169247388511605

Predicted New Error: 0.00169239051623959

Parameters:

# Old	New	Std Dev	Change/Std Sens	Summary	Name
1 34629.8978197417	34629.901522897	34.362065	0.0001 1.14932	34630(34)	v=0 A
2 2044.60911079035	2044.6091102674	.00015881	-0.0033 5.6e-6	2044.60911(16)	v=0 B
3 1928.45975254769	1928.45975344014	.00019165	0.0047 6.72e-6	1928.45975(19)	v=0 C
4 -17.188321388508	-17.188146928699	.02856865	0.0061 .001288	-17.188(29)	Cl CHlzz
5 -5.18325437891298	-5.18291124309386	.06768962	0.0051 .00142	-5.183(68)	Cl CHlxxmyy
6 65.34629980313	65.3460084776422	.02820566	-0.0103 .00097	65.346(28)	Cu CHlzz
7 -65.8366587357878	-65.8352477785581	.0894869	0.0158 .002789	-65.835(89)	Cu CHlxxmyy

Correlation Matrix

1	2	3	4	5	6	7	
1	1.000						
2	-0.611	1.000					
3	-0.436	-0.265	1.000				
4	0.032	-0.350	0.562	1.000			
5	0.057	-0.425	0.552	0.731	1.000		
6	-0.107	0.472	-0.472	-0.578	-0.828	1.000	
7	0.184	0.106	-0.538	-0.650	-0.819	0.518	1.000

Gpogher 8.0.102 08 Dec 2013 16:55 32 bit (Delphi 18.5/18)

Mixture: Cavity 12C2 D2 --- 63Cu 35Cl.pgo

Units MHz
PrintLevel Detail
Precision 4
BasisOrder boDefault
QuantumNumberFormat J
FitCycles 1
FitDetails False
AutoReplot True
AllowComplex False
NoLineList False
ShowEstUnc False
ShowDerivatives False
SVDlimit 5
SVDThresh 1E-15
ScaleChanges 1
Species: Species
Jmin 0
Jmax 30
Concentration 1
AsymmetricMolecule: 12C-D2---63Cu-35Cl
nNuclei 2
Jmax 30
Colour Olive
JAdjustSym False
BlockMatrix True
PointGroup C2v
Representation Ir
SReduction False
eeWt 1

Residuals before fit for 12C-D2---63Cu-35Cl for the Ground manifold

J'S' #'	J"S' #"	Observed	Calculated	Obs-Calc	StdDev	
5 B2 1	4 B1 1	7605.9718	7605.9753	-0.0035 1	.00019	0 : qR1,1(1)3.5,5,2,5,4 : v=0 2 1 2 3.5 5 - v=0 1 1 1 2.5 4 : 1:<LineList>
3 A1 4	2 A2 3	7753.9562	7753.9531	0.0031 1	.00019	0 : qR0,1(1)2.5,3,0,5,2 : v=0 2 0 2 2.5 3 - v=0 1 0 1 0.5 2 : 2:<LineList>
3 A1 2	2 A2 2	7755.8862	7755.8893	-0.0031 1	.00022	0 : qR0,1(1)1.5,3,2,5,2 : v=0 2 0 2 1.5 3 - v=0 1 0 1 2.5 2 : 3:<LineList>
4 A1 1	3 A2 1	7757.4101	7757.4064	0.0037 1	.00036	0 : qR0,1(1)2.5,4,1,5,3 : v=0 2 0 2 2.5 4 - v=0 1 0 1 1.5 3 : 4:<LineList>
2 A1 3	1 A2 2	7758.0386	7758.0458	-0.0072 1	.00017	0 : qR0,1(1)1.5,2,0,5,1 : v=0 2 0 2 1.5 2 - v=0 1 0 1 0.5 1 : 5:<LineList>
5 A1 1	4 A2 1	7758.2185	7758.2180	0.0005 1	.00054	0 : qR0,1(1)3.5,5,2,5,4 : v=0 2 0 2 3.5 5 - v=0 1 0 1 2.5 4 : 6:<LineList>
5 B1 1	4 B2 1	7908.2497	7908.2490	0.0007 1	.0002	0 : qR1,0(1)3.5,5,2,5,4 : v=0 2 1 1 3.5 5 - v=0 1 1 1 0.2 5 4 : 7:<LineList>
5 B1 2	4 B2 2	11409.4673	11409.4652	0.0021 1	.00023	0 : qR1,2(2)3.5,5,2,5,4 : v=0 3 1 3 3.5 5 - v=0 2 1 2 2.5 4 : 8:<LineList>
6 B1 1	5 B2 1	11410.5581	11410.5587	-0.0006 1	.00032	0 : qR1,2(2)4.5,6,3,5,5 : v=0 3 1 3 4.5 6 - v=0 2 1 2 3.5 5 : 9:<LineList>
4 B1 6	3 B2 5	11413.1989	11413.1936	0.0053 1	.0002	0 : qR1,2(2)4.5,4,3,5,3 : v=0 3 1 3 4.5 4 - v=0 2 1 2 3.5 3 : 10:<LineList>
5 B1 3	4 B2 3	11414.3505	11414.3520	-0.0015 1	.00024	0 : qR1,2(2)4.5,5,3,5,4 : v=0 3 1 3 4.5 5 - v=0 2 1 2 3.5 4 : 11:<LineList>
3 A2 6	2 A1 5	11634.8787	11634.8763	0.0024 1	.00024	0 : qR0,2(2)2.5,3,0,5,2 : v=0 3 0 3 2.5 3 - v=0 2 0 2 0.5 2 : 12:<LineList>
4 A2 4	3 A1 4	11635.2495	11635.2422	0.0073 1	.00041	0 : qR0,2(2)4.5,4,2,5,3 : v=0 3 0 3 4.5 4 - v=0 2 0 2 2.5 3 : 13:<LineList>
6 A2 1	5 A1 1	11636.3205	11636.3253	-0.0048 1	.00072	0 : qR0,2(2)4.5,6,3,5,5 : v=0 3 0 3 4.5 6 - v=0 2 0 2 3.5 5 : 14:<LineList>
5 A2 2	4 A1 2	11636.5516	11636.5484	0.0032 1	.00054	0 : qR0,2(2)4.5,5,3,5,4 : v=0 3 0 3 4.5 5 - v=0 2 0 2 3.5 4 : 15:<LineList>
3 A2 5	2 A1 4	11638.2664	11638.2704	-0.0040 1	.00028	0 : qR0,2(2)3.5,3,3,5,2 : v=0 3 0 3 3.5 3 - v=0 2 0 2 3.5 2 : 16:<LineList>
5 B2 2	4 B1 2	11864.0649	11864.0667	-0.0018 1	.00026	0 : qR1,1(2)3.5,5,2,5,4 : v=0 3 1 2 3.5 5 - v=0 2 1 1 2.5 4 : 17:<LineList>
6 B2 1	5 B1 1	11865.4290	11865.4276	0.0014 1	.00033	0 : qR1,1(2)4.5,6,3,5,5 : v=0 3 1 2 4.5 6 - v=0 2 1 1 3.5 5 : 18:<LineList>
7 B2 1	6 B1 1	15213.7990	15213.7988	0.0002 1	.00035	0 : qR1,3(3)5.7,4,5,6 : v=0 4 1 4 5.5 7 - v=0 3 1 3 4.5 6 : 19:<LineList>
6 B2 3	5 B1 3	15215.4384	15215.4409	-0.0025 1	.00029	0 : qR1,3(3)5.5,6,4,5,5 : v=0 4 1 4 5.5 6 - v=0 3 1 3 4.5 5 : 20:<LineList>
5 A1 2	4 A2 2	15511.5770	15511.5803	-0.0033 1	.00051	0 : qR0,3(3)3.5,5,2,5,4 : v=0 4 0 4 3.5 5 - v=0 3 0 3 2.5 4 : 21:<LineList>
6 A1 1	5 A2 1	15511.7804	15511.7820	-0.0016 1	.00062	0 : qR0,3(3)4.5,6,3,5,5 : v=0 4 0 4 4.5 6 - v=0 3 0 3 3.5 5 : 22:<LineList>
7 A1 1	6 A2 1	15511.9495	15511.9480	0.0015 1	.00075	0 : qR0,3(3)5.5,7,4,5,6 : v=0 4 0 4 5.5 7 - v=0 3 0 3 4.5 6 : 23:<LineList>
5 A1 3	4 A2 3	15513.7022	15513.7003	0.0019 1	.00042	0 : qR0,3(3)4.5,5,3,5,4 : v=0 4 0 4 4.5 5 - v=0 3 0 3 3.5 4 : 24:<LineList>
7 B1 1	6 B2 1	15820.8772	15820.8762	0.0010 1	.00035	0 : qR1,2(3)5.5,7,4,5,6 : v=0 4 1 3 5.5 7 - v=0 3 1 2 4.5 6 : 25:<LineList>
6 B1 3	5 B2 3	15822.5509	15822.5509	-0.0000 1	.00028	0 : qR1,2(3)5.5,6,4,5,5 : v=0 4 1 3 5.5 6 - v=0 3 1 2 4.5 5 : 26:<LineList>
4 B1 2	3 B2 2	7903.1286	7903.1301	-0.0015 1	9.5e-5	0 : qR1,0(1)2.5,4,1,5,3 : v=0 2 1 1 2.5 4 - v=0 1 1 0 1.5 3 : 27:<LineList>

27 Observations, 9 Parameters

Initial Average Error: 0.00391060060487059

Predicted New Error: 0.00390905184858259

Parameters:

# Old	New	Std Dev	Change/Std Sens	Summary	Name
1 25101.9081604735	25102.0376321841	30.78921	0.0042 .295153	25102.0(308)	v=0 A
2 2015.92452486474	2015.92452608432	.00069846	0.0017 1.37e-5	2015.92453(70)	v=0 B
3 1864.01322280752	1864.0132225452	.00072859	-0.0004 1.28e-5	1864.01322(73)	v=0 C
4 .0294150895672294	.029411831324242	.00083568	-0.0039 9.45e-7	0.029412(836)	v=0 DJK
5 .000242611496502316	.000242786703264415	3.5578e-5	0.0049 7.93e-9	2.4279(3558)e-4	v=0 DJ
6 -21.7653278541012	-21.7650020349673	.05998125	0.0054 .000467	-21.7650(600)	Cl CHlzz
7 -6.59968302558134	-6.59698415066277	.71385048	0.0038 .000215	-6.5970(7139)	Cl CHlxxmyy
8 65.4381665553303	65.4351758571077	.56059649	-0.0053 .000882	65.435(561)	Cu CHlzz
9 -65.931628619467	-65.926569904313	.40901363	0.0124 .001921	-65.927(409)	Cu CHlxxmyy

Correlation Matrix

1	2	3	4	5	6	7	8	9
1 1.000								
2 -0.189	1.000							
3 -0.310	0.098	1.000						
4 -0.946	0.193	0.321	1.000					
5 0.854	0.176	0.074	-0.835	1.000				
6 0.808	0.246	-0.155	-0.771	0.891	1.000			
7 0.781	0.232	0.204	-0.753	0.988	0.841	1.000		
8 -0.797	-0.301	0.071	0.736	-0.922	-0.967	-0.887	1.000	
9 -0.787	-0.281	-0.116	0.772	-0.981	-0.884	-0.981	0.907	1.000

AsymmetricTopNucleus: Cu
Spin 1.5
AsNext False
CHlzz 65.4381665553303 Float
CHlxxmyy -65.931628619467 Float
Caa 0.0309
Cbb 0.00907
Ccc 0.00708
<N ,K |A|N,K> = K^2
<N ,K+2|B|N,K> = sqrt((N*(N+1)+(-K+1)*(K-2))*(N*(N+1)-K*(K-1)))/4
<N ,K |B|N,K> = (N*(N+1)-K^2)/2
<N ,K+2|B|N,K> = sqrt((N*(N+1)+(-K-1)*(K+2))*(N*(N+1)-K*(K+1)))/4
<N ,K+2|C|N,K> = (-sqrt((N*(N+1)+(-K+1)*(K-2))*(N*(N+1)-K*(K-1)))/4
<N ,K |C|N,K> = (N*(N+1)-K^2)/2
<N ,K+2|C|N,K> = (-sqrt((N*(N+1)+(-K-1)*(K+2))*(N*(N+1)-K*(K+1)))/4
<N ,K |DJK|N,K> = -N*(N+1)*K^2
<N ,K |D|N,K> = -N^2*(N+1)^2
<N ,K+2|deltaJ|N,K> = -N*(N+1)*sqrt((N*(N+1)+(-K+1)*(K-2))*(N*(N+1)-K*(K-1))
<N ,K+2|deltaJ|N,K> = -N*(N+1)*sqrt((N*(N+1)+(-K-1)*(K+2))*(N*(N+1)-K*(K+1))
TransitionMoments: <Ground|mu|Ground>
CartesianTransitionMoment: <v=0|a|v=0>
Axis a
Strength 1
Symbolic Matrix Elements not available for <v=0|a|v=0>

¹³C₂H₂ --- ⁶³Cu³⁵Cl (Page 1 of 2)

Pgopher 8.0.102 08 Dec 2013 16:55 32 bit (Delphi 18.5/18)

Mixture: Cavity_13C2H2_63_35_with_spin_rotation.pgo

Units MHz

PrintLevel Detail

Precision 4

BasisOrder boDefault

QuantumNumberFormat J

FitCycles 1

FitDetails False

AutoReplot True

AllowComplex False

NoLineList False

ShowEstUnc False

ShowDerivatives False

SVDlimit 5

SVDThresh 1E-15

ScaleChanges 1

Species: C2H2_CuCl

Jmax 30

Concentration 1

AsymmetricMolecule: 13C2H2_63-35

nNuclei 2

Colour Teal

JAdjustSym False

BlockMatrix True

PointGroup C2v

Representation Ir

SReduction False

eeWt 1

eoWt 1

oeWt 1

ooWt 1

C2zAxis a

C2xAxis c

PseudoC2v False

FakeSym False

PhaseAdjust False

Abundance 1

AsymmetricManifold: 13C2H2_63-35 Ground

Initial True

EigenSearch True

LimitSearch True

AutoQConverge True

UsePopParams False

AsymmetricTop: 13C2H2_63-35 v=0

Symmetry A1

Kmin all

Kmax all

A 32881.7572779183 Float

B 2032.35982226355 Float

C 1912.01641954713 Float

DJK 0.0284488913420128 Float

DJ 0.000275484427778471 Float

deltaJ 1.53E-5

AsymmetricTopNucleus: 13C2H2_63-35 Cl

Spin 1.5

AsNext False

CHlzz -21.748282235954 Float

CHlxxmyy -6.35458189042727 Float

AsymmetricTopNucleus: 13C2H2_63-35 Cu

Spin 1.5

AsNext False

CHlzz 64.8699969764716 Float

CHlxxmyy -65.2160627201671 Float

Caa 0.0309436432952066 Float

Cbb 0.00668574169311811 Float

Ccc 0.00862457936172966 Float

<N ,K |A|N,K> = K^2

<N ,K-2|B|N,K> = sqrt(((N*(N+1)+(-K+1)*(K-2))*(N*(N+1)-K*(K-1)))/4

<N ,K |B|N,K> = (N*(N+1)-K^2)/2

<N ,K+2|B|N,K> = sqrt(((N*(N+1)+(-K-1)*(K+2))*(N*(N+1)-K*(K+1)))/4

<N ,K-2|C|N,K> = (-sqrt(((N*(N+1)+(-K+1)*(K-2))*(N*(N+1)-K*(K-1)))/4

<N ,K |C|N,K> = (N*(N+1)-K^2)/2

<N ,K+2|C|N,K> = (-sqrt(((N*(N+1)+(-K-1)*(K+2))*(N*(N+1)-K*(K+1)))/4

<N ,K |DJK|N,K> = -N*(N+1)*K^2

<N ,K |DJ|N,K> = -N^2*(N+1)^2

<N ,K-2|deltaJ|N,K> = -N*(N+1)*sqrt(((N*(N+1)+(-K+1)*(K-2))*(N*(N+1)-K*(K-1))

<N ,K+2|deltaJ|N,K> = -N*(N+1)*sqrt(((N*(N+1)+(-K-1)*(K+2))*(N*(N+1)-K*(K+1))

TransitionMoments: 13C2H2_63-35 <Ground|mu|Ground>

CartesianTransitionMoment: 13C2H2_63-35 <v=0|a|v=0>

Axis a

Strength 1

Symbolic Matrix Elements not available for <v=0|a|v=0>

Residuals before fit for 13C2H2_63-35 for the Ground manifold

J"S' #"	J"S" #"	Observed	Calculated	Obs-Calc	StdDev	
3 A1 2	2 A2 2	7885.1582	7885.1603	-0.0021 1	.00065	0 : qR0,1(1)1.5,3,2,5,2 : 13C2H2_63-35 v=0 2 0 2 1.5 3 - v=0 1 0 1 2.5 2 : 1:<LineList>
4 A1 1	3 A2 1	7886.6752	7886.6861	-0.0109 1	.00108	0 : qR0,1(1)2.5,4,1.5,3 : 13C2H2_63-35 v=0 2 0 2 2.5 4 - v=0 1 0 1 1.5 3 : 2:<LineList>
5 A1 1	4 A2 1	7887.4835	7887.4937	-0.0102 1	.00155	0 : qR0,1(1)3.5,5,2.5,4 : 13C2H2_63-35 v=0 2 0 2 3.5 5 - v=0 1 0 1 2.5 4 : 3:<LineList>
5 B1 2	4 B2 2	11650.3813	11650.3859	-0.0046 1	.00026	0 : qR1,2(2)3.5,5,2.5,4 : 13C2H2_63-35 v=0 3 1 3 3.5 5 - v=0 2 1 2 2.5 4 : 4:<LineList>
6 B1 1	5 B2 1	11651.4742	11651.4821	-0.0079 1	.00037	0 : qR1,2(2)4.5,6,3.5,5 : 13C2H2_63-35 v=0 3 1 3 4.5 6 - v=0 2 1 2 3.5 5 : 5:<LineList>
4 B1 6	3 B2 5	11654.1098	11654.1027	0.0071 1	.00023	0 : qR1,2(2)4.5,4,3.5,3 : 13C2H2_63-35 v=0 3 1 3 4.5 4 - v=0 2 1 2 3.5 3 : 6:<LineList>
5 B1 3	4 B2 3	11655.2696	11655.2513	0.0183 1	.00028	0 : qR1,2(2)4.5,5,3.5,4 : 13C2H2_63-35 v=0 3 1 3 4.5 5 - v=0 2 1 2 3.5 4 : 7:<LineList>
4 A2 4	3 A1 4	11830.1573	11830.1678	-0.0105 1	.00105	0 : qR0,2(2)4.5,4,2.5,3 : 13C2H2_63-35 v=0 3 0 3 4.5 4 - v=0 2 0 2 2.5 3 : 8:<LineList>
5 A2 1	4 A1 1	11830.8855	11830.8952	-0.0097 1	.00143	0 : qR0,2(2)3.5,5,2.5,4 : 13C2H2_63-35 v=0 3 0 3 3.5 5 - v=0 2 0 2 2.5 4 : 9:<LineList>
4 A2 2	3 A1 2	11830.9037	11830.9079	-0.0042 1	.00111	0 : qR0,2(2)2.5,4,1.5,3 : 13C2H2_63-35 v=0 3 0 3 2.5 4 - v=0 2 0 2 1.5 3 : 10:<LineList>
6 A2 1	5 A1 1	11831.2075	11831.2128	-0.0053 1	.00185	0 : qR0,2(2)4.5,6,3.5,5 : 13C2H2_63-35 v=0 3 0 3 4.5 6 - v=0 2 0 2 3.5 5 : 11:<LineList>
5 A2 2	4 A1 2	11831.4652	11831.4693	-0.0041 1	.00137	0 : qR0,2(2)4.5,5,3.5,4 : 13C2H2_63-35 v=0 3 0 3 4.5 5 - v=0 2 0 2 3.5 4 : 12:<LineList>
2 A2 6	1 A1 4	11831.8449	11831.8502	-0.0053 1	.00042	0 : qR0,2(2)1.5,2,0.5,1 : 13C2H2_63-35 v=0 3 0 3 1.5 2 - v=0 2 0 2 0.5 1 : 13:<LineList>
4 A2 2	4 A1 1	11832.4570	11832.4626	-0.0056 1	.00012	0 : qR0,2(2)2.5,4,2.5,4 : 13C2H2_63-35 v=0 3 0 3 2.5 4 - v=0 2 0 2 2.5 4 : 14:<LineList>
2 A2 4	2 A1 2	11832.5092	11832.4867	0.0225 1	.00027	0 : qR0,2(2)3.5,2,2.5,2 : 13C2H2_63-35 v=0 3 0 3 3.5 2 - v=0 2 0 2 2.5 2 : 15:<LineList>
3 A2 5	2 A1 4	11833.1747	11833.1532	0.0215 1	.00007	0 : qR0,2(2)3.5,3,3.5,2 : 13C2H2_63-35 v=0 3 0 3 3.5 3 - v=0 2 0 2 3.5 2 : 16:<LineList>
4 A2 3	3 A1 3	11835.1377	11835.1088	0.0289 1	.00083	0 : qR0,2(2)3.5,4,3.5,3 : 13C2H2_63-35 v=0 3 0 3 3.5 4 - v=0 2 0 2 3.5 3 : 17:<LineList>
5 B2 2	4 B1 2	12010.2782	12010.2956	-0.0174 1	.0002	0 : qR1,1(2)3.5,5,2.5,4 : 13C2H2_63-35 v=0 3 1 2 3.5 5 - v=0 2 1 1 2.5 4 : 18:<LineList>
6 B2 1	5 B1 1	12011.6399	12011.6571	-0.0172 1	.00026	0 : qR1,1(2)4.5,6,3.5,5 : 13C2H2_63-35 v=0 3 1 2 4.5 6 - v=0 2 1 1 3.5 5 : 19:<LineList>
5 B2 3	4 B1 3	12015.7118	12015.7006	0.0112 1	.00019	0 : qR1,1(2)4.5,5,3.5,4 : 13C2H2_63-35 v=0 3 1 2 4.5 5 - v=0 2 1 1 3.5 4 : 20:<LineList>
4 B2 5	3 B1 4	12017.6841	12017.6476	0.0365 1	.00013	0 : qR1,1(2)4.5,4,3.5,3 : 13C2H2_63-35 v=0 3 1 2 4.5 4 - v=0 2 1 1 3.5 3 : 21:<LineList>
6 B2 2	5 B1 2	15534.8886	15534.8889	-0.0003 1	.00027	0 : qR1,3(3)4.5,6,3.5,5 : 13C2H2_63-35 v=0 4 1 4 4.5 6 - v=0 3 1 3 3.5 5 : 22:<LineList>
5 B2 4	4 B1 4	15534.9648	15534.9715	-0.0067 1	.00022	0 : qR1,3(3)3.5,5,2.5,4 : 13C2H2_63-35 v=0 4 1 4 3.5 5 - v=0 3 1 3 2.5 4 : 23:<LineList>
7 B2 1	6 B1 1	15535.4710	15535.4756	-0.0046 1	.00033	0 : qR1,3(3)5.5,7,4.5,6 : 13C2H2_63-35 v=0 4 1 4 5.5 7 - v=0 3 1 3 4.5 6 : 24:<LineList>
4 B2 9	3 B1 7	15535.8550	15535.8555	-0.0005 1	.00015	0 : qR1,3(3)3.5,4,4.5,3 : 13C2H2_63-35 v=0 4 1 4 3.5 4 - v=0 3 1 3 4.5 3 : 25:<LineList>
4 B2 7	3 B1 6	15535.8550	15535.8570	-0.0020 1	.00015	0 : qR1,3(3)4.5,4,3.5,3 : 13C2H2_63-35 v=0 4 1 4 4.5 4 - v=0 3 1 3 3.5 3 : 26:<LineList>
6 B2 3	5 B1 3	15537.1222	15537.1137	0.0085 1	.00027	0 : qR1,3(3)5.5,6,4.5,5 : 13C2H2_63-35 v=0 4 1 4 5.5 6 - v=0 3 1 3 4.5 5 : 27:<LineList>
6 A1 1	5 A2 1	15773.4705	15773.4737	-0.0032 1	.00126	0 : qR0,3(3)4.5,6,3.5,5 : 13C2H2_63-35 v=0 4 0 4 4.5 6 - v=0 3 0 3 3.5 5 : 28:<LineList>
4 A1 4	3 A2 4	15773.5451	15773.5514	-0.0063 1	.00087	0 : qR0,3(3)2.5,4,1.5,3 : 13C2H2_63-35 v=0 4 0 4 2.5 4 - v=0 3 0 3 1.5 3 : 29:<LineList>
7 A1 1	6 A2 1	15773.6322	15773.6348	-0.0026 1	.00154	0 : qR0,3(3)5.5,7,4.5,6 : 13C2H2_63-35 v=0 4 0 4 5.5 7 - v=0 3 0 3 4.5 6 : 30:<LineList>
6 A1 2	5 A2 2	15773.7139	15773.7177	-0.0038 1	.00123	0 : qR0,3(3)5.5,6,4.5,5 : 13C2H2_63-35 v=0 4 0 4 5.5 6 - v=0 3 0 3 4.5 5 : 31:<LineList>
4 A1 5	3 A2 5	15774.6719	15774.6643	0.0076 1	.00076	0 : qR0,3(3)4.5,4,3.5,3 : 13C2H2_63-35 v=0 4 0 4 4.5 4 - v=0 3 0 3 3.5 3 : 32:<LineList>
3 A1 6	2 A2 5	15774.7288	15774.7161	0.0127 1	.00053	0 : qR0,3(3)3.5,3,2.5,2 : 13C2H2_63-35 v=0 4 0 4 3.5 3 - v=0 3 0 3 2.5 2 : 33:<LineList>
3 A1 5	2 A2 4	15775.0098	15774.9991	0.0107 1	.00051	0 : qR0,3(3)4.5,3,3.5,2 : 13C2H2_63-35 v=0 4 0 4 4.5 3 - v=0 3 0 3 3.5 2 : 34:<LineList>
5 A1 3	4 A2 3	15775.4268	15775.4116	0.0152 1	.00087	0 : qR0,3(3)4.5,5,3.5,4 : 13C2H2_63-35 v=0 4 0 4 4.5 5 - v=0 3 0 3 3.5 4 : 35:<LineList>
4 A1 3	3 A2 3	15775.9339	15775.9239	0.0100 1	.00076	0 : qR0,3(3)5.5,4,4.5,3 : 13C2H2_63-35 v=0 4 0 4 5.5 4 - v=0 3 0 3 4.5 3 : 36:<LineList>
6 B1 2	5 B2 2	16015.6682	16015.6769	-0.0087 1	.00027	0 : qR1,2(3)4.5,6,3.5,5 : 13C2H2_63-35 v=0 4 1 3 4.5 6 - v=0 3 1 2 3.5 5 : 37:<LineList>
7 B1 1	6 B2 1	16016.2827	16016.2950	-0.0123 1	.00032	0 : qR1,2(3)5.5,7,4.5,6 : 13C2H2_63-35 v=0 4 1 3 5.5 7 - v=0 3 1 2 4.5 6 : 38:<LineList>
4 B1 10	3 B2 9	16017.1638	16017.1575	0.0063 1	.00015	0 : qR1,2(3)3.5,4,2.5,3 : 13C2H2_63-35 v=0 4 1 3 3.5 4 - v=0 3 1 2 2.5 3 : 39:<LineList>
6 B1 3	5 B2 3	16017.9693	16017.9687	0.0006 1	.00026	0 : qR1,2(3)5.5,6,4.5,5 : 13C2H2_63-35 v=0 4 1 3 5.5 6 - v=0 3 1 2 4.5 5 : 40:<LineList>

40 Observations, 12 Parameters

Initial Average Error: 0.0146650524674515

Predicted New Error: 0.00181243329985312

Parameters:

# Old	New	Std Dev	Change/Std Sens		Summary	Name
1 32881.7572779183		32882.9678128181	35.898037	0.0337 .252811	32883.0(359)	13C2H2_63-35 v=0 A
2 2032.35982226355		2032.35980358696	.00036248	-0.0515 4.28e-6	2032.35980(36)	13C2H2_63-35 v=0 B
3 1912.01641954713		1912.01641832488	.00029288	-0.0042 3.98e-6	1912.01642(29)	13C2H2_63-35 v=0 C
4 .0284488913420128		.0284393036431333	.00034812	-0.0275 3.14e-6	0.028439(348)	13C2H2_63-35 v=0 DJK
5 .000275484427778471		.000275804312955605	1.3489e-5	0.0237 7.91e-8	2.758(135)e-4	13C2H2_63-35 v=0 DJ
6 -21.748282235954		-21.7520288614397	.00929514	-0.4031 .000407	-21.7520(93)	13C2H2_63-35 Cl CHlzz
7 -6.35458189042727		-6.5087326346989	.079336	-1.9430 .002622	-6.509(79)	13C2H2_63-35 Cl CHlxxmyy
8 64.8699969764716		65.3587857623401	.02378011	20.5545 .000572	65.359(24)	13C2H2_63-35 Cu CHlzz
9 -65.2160627201671		-65.8667850067581	.06155035	-10.5722 .001892	-65.867(62)	13C2H2_63-35 Cu CHlxxmyy
10 .0309436432952066		.0311267230434281	.00575904	0.0318 .000236	0.0311(58)	13C2H2_63-35 Cu Caa
11 .00668574169311811		.00677851651348232	.00184449	0.0503 2.42e-5	6.8(18)e-3	13C2H2_63-35 Cu Cbb
12 .00862457936172966		.00856972403054351	.00130178	-0.0421 1.99e-5	8.6(13)e-3	13C2H2_63-35 Cu Ccc

Correlation Matrix

1	2	3	4	5	6	7	8	9	10	11	12
1 1.000											
2 -0.246	1.000										
3 -0.375	-0.127	1.000									
4 -0.963	0.247	0.354	1.000								
5 0.879	0.085	-0.118	-0.863	1.000							
6 0.182	-0.220	-0.036	-0.233	0.083	1.000						
7 -0.179	-0.358	0.421	0.087	-0.240	0.271	1.000					
8 -0.106	-0.248	-0.041	0.167	-0.161	-0.375	-0.341	1.000				
9 0.078	0.431	-0.294	-0.106	0.125	0.204	-0.059	-0.520	1.000			
10 0.119	-0.119	-0.080	-0.116	0.037	0.344	0.118	-0.372	0.193	1.000		
11 0.008	-0.713	0.340	0.034	-0.122	-0.022	0.087	0.524	-0.725	0.044	1.000	
12 0.048	0.611	-0.557	-0.037	0.102	-0.032	-0.291	-0.162	0.679	-0.009	-0.837	1.000

Gpghor 8.0.102 08 Dec 2013 16:55 32 bit (Delphi 18.5/18)

Mixture: 63-35 recovered.pgo

Units MHz
PrintLevel Detail
Precision 4
BasisOrder boDefault
QuantumNumberFormat J
FitCycles 1
FitDetails False
AutoReplot True
AllowComplex False
NoLineList False
ShowEstUnc False
ShowDerivatives False
SVDlimit 5
SVDThresh 1E-15
ScaleChanges 1
Species: C2H4-Cu-Cl
Jmax 30
Concentration 1
AsymmetricMolecule: C2H4-63Cu-35Cl
C2H4-63Cu-35Cl Fri OffFri Feb 18 18:55:10 2011
nNuclei 2
Jmax 30
Colour Fuchsia
JAdjustSym False
BlockMatrix True
PointGroup C2v
Representation Ir
SReduction False
eeWt 1
eoWt 1
oeWt 1
ooWt 1
C2zAxis a
C2xAxis c
PseudoC2v False
FakeSym False
PhaseAdjust False
Abundance 1

AsymmetricManifold: C2H4-63Cu-35Cl Ground

Jmax 30
Initial True
EigenSearch True
LimitSearch True
AutoQConverge True
UsePopParams False
AsymmetricTop: C2H4-63Cu-35Cl v=0
Symmetry A1
Kmin all
Kmax all
A 23920.3429096552 Float
B 1988.93165476155 Float
C 1882.69416025887 Float
DJK 0.0194038016596251 Float
DJ 0.0002678763750342 Float
AsymmetricTopNucleus: C2H4-63Cu-35Cl Copper
Spin 1.5
AsNext False
CHlzz 63.776258849643 Float
CHlxxmyy -44.505579698344 Float
AsymmetricTopNucleus: C2H4-63Cu-35Cl Chlorine
Spin 1.5
AsNext False
CHlzz -20.9938683685614 Float
CHlxxmyy -5.12019498024267 Float
<N ,K |A|N,K> = K^2
<N ,K-2|B|N,K> = sqrt((N*(N+1)+(-K+1)*(K-2))*(N*(N+1)-K*(K-1)))/4
<N ,K |B|N,K> = (N*(N+1)-K^2)/2
<N ,K+2|B|N,K> = sqrt((N*(N+1)+(-K-1)*(K+2))*(N*(N+1)-K*(K+1)))/4
<N ,K-2|C|N,K> = (-sqrt((N*(N+1)+(-K+1)*(K-2))*(N*(N+1)-K*(K-1)))/4
<N ,K |C|N,K> = (N*(N+1)-K^2)/2
<N ,K+2|C|N,K> = (-sqrt((N*(N+1)+(-K-1)*(K+2))*(N*(N+1)-K*(K+1)))/4
<N ,K |DJK|N,K> = -N*(N+1)*K^2
<N ,K |DJ|N,K> = -N^2*(N+1)^2
TransitionMoments: C2H4-63Cu-35Cl <Ground|mu|Ground>
CartesianTransitionMoment: C2H4-63Cu-35Cl <v=0|a|v=0>
Axis a
Strength 1
Symbolic Matrix Elements not available for <v=0|a|v=0>

Residuals before fit for C2H4-63Cu-35Cl for the Ground manifold

J'S' #'	J"S' #"	Observed	Calculated	Obs-Calc	StdDev	
4 B2 2	3 B1 2	7630.5260	7630.5452	-0.0192 1	.0002	0 : qR1,1(1)3.5,4,2.5,3 : C2H4-63Cu-35Cl v=0 2 1 2 3.5 4 - v=0 1 1 1 2.5 3 : 1:<LineList>
5 B2 1	4 B1 1	7634.8720	7634.8671	0.0049 1	.00032	0 : qR1,1(1)3.5,5,2.5,4 : C2H4-63Cu-35Cl v=0 2 1 2 3.5 5 - v=0 1 1 1 2.5 4 : 2:<LineList>
1 A1 3	2 A2 3	7727.2690	7727.2755	-0.0065 1	1e-4	0 : qR0,1(1)1.5,1,1.5,2 : C2H4-63Cu-35Cl v=0 2 0 2 1.5 1 - v=0 1 0 1 1.5 2 : 3:<LineList>
2 A1 4	2 A2 3	7727.2970	7727.2858	0.0112 1	7.5e-5	0 : qR0,1(1)1.5,2,1.5,2 : C2H4-63Cu-35Cl v=0 2 0 2 1.5 2 - v=0 1 0 1 1.5 2 : 4:<LineList>
3 A1 3	3 A2 2	7730.5950	7730.6054	-0.0104 1	.00035	0 : qR0,1(1)1.5,3,1.5,3 : C2H4-63Cu-35Cl v=0 2 0 2 1.5 3 - v=0 1 0 1 1.5 3 : 5:<LineList>
3 A1 4	2 A2 3	7737.9000	7737.8728	0.0272 1	.00046	0 : qR0,1(1)2.5,3,1.5,2 : C2H4-63Cu-35Cl v=0 2 0 2 2.5 3 - v=0 1 0 1 1.5 2 : 6:<LineList>
3 A1 2	2 A2 2	7739.7290	7739.7205	0.0085 1	.00052	0 : qR0,1(1)3.5,3,2.5,2 : C2H4-63Cu-35Cl v=0 2 0 2 3.5 3 - v=0 1 0 1 2.5 2 : 7:<LineList>
4 A1 1	3 A2 1	7741.1830	7741.1715	0.0115 1	.00087	0 : qR0,1(1)3.5,4,2.5,3 : C2H4-63Cu-35Cl v=0 2 0 2 3.5 4 - v=0 1 0 1 2.5 3 : 8:<LineList>
2 A1 3	1 A2 2	7741.7920	7741.7897	0.0023 1	.00039	0 : qR0,1(1)3.5,2,2.5,1 : C2H4-63Cu-35Cl v=0 2 0 2 3.5 2 - v=0 1 0 1 2.5 1 : 9:<LineList>
5 A1 1	4 A2 1	7741.9670	7741.9538	0.0132 1	.00125	0 : qR0,1(1)3.5,5,2.5,4 : C2H4-63Cu-35Cl v=0 2 0 2 3.5 5 - v=0 1 0 1 2.5 4 : 10:<LineList>
4 A1 2	3 A2 2	7742.7060	7742.7037	0.0023 1	.00076	0 : qR0,1(1)2.5,4,1.5,3 : C2H4-63Cu-35Cl v=0 2 0 2 2.5 4 - v=0 1 0 1 1.5 3 : 11:<LineList>
2 A1 2	1 A2 1	7742.9350	7742.9411	-0.0061 1	.0002	0 : qR0,1(1)0.5,2,0.5,1 : C2H4-63Cu-35Cl v=0 2 0 2 0.5 2 - v=0 1 0 1 0.5 1 : 12:<LineList>
1 A1 4	1 A2 3	7743.4750	7743.4702	0.0048 1	.00015	0 : qR0,1(1)2.5,1,1.5,1 : C2H4-63Cu-35Cl v=0 2 0 2 2.5 1 - v=0 1 0 1 1.5 1 : 13:<LineList>
2 A1 2	2 A2 1	7743.6500	7743.6433	0.0067 1	.00025	0 : qR0,1(1)0.5,2,0.5,2 : C2H4-63Cu-35Cl v=0 2 0 2 0.5 2 - v=0 1 0 1 0.5 2 : 14:<LineList>
2 A1 4	1 A2 2	7743.8100	7743.8205	-0.0105 1	.00012	0 : qR0,1(1)1.5,2,2.5,1 : C2H4-63Cu-35Cl v=0 2 0 2 1.5 2 - v=0 1 0 1 2.5 1 : 15:<LineList>
4 A1 2	4 A2 1	7757.1060	7757.1226	-0.0166 1	.00024	0 : qR0,1(1)2.5,4,2.5,4 : C2H4-63Cu-35Cl v=0 2 0 2 2.5 4 - v=0 1 0 1 2.5 4 : 16:<LineList>
2 A1 4	2 A2 1	7759.8690	7759.8675	0.0015 1	7.9e-5	0 : qR0,1(1)1.5,2,0.5,2 : C2H4-63Cu-35Cl v=0 2 0 2 1.5 2 - v=0 1 0 1 0.5 2 : 17:<LineList>
3 A1 3	2 A2 1	7759.8620	7759.8572	0.0048 1	.00023	0 : qR0,1(1)1.5,3,0.5,2 : C2H4-63Cu-35Cl v=0 2 0 2 1.5 3 - v=0 1 0 1 0.5 2 : 18:<LineList>
4 B1 2	3 B2 2	7841.9170	7841.9192	-0.0022 1	.00021	0 : qR1,0(1)3.5,4,2.5,3 : C2H4-63Cu-35Cl v=0 2 1 1 3.5 4 - v=0 1 1 0 2.5 3 : 19:<LineList>
5 B1 1	4 B2 1	7846.3060	7846.2818	0.0242 1	.00033	0 : qR1,0(1)3.5,5,2.5,4 : C2H4-63Cu-35Cl v=0 2 1 1 3.5 5 - v=0 1 1 0 2.5 4 : 20:<LineList>
4 B1 3	3 B2 1	7861.3800	7861.3757	0.0043 1	.0002	0 : qR1,0(1)2.5,4,1.5,3 : C2H4-63Cu-35Cl v=0 2 1 1 2.5 4 - v=0 1 1 0 1.5 3 : 21:<LineList>
2 B1 8	2 B2 4	11450.7500	11450.7628	-0.0128 1	.00011	0 : qR1,2(2)1.5,2,0.5,2 : C2H4-63Cu-35Cl v=0 3 1 3 1.5 2 - v=0 2 1 2 0.5 2 : 22:<LineList>
2 B1 8	1 B2 4	11451.2070	11451.2013	0.0057 1	.00013	0 : qR1,2(2)1.5,2,0.5,1 : C2H4-63Cu-35Cl v=0 3 1 3 1.5 2 - v=0 2 1 2 0.5 1 : 23:<LineList>
5 B1 2	4 B2 2	11453.0230	11453.0163	0.0067 1	.00051	0 : qR1,2(2)4.5,5,3.5,4 : C2H4-63Cu-35Cl v=0 3 1 3 4.5 5 - v=0 2 1 2 3.5 4 : 24:<LineList>
3 B1 6	2 B2 4	11453.2850	11453.3008	-0.0158 1	.00021	0 : qR1,2(2)1.5,3,0.5,2 : C2H4-63Cu-35Cl v=0 3 1 3 1.5 3 - v=0 2 1 2 0.5 2 : 25:<LineList>
4 B1 5	4 B2 3	11453.4530	11453.4594	-0.0064 1	9.7e-5	0 : qR1,2(2)2.5,4,2.5,4 : C2H4-63Cu-35Cl v=0 3 1 3 2.5 4 - v=0 2 1 2 2.5 4 : 26:<LineList>
4 B1 4	3 B2 3	11453.7530	11453.7411	0.0119 1	.00033	0 : qR1,2(2)4.5,4,3.5,3 : C2H4-63Cu-35Cl v=0 3 1 3 4.5 4 - v=0 2 1 2 3.5 3 : 27:<LineList>
6 B1 1	5 B2 1	11454.2950	11454.2910	0.0040 1	.00068	0 : qR1,2(2)4.5,6,3.5,5 : C2H4-63Cu-35Cl v=0 3 1 3 4.5 6 - v=0 2 1 2 3.5 5 : 28:<LineList>
3 B1 7	2 B2 6	11454.8250	11454.8121	0.0129 1	7.4e-5	0 : qR1,2(2)4.5,3,1.5,2 : C2H4-63Cu-35Cl v=0 3 1 3 4.5 3 - v=0 2 1 2 1.5 2 : 29:<LineList>
3 B1 7	2 B2 5	11454.9420	11454.9433	-0.0013 1	.00022	0 : qR1,2(2)4.5,3,3.5,2 : C2H4-63Cu-35Cl v=0 3 1 3 4.5 3 - v=0 2 1 2 3.5 2 : 30:<LineList>
3 B1 8	2 B2 6	11455.1000	11455.1040	-0.0040 1	.0002	0 : qR1,2(2)2.5,3,1.5,2 : C2H4-63Cu-35Cl v=0 3 1 3 2.5 3 - v=0 2 1 2 1.5 2 : 31:<LineList>
1 B1 8	1 B2 6	11455.1420	11455.1519	-0.0099 1	7e-5	0 : qR1,2(2)2.5,1,2.5,1 : C2H4-63Cu-35Cl v=0 3 1 3 2.5 1 - v=0 2 1 2 2.5 1 : 32:<LineList>
3 B1 8	2 B2 5	11455.2290	11455.2352	-0.0062 1	.00011	0 : qR1,2(2)2.5,3,3.5,2 : C2H4-63Cu-35Cl v=0 3 1 3 2.5 3 - v=0 2 1 2 3.5 2 : 33:<LineList>
2 B1 9	1 B2 5	11455.5220	11455.5350	-0.0130 1	.00013	0 : qR1,2(2)2.5,2,1.5,1 : C2H4-63Cu-35Cl v=0 3 1 3 2.5 2 - v=0 2 1 2 1.5 1 : 34:<LineList>
4 B1 5	3 B2 4	11455.8400	11455.8405	-0.0005 1	.00022	0 : qR1,2(2)2.5,4,1.5,3 : C2H4-63Cu-35Cl v=0 3 1 3 2.5 4 - v=0 2 1 2 1.5 3 : 35:<LineList>
3 B1 9	2 B2 7	11456.1950	11456.1915	0.0035 1	.0002	0 : qR1,2(2)3.5,2,2.5,2 : C2H4-63Cu-35Cl v=0 3 1 3 3.5 3 - v=0 2 1 2 2.5 2 : 36:<LineList>
4 B1 6	3 B2 5	11457.1330	11457.1305	0.0025 1	.00042	0 : qR1,2(2)3.5,4,2.5,3 : C2H4-63Cu-35Cl v=0 3 1 3 3.5 4 - v=0 2 1 2 2.5 3 : 37:<LineList>
5 B1 3	4 B2 3	11458.2300	11458.2237	0.0063 1	.00051	0 : qR1,2(2)3.5,5,2.5,4 : C2H4-63Cu-35Cl v=0 3 1 3 3.5 5 - v=0 2 1 2 2.5 4 : 38:<LineList>
2 B1 10	1 B2 6	11458.5190	11458.5097	0.0093 1	.00013	0 : qR1,2(2)3.5,2,2.5,1 : C2H4-63Cu-35Cl v=0 3 1 3 3.5 2 - v=0 2 1 2 2.5 1 : 39:<LineList>
2 B1 10	2 B2 7	11458.8070	11458.8041	0.0029 1	.0001	0 : qR1,2(2)3.5,2,2.5,2 : C2H4-63Cu-35Cl v=0 3 1 3 3.5 2 - v=0 2 1 2 2.5 2 : 40:<LineList>
1 B1 8	0 B2 2	11458.9800	11458.9891	-0.0091 1	4.1e-5	0 : qR1,2(2)2.5,1,1.5,0 : C2H4-63Cu-35Cl v=0 3 1 3 2.5 1 - v=0 2 1 2 1.5 0 : 41:<LineList>

1 B1 8	1 B2 5	11458.9800	11458.9894	-0.0094 1	1.4e-5	0 : qR1,2(2)2.5,1,1.5,1 : C2H4-63Cu-35Cl v=0 3 1 3 2.5 1 -v=0 2 1 2 1.5 1 : 42:<LineList>
3 B1 9	3 B2 4	11459.7730	11459.7617	0.0113 1	8.6e-5	0 : qR1,2(2)3.5,3,1.5,3 : C2H4-63Cu-35Cl v=0 3 1 3 3.5 3 -v=0 2 1 2 1.5 3 : 43:<LineList>
5 B1 3	5 B2 1	11460.3760	11460.3832	-0.0072 1	6.1e-5	0 : qR1,2(2)3.5,5,3,5,5 : C2H4-63Cu-35Cl v=0 3 1 3 3.5 5 -v=0 2 1 2 3.5 5 : 44:<LineList>
2 A2 4	2 A1 4	11597.9040	11597.9121	-0.0081 1	4.5e-5	0 : qR0,2(2)1.5,2,1.5,2 : C2H4-63Cu-35Cl v=0 3 0 3 1.5 2 -v=0 2 0 2 1.5 2 : 45:<LineList>
2 A2 4	3 A1 3	11597.9040	11597.9225	-0.0185 1	6.3e-5	0 : qR0,2(2)1.5,2,1.5,3 : C2H4-63Cu-35Cl v=0 3 0 3 1.5 2 -v=0 2 0 2 1.5 3 : 46:<LineList>
2 A2 4	1 A1 3	11597.9040	11597.9225	-0.0185 1	4.9e-5	0 : qR0,2(2)1.5,2,1.5,1 : C2H4-63Cu-35Cl v=0 3 0 3 1.5 2 -v=0 2 0 2 1.5 1 : 47:<LineList>
3 A2 3	3 A1 3	11601.1400	11601.1608	-0.0208 1	.00029	0 : qR0,2(2)1.5,3,1.5,3 : C2H4-63Cu-35Cl v=0 3 0 3 1.5 3 -v=0 2 0 2 1.5 3 : 48:<LineList>
2 A2 5	2 A1 5	11603.6080	11603.6193	-0.0113 1	8.7e-5	0 : qR0,2(2)2.5,2,2.5,2 : C2H4-63Cu-35Cl v=0 3 0 3 2.5 2 -v=0 2 0 2 2.5 2 : 49:<LineList>
4 A2 3	4 A1 2	11604.5800	11604.5851	-0.0051 1	.00043	0 : qR0,2(2)2.5,4,2.5,4 : C2H4-63Cu-35Cl v=0 3 0 3 2.5 4 -v=0 2 0 2 2.5 4 : 50:<LineList>
1 A2 5	1 A1 4	11605.6120	11605.6283	-0.0163 1	.00014	0 : qR0,2(2)2.5,1,2.5,1 : C2H4-63Cu-35Cl v=0 3 0 3 2.5 1 -v=0 2 0 2 2.5 1 : 51:<LineList>
5 A2 1	5 A1 1	11608.0170	11608.0098	0.0072 1	.00016	0 : qR0,2(2)4.5,5,3.5,5 : C2H4-63Cu-35Cl v=0 3 0 3 4.5 5 -v=0 2 0 2 3.5 5 : 52:<LineList>
3 A2 6	2 A1 5	11611.4670	11611.4711	-0.0041 1	.00075	0 : qR0,2(2)3.5,3,2.5,2 : C2H4-63Cu-35Cl v=0 3 0 3 3.5 3 -v=0 2 0 2 2.5 2 : 53:<LineList>
4 A2 4	3 A1 4	11611.8270	11611.8152	0.0118 1	.00129	0 : qR0,2(2)3.5,4,2.5,3 : C2H4-63Cu-35Cl v=0 3 0 3 3.5 4 -v=0 2 0 2 2.5 3 : 54:<LineList>
5 A2 1	4 A1 1	11612.5280	11612.5097	0.0183 1	.00175	0 : qR0,2(2)4.5,5,3.5,4 : C2H4-63Cu-35Cl v=0 3 0 3 4.5 5 -v=0 2 0 2 3.5 4 : 55:<LineList>
4 A2 2	3 A1 2	11612.5280	11612.5151	0.0129 1	.00136	0 : qR0,2(2)4.5,4,3.5,3 : C2H4-63Cu-35Cl v=0 3 0 3 4.5 4 -v=0 2 0 2 3.5 3 : 56:<LineList>
6 A2 1	5 A1 1	11612.8150	11612.8177	-0.0027 1	.00226	0 : qR0,2(2)4.5,6,3.5,5 : C2H4-63Cu-35Cl v=0 3 0 3 4.5 6 -v=0 2 0 2 3.5 5 : 57:<LineList>
3 A2 4	2 A1 3	11612.8500	11612.8612	-0.0112 1	.00107	0 : qR0,2(2)4.5,3,3.5,2 : C2H4-63Cu-35Cl v=0 3 0 3 4.5 3 -v=0 2 0 2 3.5 2 : 58:<LineList>
5 A2 2	4 A1 2	11613.0880	11613.0795	0.0085 1	.00167	0 : qR0,2(2)3.5,5,2.5,4 : C2H4-63Cu-35Cl v=0 3 0 3 3.5 5 -v=0 2 0 2 2.5 4 : 59:<LineList>
2 A2 6	1 A1 4	11613.4610	11613.4501	0.0109 1	.00052	0 : qR0,2(2)3.5,2,2.5,1 : C2H4-63Cu-35Cl v=0 3 0 3 3.5 2 -v=0 2 0 2 2.5 1 : 60:<LineList>
2 A2 4	2 A1 2	11614.1330	11614.1363	-0.0033 1	.00033	0 : qR0,2(2)1.5,2,0.5,2 : C2H4-63Cu-35Cl v=0 3 0 3 1.5 2 -v=0 2 0 2 0.5 2 : 61:<LineList>
2 A2 4	1 A1 2	11614.5140	11614.5194	-0.0054 1	.00036	0 : qR0,2(2)1.5,2,0.5,1 : C2H4-63Cu-35Cl v=0 3 0 3 1.5 2 -v=0 2 0 2 0.5 1 : 62:<LineList>
3 A2 5	2 A1 4	11614.7780	11614.7792	-0.0012 1	.00086	0 : qR0,2(2)2.5,3,1.5,2 : C2H4-63Cu-35Cl v=0 3 0 3 2.5 3 -v=0 2 0 2 1.5 2 : 63:<LineList>
2 A2 6	2 A1 5	11614.8870	11614.8829	0.0041 1	.00026	0 : qR0,2(2)3.5,2,2.5,2 : C2H4-63Cu-35Cl v=0 3 0 3 3.5 2 -v=0 2 0 2 2.5 2 : 64:<LineList>
2 A2 5	1 A1 3	11615.7110	11615.7112	-0.0002 1	.00044	0 : qR0,2(2)2.5,2,1.5,1 : C2H4-63Cu-35Cl v=0 3 0 3 2.5 2 -v=0 2 0 2 1.5 1 : 65:<LineList>
4 A2 3	3 A1 3	11616.6890	11616.6833	0.0057 1	.00102	0 : qR0,2(2)2.5,4,1.5,3 : C2H4-63Cu-35Cl v=0 3 0 3 2.5 4 -v=0 2 0 2 1.5 3 : 66:<LineList>
3 A2 3	2 A1 2	11617.3710	11617.3747	-0.0037 1	.0008	0 : qR0,2(2)1.5,3,0.5,2 : C2H4-63Cu-35Cl v=0 3 0 3 1.5 3 -v=0 2 0 2 0.5 2 : 67:<LineList>
1 A2 4	1 A1 2	11617.6720	11617.6765	-0.0045 1	.00027	0 : qR0,2(2)1.5,1,0.5,1 : C2H4-63Cu-35Cl v=0 3 0 3 1.5 1 -v=0 2 0 2 0.5 1 : 68:<LineList>
1 A2 5	0 A1 2	11619.1650	11619.1570	0.0080 1	.00016	0 : qR0,2(2)2.5,1,1.5,0 : C2H4-63Cu-35Cl v=0 3 0 3 2.5 1 -v=0 2 0 2 1.5 0 : 69:<LineList>
1 A2 5	1 A1 3	11619.1650	11619.1529	0.0121 1	.00013	0 : qR0,2(2)2.5,1,1.5,1 : C2H4-63Cu-35Cl v=0 3 0 3 2.5 1 -v=0 2 0 2 1.5 1 : 70:<LineList>
5 A2 2	5 A1 1	11628.2490	11628.2483	0.0007 1	.00022	0 : qR0,2(2)3.5,5,3.5,5 : C2H4-63Cu-35Cl v=0 3 0 3 3.5 5 -v=0 2 0 2 3.5 5 : 71:<LineList>
3 A2 6	3 A1 2	11629.6070	11629.6258	-0.0188 1	.00011	0 : qR0,2(2)3.5,3,3.5,3 : C2H4-63Cu-35Cl v=0 3 0 3 3.5 3 -v=0 2 0 2 3.5 3 : 72:<LineList>
4 A2 4	4 A1 1	11629.9780	11629.9830	-0.0050 1	.00019	0 : qR1,1(2)1.5,3,4,3.5,4 : C2H4-63Cu-35Cl v=0 3 0 3 3.5 4 -v=0 2 0 2 3.5 4 : 73:<LineList>
3 B2 6	3 B1 4	11760.2810	11760.2854	-0.0044 1	9.1e-5	0 : qR1,1(2)1.5,3,1.5,3 : C2H4-63Cu-35Cl v=0 3 1 2 1.5 3 -v=0 2 1 1 1.5 3 : 74:<LineList>
4 B2 5	4 B1 3	11767.7630	11767.7685	-0.0055 1	.00013	0 : qR1,1(2)2.5,4,2.5,4 : C2H4-63Cu-35Cl v=0 3 1 2 2.5 4 -v=0 2 1 1 2.5 4 : 75:<LineList>
5 B2 2	4 B1 2	11771.0880	11771.0906	-0.0026 1	.00055	0 : qR1,1(2)4.5,5,3.5,4 : C2H4-63Cu-35Cl v=0 3 1 2 4.5 5 -v=0 2 1 1 3.5 4 : 76:<LineList>
4 B2 4	3 B1 3	11771.4250	11771.4128	0.0122 1	.00043	0 : qR1,1(2)4.5,4,3.5,3 : C2H4-63Cu-35Cl v=0 3 1 2 4.5 4 -v=0 2 1 1 3.5 3 : 77:<LineList>
2 B2 8	2 B1 4	11771.7730	11771.7669	0.0061 1	1e-4	0 : qR1,1(2)1.5,2,0.5,2 : C2H4-63Cu-35Cl v=0 3 1 2 1.5 2 -v=0 2 1 1 0.5 2 : 78:<LineList>
2 B2 8	1 B1 4	11771.8500	11771.8393	0.0107 1	.0001	0 : qR1,1(2)1.5,2,0.5,1 : C2H4-63Cu-35Cl v=0 3 1 2 1.5 2 -v=0 2 1 1 0.5 1 : 79:<LineList>
4 B2 4	4 B1 2	11772.0330	11772.0317	0.0013 1	4.9e-5	0 : qR1,1(2)4.5,4,3.5,4 : C2H4-63Cu-35Cl v=0 3 1 2 4.5 4 -v=0 2 1 1 3.5 4 : 80:<LineList>
6 B2 1	5 B1 1	11772.4170	11772.4134	0.0036 1	.0007	0 : qR1,1(2)4.5,6,3.5,5 : C2H4-63Cu-35Cl v=0 3 1 2 4.5 6 -v=0 2 1 1 3.5 5 : 81:<LineList>
3 B2 7	2 B1 5	11772.6740	11772.6674	0.0066 1	.00034	0 : qR1,1(2)4.5,3,3.5,2 : C2H4-63Cu-35Cl v=0 3 1 2 4.5 3 -v=0 2 1 1 3.5 2 : 82:<LineList>
3 B2 6	2 B1 4	11773.8360	11773.8465	-0.0105 1	.00026	0 : qR1,1(2)1.5,3,0.5,2 : C2H4-63Cu-35Cl v=0 3 1 2 1.5 3 -v=0 2 1 1 0.5 2 : 83:<LineList>
4 B2 6	3 B1 5	11775.0920	11775.0817	0.0103 1	.00039	0 : qR1,1(2)3.5,4,2.5,3 : C2H4-63Cu-35Cl v=0 3 1 2 3.5 4 -v=0 2 1 1 2.5 3 : 84:<LineList>
3 B2 9	2 B1 7	11775.4440	11775.4335	0.0105 1	.00025	0 : qR1,1(2)3.5,3,2.5,2 : C2H4-63Cu-35Cl v=0 3 1 2 3.5 3 -v=0 2 1 1 2.5 2 : 85:<LineList>
3 B2 9	3 B1 5	11775.8730	11775.8744	-0.0014 1	6.9e-5	0 : qR1,1(2)3.5,3,2.5,3 : C2H4-63Cu-35Cl v=0 3 1 2 3.5 3 -v=0 2 1 1 2.5 3 : 86:<LineList>
3 B2 8	2 B1 6	11776.2500	11776.2500	0.0000 1	.00025	0 : qR1,1(2)2.5,3,1.5,2 : C2H4-63Cu-35Cl v=0 3 1 2 2.5 3 -v=0 2 1 1 1.5 2 : 87:<LineList>
5 B2 3	4 B1 3	11776.4000	11776.3996	0.0004 1	.00051	0 : qR1,1(2)3.5,5,2.5,4 : C2H4-63Cu-35Cl v=0 3 1 2 3.5 5 -v=0 2 1 1 2.5 4 : 88:<LineList>
4 B2 5	3 B1 4	11777.6810	11777.6793	0.0017 1	.00035	0 : qR1,1(2)2.5,4,1.5,3 : C2H4-63Cu-35Cl v=0 3 1 2 2.5 4 -v=0 2 1 1 1.5 3 : 89:<LineList>
4 B2 6	4 B1 2	11789.3490	11789.3596	-0.0106 1	6.2e-5	0 : qR1,1(2)3.5,4,3.5,4 : C2H4-63Cu-35Cl v=0 3 1 2 3.5 4 -v=0 2 1 1 3.5 4 : 90:<LineList>
3 B2 9	3 B1 3	11789.5250	11789.5333	-0.0083 1	4.1e-5	0 : qR1,1(2)3.5,3,3.5,3 : C2H4-63Cu-35Cl v=0 3 1 2 3.5 3 -v=0 2 1 1 3.5 3 : 91:<LineList>
5 B2 3	5 B1 1	11789.6030	11789.6190	-0.0160 1	7.3e-5	0 : qR1,1(2)3.5,5,3.5,5 : C2H4-63Cu-35Cl v=0 3 1 2 3.5 5 -v=0 2 1 1 3.5 5 : 92:<LineList>
3 B2 10	3 B1 6	15269.4110	15269.4046	0.0064 1	8.8e-5	0 : qR1,3(3)2.5,3,1.5,3 : C2H4-63Cu-35Cl v=0 4 1 4 2.5 3 -v=0 3 1 3 1.5 3 : 93:<LineList>
2 B2 11	1 B1 7	15271.4230	15271.4398	-0.0168 1	.00016	0 : qR1,3(3)2.5,2,1.5,1 : C2H4-63Cu-35Cl v=0 4 1 4 2.5 2 -v=0 3 1 3 1.5 1 : 94:<LineList>
3 B2 10	2 B1 8	15271.9500	15271.9426	0.0074 1	.00027	0 : qR1,3(3)2.5,3,1.5,2 : C2H4-63Cu-35Cl v=0 4 1 4 2.5 3 -v=0 3 1 3 1.5 2 : 95:<LineList>
6 B2 2	5 B1 2	15272.0050	15272.0050	-0.0000 1	.00066	0 : qR1,3(3)5.5,6,4.5,5 : C2H4-63Cu-35Cl v=0 4 1 4 5.5 6 -v=0 3 1 3 4.5 5 : 96:<LineList>
5 B2 4	4 B1 4	15272.0050	15271.9993	0.0057 1	.00055	0 : qR1,3(3)5.5,5,4.5,4 : C2H4-63Cu-35Cl v=0 4 1 4 5.5 5 -v=0 3 1 3 4.5 4 : 97:<LineList>
7 B2 1	6 B1 1	15272.6100	15272.6001	0.0099 1	.00081	0 : qR1,3(3)5.5,7,4.5,6 : C2H4-63Cu-35Cl v=0 4 1 4 5.5 7 -v=0 3 1 3 4.5 6 : 98:<LineList>
4 B2 8	3 B1 7	15272.8010	15272.7909	0.0101 1	.00045	0 : qR1,3(3)5.5,4,4.5,3 : C2H4-63Cu-35Cl v=0 4 1 4 5.5 4 -v=0 3 1 3 4.5 3 : 99:<LineList>
4 B2 10	3 B1 9	15272.9780	15272.9720	0.0060 1	.00036	0 : qR1,3(3)4.5,4,3.5,3 : C2H4-63Cu-35Cl v=0 4 1 4 4.5 4 -v=0 3 1 3 3.5 3 : 100:<LineList>
4 B2 7	3 B1 6	15273.1360	15273.1328	0.0032 1	.00038	0 : qR1,3(3)2.5,4,1.5,3 : C2H4-63Cu-35Cl v=0 4 1 4 2.5 4 -v=0 3 1 3 1.5 3 : 101:<LineList>
4 B2 9	3 B1 8	15273.2800	15273.2734	0.0066 1	.00043	0 : qR1,3(3)3.5,4,2.5,3 : C2H4-63Cu-35Cl v=0 4 1 4 3.5 4 -v=0 3 1 3 2.5 3 : 102:<LineList>
3 B2 11	2 B1 9	15273.4920	15273.4896	0.0024 1	.00028	0 : qR1,3(3)3.5,3,2.5,2 : C2H4-63Cu-35Cl v=0 4 1 4 3.5 3 -v=0 3 1 3 2.5 2 : 103:<LineList>
5 B2 5	4 B1 5	15273.8200	15273.8102	0.0098 1	.00043	0 : qR1,3(3)4.5,5,2.5,4 : C2H4-63Cu-35Cl v=0 4 1 4 4.5 5 -v=0 3 1 3 2.5 4 : 104:<LineList>
5 B2 6	4 B1 6	15273.9390	15273.9290	0.0100 1	.00055	0 : qR1,3(3)3.5,5,3.5,4 : C2H4-63Cu-35Cl v=0 4 1 4 3.5 5 -v=0 3 1 3 3.5 4 : 105:<LineList>
3 B2 12	2 B1 10	15274.1470	15274.1418	0.0052 1	.00028	0 : qR1,3(3)4.5,3,3.5,2 : C2H4-63Cu-35Cl v=0 4 1 4 4.5 3 -v=0 3 1 3 3.5 2 : 106:<LineList>
6 B2 3	5 B1 3	15274.2540	15274.2469	0.0071 1	.00065	0 : qR1,3(3)4.5,6,3.5,5 : C2H4-63Cu-35Cl v=0 4 1 4 4.5 6 -v=0 3 1 3 3.5 5 : 107:<LineList>
2 B2 12	1 B1 8	15274.4800	15274.4784	0.0016 1	.00017	0 : qR1,3(3)3.5,2,2.5,1 : C2H4-63Cu-35Cl v=0 4 1 4 3.5 2 -v=0 3 1 3 2.5 1 : 108:<LineList>
3 B2 12	3 B1 9	15276.7470	15276.7544	-0.0074 1	8.5e-5	0 : qR1,3(3)4.5,3,3.5,3 : C2H4-63Cu-35Cl v=0 4 1 4 4.5 3 -v=0 3 1 3 3.5 3 : 109:<LineList>
4 B2 10	4 B1 5	15276.8740	15276.8932	-0.0192 1	5.2e-5	0 : qR1,3(3)4.5,4,2.5,4 : C2H4-63Cu-35Cl v=0 4 1 4 4.5 4 -v=0 3 1 3 2.5 4 : 110:<LineList>
5 B2 5	5 B1 2	15279.3920	15279.4111	-0.0191 1	5e-5	0 : qR1,3(3)4.5,5,4.5,5 : C2H4-63Cu-35Cl v=0 4 1 4 4.5 5 -v=0 3 1 3 4.5 5 : 111:<LineList>
6 B2 3	6 B1 1	15280.3370	15280.3391	-0.0021 1	4.7e-5	0 : qR1,3(3)4.5,6,4.5,6 : C2H4-63Cu-35Cl v=0 4 1 4 4.5 6 -v=0 3 1 3 4.5 6 : 112:<LineList>
4 B2 10	4 B1 4	15281.1750	15281.1886	-0.0136 1	3.5e-5	0 : qR1,3(3)4.5,4,4.5,4 : C2H4-63Cu-35Cl v=0 4 1 4 4.5 4 -v=0 3 1 3 4.5 4 : 113:<LineList>
3 A1 5	3 A2 5	15466.7980	15466.7884	0.0096 1	6.2e-5	0 : qR0,3(3)2.5,3,2.5,3 : C2H4-63Cu-35Cl v=0 4 0 4 2.5 3 -v=0 3 0 3 2.5 3 : 114:<LineList>
2 A1 6	2 A2 5	15468.1230	15468.1200	0.0030 1	7.1e-5	0 : qR0,3(3)2.5,2,2.5,2 : C2H4-63Cu-35Cl v=0 4 0 4 2.5 2 -v=0 3 0 3 2.5 2 : 115:<LineList>
4 A1 3	4 A2 3	15469.0150	15469.0264	-0.0114 1	.0002	0 : qR0,3(3)2.5,4,2.5,4 : C2H4-63Cu-35Cl v=0 4 0 4 2.5 4 -v=0 3 0 3 2.5 4 : 116:<LineList>
1 A1 5	1 A2 5	15469.1710	15469.1870	-0.0160 1	7.9e-5	0 : qR0,3(3)2.5,1,2.5,1 : C2H4-63Cu-35Cl v=0 4 0 4 2.5 1 -v=0 3 0 3 2.5 1 : 117:<LineList>
5 A1 3	5 A2 2	15475.5810	15475.5685	0.0125 1	.00032	0 : qR0,3(3)3.5,5,3.5,5 : C2H4-63Cu-35Cl v=0 4 0 4 3.5 5 -v=0 3 0 3 3.5 5 : 118:<LineList>
2 A1 7	2 A2 6	15476.4240	15476.4401	-0.0161 1	.00015	0 : qR0,3(3)3.5,2,3.5,2 : C2H4-63Cu-35Cl v=0 4 0 4 3.5 2 -v=0 3 0 3 3.5 2 : 11

7 A1 1	6 A2 1	15482.2890	15482.2860	0.0030 1	.00252	0 : qR0,3(3)5.5,7,4.5,6 : C2H4-63Cu-35Cl v=0 4 0 4 5.5 7 - v=0 3 0 3 4.5 6 : 126:<LineList>
6 A1 2	5 A2 2	15482.3780	15482.3815	-0.0035 1	.00202	0 : qR0,3(3)4.5,6,3.5,5 : C2H4-63Cu-35Cl v=0 4 0 4 4.5 6 - v=0 3 0 3 3.5 5 : 127:<LineList>
2 A1 6	1 A2 4	15482.7580	15482.7515	0.0065 1	.00048	0 : qR0,3(3)2.5,2,1.5,1 : C2H4-63Cu-35Cl v=0 4 0 4 2.5 2 - v=0 3 0 3 1.5 1 : 128:<LineList>
4 A1 5	3 A2 5	15483.3300	15483.3337	-0.0037 1	.00125	0 : qR0,3(3)3.5,4,2.5,3 : C2H4-63Cu-35Cl v=0 4 0 4 3.5 4 - v=0 3 0 3 2.5 3 : 129:<LineList>
3 A1 6	2 A2 5	15483.3750	15483.3823	-0.0073 1	.00087	0 : qR0,3(3)3.5,3,2.5,2 : C2H4-63Cu-35Cl v=0 4 0 4 3.5 3 - v=0 3 0 3 2.5 2 : 130:<LineList>
5 A1 2	5 A2 1	15483.4370	15483.4465	-0.0095 1	.00012	0 : qR0,3(3)5.5,5,4.5,5 : C2H4-63Cu-35Cl v=0 4 0 4 5.5 5 - v=0 3 0 3 4.5 5 : 131:<LineList>
1 A1 5	0 A2 2	15483.5250	15483.5399	-0.0149 1	.00022	0 : qR0,3(3)2.5,1,1.5,0 : C2H4-63Cu-35Cl v=0 4 0 4 2.5 1 - v=0 3 0 3 1.5 0 : 132:<LineList>
3 A1 5	2 A2 4	15483.6630	15483.6555	0.0075 1	.00084	0 : qR0,3(3)2.5,3,1.5,2 : C2H4-63Cu-35Cl v=0 4 0 4 2.5 3 - v=0 3 0 3 1.5 2 : 133:<LineList>
5 A1 3	4 A2 3	15484.0840	15484.0629	0.0211 1	.00143	0 : qR0,3(3)3.5,5,2.5,4 : C2H4-63Cu-35Cl v=0 4 0 4 3.5 5 - v=0 3 0 3 2.5 4 : 134:<LineList>
2 A1 7	1 A2 5	15484.2750	15484.2619	0.0131 1	.00056	0 : qR0,3(3)3.5,2,2.5,1 : C2H4-63Cu-35Cl v=0 4 0 4 3.5 2 - v=0 3 0 3 2.5 1 : 135:<LineList>
4 A1 3	3 A2 3	15484.5550	15484.5490	0.0060 1	.00126	0 : qR0,3(3)2.5,4,1.5,3 : C2H4-63Cu-35Cl v=0 4 0 4 2.5 4 - v=0 3 0 3 1.5 3 : 136:<LineList>
3 A1 7	3 A2 6	15485.6280	15485.6085	0.0195 1	.0002	0 : qR0,3(3)4.5,3,3.5,3 : C2H4-63Cu-35Cl v=0 4 0 4 4.5 3 - v=0 3 0 3 3.5 3 : 137:<LineList>
2 A1 6	2 A2 4	15485.9020	15485.9087	-0.0067 1	.00023	0 : qR0,3(3)2.5,2,1.5,2 : C2H4-63Cu-35Cl v=0 4 0 4 2.5 2 - v=0 3 0 3 1.5 2 : 138:<LineList>
1 A1 5	1 A2 4	15487.2690	15487.2603	0.0087 1	.00016	0 : qR0,3(3)2.5,1,1.5,1 : C2H4-63Cu-35Cl v=0 4 0 4 2.5 1 - v=0 3 0 3 1.5 1 : 139:<LineList>
5 A1 3	5 A2 1	15495.7820	15495.8069	-0.0249 1	5.7e-5	0 : qR0,3(3)3.5,5,4.5,5 : C2H4-63Cu-35Cl v=0 4 0 4 3.5 5 - v=0 3 0 3 4.5 5 : 140:<LineList>
6 A1 2	6 A2 1	15497.8080	15497.8121	-0.0041 1	.00016	0 : qR0,3(3)4.5,6,4.5,6 : C2H4-63Cu-35Cl v=0 4 0 4 4.5 6 - v=0 3 0 3 4.5 6 : 141:<LineList>
4 A1 6	4 A2 2	15498.5430	15498.5463	-0.0033 1	.00011	0 : qR0,3(3)4.5,4,4.5,4 : C2H4-63Cu-35Cl v=0 4 0 4 4.5 4 - v=0 3 0 3 4.5 4 : 142:<LineList>
5 A1 4	5 A2 1	15499.4530	15499.4620	-0.0090 1	.00011	0 : qR0,3(3)4.5,5,4.5,5 : C2H4-63Cu-35Cl v=0 4 0 4 4.5 5 - v=0 3 0 3 4.5 5 : 143:<LineList>
4 B1 9	4 B2 6	15691.1700	15691.1913	-0.0213 1	3.2e-5	0 : qR1,2(3)3.5,4,3.5,4 : C2H4-63Cu-35Cl v=0 4 1 3 3.5 4 - v=0 3 1 2 3.5 4 : 144:<LineList>
5 B1 5	5 B2 3	15691.5870	15691.6036	-0.0166 1	9.8e-5	0 : qR1,2(3)3.5,5,3.5,5 : C2H4-63Cu-35Cl v=0 4 1 3 3.5 5 - v=0 3 1 2 3.5 5 : 145:<LineList>
5 B1 4	4 B2 4	15696.5750	15696.5722	0.0028 1	.00056	0 : qR1,2(3)5.5,5,4.5,4 : C2H4-63Cu-35Cl v=0 4 1 3 5.5 5 - v=0 3 1 2 4.5 4 : 146:<LineList>
6 B1 2	5 B2 2	15696.5750	15696.5704	0.0046 1	.00068	0 : qR1,2(3)5.5,6,4.5,5 : C2H4-63Cu-35Cl v=0 4 1 3 5.5 6 - v=0 3 1 2 4.5 5 : 147:<LineList>
7 B1 1	6 B2 1	15697.1670	15697.1697	-0.0027 1	.00082	0 : qR1,2(3)5.5,7,4.5,6 : C2H4-63Cu-35Cl v=0 4 1 3 5.5 7 - v=0 3 1 2 4.5 6 : 148:<LineList>
4 B1 8	3 B2 7	15697.1850	15697.1877	-0.0027 1	.00047	0 : qR1,2(3)5.5,4,4.5,3 : C2H4-63Cu-35Cl v=0 4 1 3 5.5 4 - v=0 3 1 2 4.5 3 : 149:<LineList>
2 B1 11	1 B2 7	15697.4550	15697.4662	-0.0112 1	.00015	0 : qR1,2(3)2.5,2,1.5,1 : C2H4-63Cu-35Cl v=0 4 1 3 2.5 2 - v=0 3 1 2 1.5 1 : 150:<LineList>
3 B1 10	2 B2 8	15697.8250	15697.8244	0.0006 1	.00027	0 : qR1,2(3)2.5,3,1.5,2 : C2H4-63Cu-35Cl v=0 4 1 3 2.5 3 - v=0 3 1 2 1.5 2 : 151:<LineList>
4 B1 10	3 B2 9	15698.0220	15698.0126	0.0094 1	.00039	0 : qR1,2(3)4.5,4,3.5,3 : C2H4-63Cu-35Cl v=0 4 1 3 4.5 4 - v=0 3 1 2 3.5 3 : 152:<LineList>
5 B1 6	4 B2 6	15698.0940	15698.0874	0.0066 1	.00054	0 : qR1,2(3)4.5,5,3.5,4 : C2H4-63Cu-35Cl v=0 4 1 3 4.5 5 - v=0 3 1 2 3.5 4 : 153:<LineList>
1 B1 9	0 B2 3	15698.4240	15698.4419	-0.0179 1	7.1e-5	0 : qR1,2(3)2.5,1,1.5,0 : C2H4-63Cu-35Cl v=0 4 1 3 2.5 1 - v=0 3 1 2 1.5 0 : 154:<LineList>
4 B1 7	3 B2 6	15698.8000	15698.8059	-0.0059 1	.00041	0 : qR1,2(3)2.5,4,1.5,3 : C2H4-63Cu-35Cl v=0 4 1 3 2.5 4 - v=0 3 1 2 1.5 3 : 155:<LineList>
6 B1 3	5 B2 3	15698.8320	15698.8229	0.0091 1	.00066	0 : qR1,2(3)4.5,6,3.5,5 : C2H4-63Cu-35Cl v=0 4 1 3 4.5 6 - v=0 3 1 2 3.5 5 : 156:<LineList>
3 B1 12	2 B2 10	15698.9050	15698.9010	0.0040 1	.0003	0 : qR1,2(3)4.5,3,3.5,2 : C2H4-63Cu-35Cl v=0 4 1 3 4.5 3 - v=0 3 1 2 3.5 2 : 157:<LineList>
4 B1 9	3 B2 8	15699.3360	15699.3307	0.0053 1	.00039	0 : qR1,2(3)3.5,4,2.5,3 : C2H4-63Cu-35Cl v=0 4 1 3 3.5 4 - v=0 3 1 2 2.5 3 : 158:<LineList>
3 B1 11	2 B2 9	15699.4500	15699.4461	0.0039 1	.00028	0 : qR1,2(3)3.5,3,2.5,2 : C2H4-63Cu-35Cl v=0 4 1 3 3.5 3 - v=0 3 1 2 2.5 2 : 159:<LineList>
5 B1 5	4 B2 5	15700.2370	15700.2347	0.0023 1	.0005	0 : qR1,2(3)3.5,5,2.5,4 : C2H4-63Cu-35Cl v=0 4 1 3 3.5 5 - v=0 3 1 2 2.5 4 : 160:<LineList>
2 B1 12	1 B2 8	15700.4910	15700.4811	0.0099 1	.00018	0 : qR1,2(3)3.5,2,2.5,1 : C2H4-63Cu-35Cl v=0 4 1 3 3.5 2 - v=0 3 1 2 2.5 1 : 161:<LineList>
1 B1 9	1 B2 7	15700.6960	15700.6894	0.0066 1	5.8e-5	0 : qR1,2(3)2.5,1,1.5,1 : C2H4-63Cu-35Cl v=0 4 1 3 2.5 1 - v=0 3 1 2 1.5 1 : 162:<LineList>
3 A1 4	3 A2 1	7759.3400	7759.3393	0.0007 1	.00021	0 : qR0,1(1)2.5,3,2.5,3 : C2H4-63Cu-35Cl v=0 2 0 2 2.5 3 - v=0 1 0 1 2.5 3 : 163:<LineList>
2 A1 4	1 A2 1	7759.1770	7759.1653	0.0117 1	.0001	0 : qR0,1(1)1.5,2,0.5,1 : C2H4-63Cu-35Cl v=0 2 0 2 1.5 2 - v=0 1 0 1 0.5 1 : 164:<LineList>
1 A1 3	1 A2 1	7759.1580	7759.1549	0.0031 1	9.3e-5	0 : qR0,1(1)1.5,1,0.5,1 : C2H4-63Cu-35Cl v=0 2 0 2 1.5 1 - v=0 1 0 1 0.5 1 : 165:<LineList>
3 A1 6	3 A2 5	15484.3000	15484.3039	-0.0039 1	.00014	0 : qR0,3(3)3.5,3,2.5,3 : C2H4-63Cu-35Cl v=0 4 0 4 3.5 3 - v=0 3 0 3 2.5 3 : 166:<LineList>

166 Observations, 9 Parameters

Initial Average Error: 0.0103174975711399

Predicted New Error: 0.0102820729838627

Parameters:

# Old	New	Std Dev	Change/Std Sens	Summary	Name
1 23920.3429096552	23910.7763922414	56.312671	-0.1699 1.37254	23911(56)	C2H4-63Cu-35Cl v=0 A
2 1988.93165476155	1988.93172424278	.00062015	0.1120 3.26e-5	1988.93172(62)	C2H4-63Cu-35Cl v=0 B
3 1882.69416025887	1882.69423780182	.00061595	0.1259 3.12e-5	1882.69424(62)	C2H4-63Cu-35Cl v=0 C
4 .0194038016596251	.0194922749350283	.00083221	0.1063 2.28e-5	0.01949(83)	C2H4-63Cu-35Cl v=0 DJK
5 .0002678763750342	.000265888579922705	3.0623e-5	-0.0649 6.27e-7	2.66(31)e-4	C2H4-63Cu-35Cl v=0 DJ
6 63.776258849643	63.777701101865	.00895563	0.1610 .00117	63.7777(90)	C2H4-63Cu-35Cl Copper CHlzz
7 -44.505579698344	-44.5210136416758	.03021206	-0.5109 .004073	-44.521(30)	C2H4-63Cu-35Cl Copper CHlxxmyy
8 -20.9938683685614	-20.9918244490368	.01282979	0.1593 .001656	-20.992(13)	C2H4-63Cu-35Cl Chlorine CHlzz
9 -5.12019498024267	-5.09347060558684	.03931498	0.6798 .005456	-5.093(39)	C2H4-63Cu-35Cl Chlorine CHlxxmyy

Correlation Matrix

1	2	3	4	5	6	7	8	9
1 1.000								
2 -0.457	1.000							
3 -0.483	0.427	1.000						
4 -0.957	0.487	0.512	1.000					
5 0.862	-0.066	-0.095	-0.834	1.000				
6 0.015	-0.061	-0.103	0.003	-0.040	1.000			
7 0.073	0.148	-0.119	-0.045	0.100	-0.032	1.000		
8 0.055	-0.120	-0.097	-0.045	-0.013	0.387	-0.010	1.000	
9 -0.035	0.030	0.001	0.028	-0.032	-0.073	0.144	-0.188	1.000

¹²C₄H₄---⁶⁵Cu³⁵Cl (Page 1 of 2)

Pgopher 8.0.102 08 Dec 2013 16:55 32 bit (Delphi 18.5/18)

Mixture: 12C2 H4 --- 65Cu 35Cl Chirped-Pulse.pgo

Units MHz
PrintLevel Detail
Precision 4
BasisOrder boDefault
QuantumNumberFormat J
FitCycles 1
FitDetails False
AutoReplot True
AllowComplex False
NoLineList False
ShowEstUnc False
ShowDerivatives False
SVDlimit 5
SVDThresh 1E-15
ScaleChanges 1
Species: C2H4-Cu-Cl
Jmax 30
Concentration 1
AsymmetricMolecule: C2H4-Cu-Cl 12CH4---65Cu35Cl
nNuclei 2
Jmax 30
Colour \$C080FF
JAdjustSym False
BlockMatrix True
PointGroup C2v
Representation Ir
SReduction False
eeWt 1
eoWt 1
oeWt 1
ooWt 1
C2zAxis a
C2xAxis c
PseudoC2v False
FakeSym False
PhaseAdjust False
Abundance 1

AsymmetricManifold: C2H4-Cu-Cl 12CH4---65Cu35Cl Ground

Jmax 30
Initial True
EigenSearch True
LimitSearch True
AutoQConverge True
UsePopParams False
AsymmetricTop: C2H4-Cu-Cl 12CH4---65Cu35Cl v=0
Symmetry A1
Kmin all
Kmax all
A 24219.592950298 Float
B 1988.62175773136 Float
C 1882.41547839413 Float
DJK 0.0155903168771076 Float
DJ 0.000385929835526979 Float
AsymmetricTopNucleus: C2H4-Cu-Cl 12CH4---65Cu35Cl Copper
Spin 1.5
AsNext False
CHlzz 59.056998856698 Float
CHlxmymy -41.3918067112445 Float
AsymmetricTopNucleus: C2H4-Cu-Cl 12CH4---65Cu35Cl Chlorine
Spin 1.5
AsNext False
CHlzz -20.992112373059 Float
CHlxmymy -4.99384595601583 Float
<N ,K |A|N,K> = K^2
<N ,K-2|B|N,K> = sqrt((N*(N+1)+(-K+1)*(K-2))*(N*(N+1)-K*(K-1)))/4
<N ,K |B|N,K> = (N*(N+1)-K^2)/2
<N ,K+2|B|N,K> = sqrt((N*(N+1)+(-K-1)*(K+2))*(N*(N+1)-K*(K+1)))/4
<N ,K-2|C|N,K> = (-sqrt((N*(N+1)+(-K+1)*(K-2))*(N*(N+1)-K*(K-1)))/4
<N ,K |C|N,K> = (N*(N+1)-K^2)/2
<N ,K+2|C|N,K> = (-sqrt((N*(N+1)+(-K-1)*(K+2))*(N*(N+1)-K*(K+1)))/4
<N ,K |DJK|N,K> = -N*(N+1)*K^2
<N ,K |DJ|N,K> = -N^2*(N+1)^2
TransitionMoments: C2H4-Cu-Cl 12CH4---65Cu35Cl <Ground|mu|Ground>
CartesianTransitionMoment: C2H4-Cu-Cl 12CH4---65Cu35Cl <v=0|a|v=0>
Axis a
Strength 1
Symbolic Matrix Elements not available for <v=0|a|v=0>

Residuals before fit for 12CH4---65Cu35Cl for the Ground manifold

J"S" #"	J"S" #"	Observed	Calculated	Obs-Calc	StdDev	
4 B2 3	3 B1 1	7647.8740	7647.8631	0.0109 1	.00018	0 : qR1,1(1)2.5,4,1.5,3 : 12CH4---65Cu35Cl v=0 2 1 2 2.5 4 - v=0 1 1 1 1.5 3 : 1:<LineList>
1 A1 3	2 A2 3	7727.0230	7727.0166	0.0064 1	1e-4	0 : qR0,1(1)1.5,1,1.5,2 : 12CH4---65Cu35Cl v=0 2 0 2 1.5 1 - v=0 1 0 1 1.5 2 : 2:<LineList>
2 A1 4	2 A2 3	7727.0320	7727.0258	0.0062 1	7.1e-5	0 : qR0,1(1)1.5,2,1.5,2 : 12CH4---65Cu35Cl v=0 2 0 2 1.5 2 - v=0 1 0 1 1.5 2 : 3:<LineList>
3 A1 3	3 A2 2	7730.3550	7730.3455	0.0095 1	.00035	0 : qR0,1(1)1.5,3,1.5,3 : 12CH4---65Cu35Cl v=0 2 0 2 1.5 3 - v=0 1 0 1 1.5 3 : 4:<LineList>
3 A1 4	2 A2 3	7736.8100	7736.8085	0.0015 1	.00046	0 : qR0,1(1)2.5,3,1.5,2 : 12CH4---65Cu35Cl v=0 2 0 2 2.5 3 - v=0 1 0 1 1.5 2 : 5:<LineList>
4 A1 1	3 A2 1	7740.1170	7740.1072	0.0098 1	.00087	0 : qR0,1(1)3.5,4,2.5,3 : 12CH4---65Cu35Cl v=0 2 0 2 3.5 4 - v=0 1 0 1 2.5 3 : 6:<LineList>
2 A1 3	1 A2 2	7740.7130	7740.7198	-0.0068 1	.00038	0 : qR0,1(1)3.5,2,2.5,1 : 12CH4---65Cu35Cl v=0 2 0 2 3.5 2 - v=0 1 0 1 2.5 1 : 7:<LineList>
5 A1 1	4 A2 1	7740.8810	7740.8781	0.0029 1	.00125	0 : qR0,1(1)3.5,5,2.5,4 : 12CH4---65Cu35Cl v=0 2 0 2 3.5 5 - v=0 1 0 1 2.5 4 : 8:<LineList>
4 A1 2	3 A2 2	7741.6160	7741.6194	-0.0034 1	.00076	0 : qR0,1(1)2.5,4,1.5,3 : 12CH4---65Cu35Cl v=0 2 0 2 2.5 4 - v=0 1 0 1 1.5 3 : 9:<LineList>
4 A1 2	4 A2 1	7754.8710	7754.8824	-0.0114 1	.00023	0 : qR0,1(1)2.5,4,2.5,4 : 12CH4---65Cu35Cl v=0 2 0 2 2.5 4 - v=0 1 0 1 2.5 4 : 10:<LineList>
3 A1 4	3 A2 1	7757.1320	7757.1422	-0.0102 1	.00021	0 : qR0,1(1)2.5,3,2.5,3 : 12CH4---65Cu35Cl v=0 2 0 2 2.5 3 - v=0 1 0 1 2.5 3 : 11:<LineList>
4 B1 2	3 B2 2	7841.0200	7841.0120	0.0080 1	.00021	0 : qR1,0(1)3.5,4,2.5,3 : 12CH4---65Cu35Cl v=0 2 1 1 3.5 4 - v=0 1 1 0 2.5 3 : 12:<LineList>
1 B1 5	1 B2 3	7845.0970	7845.0967	0.0003 1	3.1e-5	0 : qR1,0(1)1.5,1,0.5,1 : 12CH4---65Cu35Cl v=0 2 1 1 1.5 1 - v=0 1 1 0 0.5 1 : 13:<LineList>
5 B1 1	4 B2 1	7845.3950	7845.4048	-0.0098 1	.00033	0 : qR1,0(1)3.5,5,2.5,4 : 12CH4---65Cu35Cl v=0 2 1 1 3.5 5 - v=0 1 1 0 2.5 4 : 14:<LineList>
5 B1 2	4 B2 2	11451.4240	11451.4205	0.0035 1	.00051	0 : qR1,2(2)4.5,5,3.5,4 : 12CH4---65Cu35Cl v=0 3 1 3 4.5 5 - v=0 2 1 2 3.5 4 : 15:<LineList>
6 B1 1	5 B2 1	11452.7020	11452.6920	0.0100 1	.00068	0 : qR1,2(2)4.5,6,3.5,5 : 12CH4---65Cu35Cl v=0 3 1 3 4.5 6 - v=0 2 1 2 3.5 5 : 16:<LineList>
4 B1 5	3 B2 4	11453.9630	11453.9539	0.0091 1	.00022	0 : qR1,2(2)2.5,4,1.5,3 : 12CH4---65Cu35Cl v=0 3 1 3 2.5 4 - v=0 2 1 2 1.5 3 : 17:<LineList>
4 B1 6	3 B2 5	11455.2890	11455.3018	-0.0128 1	.00042	0 : qR1,2(2)3.5,4,2.5,3 : 12CH4---65Cu35Cl v=0 3 1 3 3.5 4 - v=0 2 1 2 2.5 3 : 18:<LineList>
5 B1 3	4 B2 3	11456.3300	11456.3286	0.0014 1	.00051	0 : qR1,2(2)3.5,5,2.5,4 : 12CH4---65Cu35Cl v=0 3 1 3 3.5 5 - v=0 2 1 2 2.5 4 : 19:<LineList>
2 B1 10	1 B2 6	11456.5890	11456.5929	-0.0039 1	.00013	0 : qR1,2(2)1.5,2,0.5,2 : 12CH4---65Cu35Cl v=0 3 1 3 3.5 2 - v=0 2 1 2 2.5 1 : 20:<LineList>
2 B1 10	2 B2 7	11456.8390	11456.8540	-0.0150 1	.0001	0 : qR1,2(2)3.5,2,2.5,2 : 12CH4---65Cu35Cl v=0 3 1 3 3.5 2 - v=0 2 1 2 2.5 2 : 21:<LineList>
3 A2 3	3 A1 3	11600.2970	11600.3187	-0.0217 1	.00029	0 : qR0,2(2)1.5,3,1.5,3 : 12CH4---65Cu35Cl v=0 3 0 3 1.5 3 - v=0 2 0 2 1.5 3 : 22:<LineList>
4 A2 3	4 A1 2	11603.3460	11603.3555	-0.0095 1	.00043	0 : qR0,2(2)2.5,4,2.5,4 : 12CH4 H4 --- 65Cu 35Cl v=0 3 0 3 2.5 4 - v=0 2 0 2 2.5 4 : 23:<LineList>
3 A2 6	2 A1 5	11609.7450	11609.7398	0.0052 1	.00075	0 : qR0,2(2)3.5,3,2.5,2 : 12CH4---65Cu35Cl v=0 3 0 3 3.5 3 - v=0 2 0 2 2.5 2 : 24:<LineList>
4 A2 4	3 A1 4	11610.1620	11610.1549	0.0071 1	.00129	0 : qR0,2(2)3.5,4,2.5,3 : 12CH4---65Cu35Cl v=0 3 0 3 3.5 4 - v=0 2 0 2 2.5 3 : 25:<LineList>
5 A2 1	4 A1 1	11610.8140	11610.8127	0.0013 1	.00175	0 : qR0,2(2)4.5,5,3.5,4 : 12CH4---65Cu35Cl v=0 3 0 3 4.5 5 - v=0 2 0 2 3.5 4 : 26:<LineList>
4 A2 2	3 A1 2	11610.8500	11610.8381	0.0119 1	.00136	0 : qR0,2(2)4.5,4,3.5,3 : 12CH4---65Cu35Cl v=0 3 0 3 4.5 4 - v=0 2 0 2 3.5 3 : 27:<LineList>
6 A2 1	5 A1 1	11611.1230	11611.1154	0.0076 1	.00226	0 : qR0,2(2)4.5,6,3.5,5 : 12CH4---65Cu35Cl v=0 3 0 3 4.5 6 - v=0 2 0 2 3.5 5 : 28:<LineList>
5 A2 2	4 A1 2	11611.3740	11611.3756	-0.0016 1	.00167	0 : qR0,2(2)3.5,5,2.5,4 : 12CH4---65Cu35Cl v=0 3 0 3 3.5 5 - v=0 2 0 2 2.5 4 : 29:<LineList>
2 A2 4	2 A1 2	11612.1430	11612.1549	-0.0119 1	.00034	0 : qR0,2(2)1.5,2,0.5,2 : 12CH4---65Cu35Cl v=0 3 0 3 1.5 2 - v=0 2 0 2 0.5 2 : 30:<LineList>
2 A2 5	1 A1 3	11613.6840	11613.6992	-0.0152 1	.00044	0 : qR0,2(2)2.5,2,1.5,1 : 12CH4---65Cu35Cl v=0 3 0 3 2.5 2 - v=0 2 0 2 1.5 1 : 31:<LineList>
4 A2 3	3 A1 3	11614.6250	11614.6294	-0.0044 1	.001	0 : qR0,2(2)2.5,4,1.5,3 : 12CH4---65Cu35Cl v=0 3 0 3 2.5 4 - v=0 2 0 2 1.5 3 : 32:<LineList>
3 A2 3	2 A1 2	11615.3760	11615.3765	-0.0005 1	.0008	0 : qR0,2(2)1.5,3,0.5,2 : 12CH4---65Cu35Cl v=0 3 0 3 1.5 3 - v=0 2 0 2 0.5 2 : 33:<LineList>
1 A2 5	1 A1 3	11617.1940	11617.1869	0.0071 1	.00013	0 : qR0,2(2)2.5,1,1.5,1 : 12CH4---65Cu35Cl v=0 3 0 3 2.5 1 - v=0 2 0 2 1.5 1 : 34:<LineList>
1 A2 5	0 A1 2	11617.1940	11617.1902	0.0038 1	.00016	0 : qR0,2(2)2.5,1,1.5,0 : 12CH4---65Cu35Cl v=0 3 0 3 2.5 1 - v=0 2 0 2 1.5 0 : 35:<LineList>
4 A2 3	4 A1 1	11621.8910	11621.8725	0.0185 1	5.6e-5	0 : qR0,2(2)2.5,4,3.5,4 : 12CH4---65Cu35Cl v=0 3 0 3 2.5 4 - v=0 2 0 2 3.5 4 : 36:<LineList>
4 A2 4	4 A1 1	11627.1900	11627.1899	0.0001 1	.00019	0 : qR0,2(2)3.5,4,3.5,4 : 12CH4---65Cu35Cl v=0 3 0 3 3.5 4 - v=0 2 0 2 3.5 4 : 37:<LineList>
4 B2 5	4 B1 3	11766.3820	11766.3906	-0.0086 1	.00013	0 : qR1,1(2)2.5,4,2.5,4 : 12CH4---65Cu35Cl v=0 3 1 2 2.5 4 - v=0 2 1 1 2.5 4 : 38:<LineList>
5 B2 2	4 B1 2	11769.4400	11769.4345	0.0055 1	.00055	0 : qR1,1(2)4.5,5,3.5,4 : 12CH4---65Cu35Cl v=0 3 1 2 4.5 5 - v=0 2 1 1 3.5 4 : 39:<LineList>
4 B2 4	3 B1 3	11769.7660	11769.7608	0.0052 1	.00043	0 : qR1,1(2)4.5,4,3.5,3 : 12CH4---65Cu35Cl v=0 3 1 2 4.5 4 - v=0 2 1 1 3.5 3 : 40:<LineList>
2 B2 8	2 B1 4	11770.0080	11770.0011	0.0069 1	9.9e-5	0 : qR1,1(2)1.5,2,0.5,2 : 12CH4---65Cu35Cl v=0 3 1 2 1.5 2 - v=0 2 1 1 0.5 2 : 41:<LineList>
6 B2 1	5 B1 1	11770.7670	11770.7591	0.0079 1	.0007	0 : qR1,1(2)4.5,6,3.5,5 : 12CH4---65Cu35Cl v=0 3 1 2 4.5 6 - v=0 2 1 1 3.5 5 : 42:<LineList>

¹²C₆H₆---⁶⁵Cu³⁵Cl continued (Page 2 of 2)

3 B2 7	2 B1 5	11771.0250	11771.0113	0.0137 1	.00034	0 : qR1,1(2)4.5,3,3.5,2 : 12CH4---65Cu35Cl v=0 3 1 2 4.5 3 -v=0 2 1 1 3.5 2 : 43:<LineList>
4 B2 6	3 B1 5	11773.1480	11773.1474	0.0006 1	.00039	0 : qR1,1(2)3.5,4,2.5,3 : 12CH4---65Cu35Cl v=0 3 1 2 3.5 4 -v=0 2 1 1 2.5 3 : 44:<LineList>
3 B2 9	2 B1 7	11773.4760	11773.4848	-0.0088 1	.00025	0 : qR1,1(2)3.5,3,2.5,2 : 12CH4---65Cu35Cl v=0 3 1 2 3.5 3 -v=0 2 1 1 2.5 2 : 45:<LineList>
3 B2 8	2 B1 6	11774.1960	11774.1943	0.0017 1	.00025	0 : qR1,1(2)2.5,3,1.5,2 : 12CH4---65Cu35Cl v=0 3 1 2 2.5 3 -v=0 2 1 1 1.5 2 : 46:<LineList>
5 B2 3	4 B1 3	11774.4430	11774.4535	-0.0105 1	.00051	0 : qR1,1(2)3.5,5,2.5,4 : 12CH4---65Cu35Cl v=0 3 1 2 3.5 5 -v=0 2 1 1 2.5 4 : 47:<LineList>
2 B2 9	1 B1 5	11774.8880	11774.8895	-0.0015 1	.00013	0 : qR1,1(2)2.5,2,1.5,1 : 12CH4---65Cu35Cl v=0 3 1 2 2.5 2 -v=0 2 1 1 1.5 1 : 48:<LineList>
2 B2 9	2 B1 6	11774.8880	11774.8959	-0.0079 1	6.3e-5	0 : qR1,1(2)2.5,2,1.5,2 : 12CH4---65Cu35Cl v=0 3 1 2 2.5 2 -v=0 2 1 1 1.5 2 : 49:<LineList>
4 B2 5	3 B1 4	11775.5960	11775.6067	-0.0107 1	.00034	0 : qR1,1(2)2.5,4,1.5,3 : 12CH4---65Cu35Cl v=0 3 1 2 2.5 4 -v=0 2 1 1 1.5 3 : 50:<LineList>
6 B2 2	5 B1 2	15269.7790	15269.7840	-0.0050 1	.00066	0 : qR1,3(3)5.5,6,4.5,5 : 12CH4---65Cu35Cl v=0 4 1 4 5.5 6 -v=0 3 1 3 4.5 5 : 51:<LineList>
5 B2 4	4 B1 4	15269.7790	15269.7865	-0.0075 1	.00055	0 : qR1,3(3)5.5,5,4.5,4 : 12CH4---65Cu35Cl v=0 4 1 4 5.5 5 -v=0 3 1 3 4.5 4 : 52:<LineList>
7 B2 1	6 B1 1	15270.3800	15270.3760	0.0040 1	.00081	0 : qR1,3(3)5.5,7,4.5,6 : 12CH4---65Cu35Cl v=0 4 1 4 5.5 7 -v=0 3 1 3 4.5 6 : 53:<LineList>
4 B2 8	3 B1 7	15270.5810	15270.5753	0.0057 1	.00044	0 : qR1,3(3)5.5,4,4.5,3 : 12CH4---65Cu35Cl v=0 4 1 4 5.5 4 -v=0 3 1 3 4.5 3 : 54:<LineList>
4 B2 10	3 B1 9	15270.6130	15270.6190	-0.0060 1	.00036	0 : qR1,3(3)4.5,4,3.5,3 : 12CH4---65Cu35Cl v=0 4 1 4 4.5 4 -v=0 3 1 3 3.5 3 : 55:<LineList>
4 B2 7	3 B1 6	15270.8960	15270.8932	0.0028 1	.00038	0 : qR1,3(3)2.5,4,1.5,3 : 12CH4---65Cu35Cl v=0 4 1 4 2.5 4 -v=0 3 1 3 1.5 3 : 56:<LineList>
4 B2 9	3 B1 8	15270.9300	15270.9252	0.0048 1	.00043	0 : qR1,3(3)3.5,4,2.5,3 : 12CH4---65Cu35Cl v=0 4 1 4 3.5 4 -v=0 3 1 3 2.5 3 : 57:<LineList>
5 B2 5	4 B1 5	15271.4150	15271.4103	0.0047 1	.00043	0 : qR1,3(3)4.5,5,2.5,4 : 12CH4---65Cu35Cl v=0 4 1 4 4.5 5 -v=0 3 1 3 2.5 4 : 58:<LineList>
5 B2 6	4 B1 6	15271.6180	15271.6226	-0.0046 1	.00055	0 : qR1,3(3)3.5,5,3.5,4 : 12CH4---65Cu35Cl v=0 4 1 4 3.5 5 -v=0 3 1 3 3.5 4 : 59:<LineList>
3 B2 12	2 B1 10	15271.7950	15271.7898	0.0052 1	.00028	0 : qR1,3(3)4.5,3,3.5,2 : 12CH4---65Cu35Cl v=0 4 1 4 4.5 3 -v=0 3 1 3 3.5 2 : 60:<LineList>
6 B2 3	5 B1 3	15271.9000	15271.9034	-0.0034 1	.00065	0 : qR1,3(3)5.5,6,3.5,5 : 12CH4---65Cu35Cl v=0 4 1 4 4.5 6 -v=0 3 1 3 3.5 5 : 61:<LineList>
4 A1 3	4 A2 3	15467.7910	15467.8081	-0.0171 1	.0002	0 : qR0,3(3)2.5,4,2.5,4 : 12CH4---65Cu35Cl v=0 4 0 4 2.5 4 -v=0 3 0 3 2.5 4 : 62:<LineList>
5 A1 3	5 A2 2	15473.5600	15473.5606	-0.0006 1	.00032	0 : qR0,3(3)3.5,5,3.5,5 : 12CH4---65Cu35Cl v=0 4 0 4 3.5 5 -v=0 3 0 3 3.5 5 : 63:<LineList>
2 A1 7	2 A2 6	15474.5360	15474.5385	-0.0025 1	.00016	0 : qR0,3(3)3.5,5,2.3,5,2 : 12CH4---65Cu35Cl v=0 4 0 4 3.5 2 -v=0 3 0 3 3.5 2 : 64:<LineList>
5 A1 3	4 A2 4	15476.2650	15476.2633	0.0017 1	2.8e-5	0 : qR0,3(3)3.5,5,3.5,4 : 12CH4---65Cu35Cl v=0 4 0 4 3.5 5 -v=0 3 0 3 3.5 4 : 65:<LineList>
3 A1 5	3 A2 3	15478.0000	15478.0066	-0.0066 1	.00024	0 : qR0,3(3)2.5,3,1.5,3 : 12CH4---65Cu35Cl v=0 4 0 4 2.5 3 -v=0 3 0 3 1.5 3 : 66:<LineList>
4 A1 6	3 A2 6	15479.1340	15479.1277	0.0063 1	.00117	0 : qR1,3(3)4.5,4,3.5,3 : 12CH4---65Cu35Cl v=0 4 0 4 4.5 4 -v=0 3 0 3 3.5 3 : 67:<LineList>
5 A1 2	4 A2 2	15479.6500	15479.6415	0.0085 1	.00173	0 : qR0,3(3)5.5,5,4.5,4 : 12CH4---65Cu35Cl v=0 4 0 4 5.5 5 -v=0 3 0 3 4.5 4 : 68:<LineList>
5 A1 4	4 A2 4	15479.7500	15479.7447	0.0053 1	.00168	0 : qR0,3(3)4.5,5,3.5,4 : 12CH4---65Cu35Cl v=0 4 0 4 4.5 5 -v=0 3 0 3 3.5 4 : 69:<LineList>
6 A1 1	5 A2 1	15479.8440	15479.8357	0.0083 1	.00207	0 : qR0,3(3)5.5,6,4.5,5 : 12CH4---65Cu35Cl v=0 4 0 4 5.5 6 -v=0 3 0 3 4.5 5 : 70:<LineList>
7 A1 1	6 A2 1	15479.9930	15479.9891	0.0039 1	.00253	0 : qR1,3(3)5.5,7,4.5,6 : 12CH4---65Cu35Cl v=0 4 0 4 5.5 7 -v=0 3 0 3 4.5 6 : 71:<LineList>
6 A1 2	5 A2 2	15480.0840	15480.0865	-0.0025 1	.00203	0 : qR0,3(3)4.5,6,3.5,5 : 12CH4---65Cu35Cl v=0 4 0 4 4.5 6 -v=0 3 0 3 3.5 5 : 72:<LineList>
2 A1 6	1 A2 4	15480.3210	15480.3286	-0.0076 1	.00049	0 : qR0,3(3)2.5,2,1.5,1 : 12CH4---65Cu35Cl v=0 4 0 4 2.5 2 -v=0 3 0 3 1.5 1 : 73:<LineList>
4 A1 5	3 A2 5	15480.9080	15480.9056	0.0024 1	.00126	0 : qR0,3(3)3.5,4,2.5,3 : 12CH4---65Cu35Cl v=0 4 0 4 3.5 4 -v=0 3 0 3 2.5 3 : 74:<LineList>
3 A1 6	2 A2 5	15480.9580	15480.9590	-0.0010 1	.00087	0 : qR0,3(3)3.5,3,2.5,2 : 12CH4---65Cu35Cl v=0 4 0 4 3.5 3 -v=0 3 0 3 2.5 2 : 75:<LineList>
3 A1 5	2 A2 4	15481.2320	15481.2281	0.0039 1	.00084	0 : qR0,3(3)2.5,3,1.5,2 : 12CH4---65Cu35Cl v=0 4 0 4 2.5 3 -v=0 3 0 3 1.5 2 : 76:<LineList>
5 A1 3	4 A2 3	15481.5900	15481.5807	0.0093 1	.00141	0 : qR0,3(3)3.5,5,2.5,4 : 12CH4---65Cu35Cl v=0 4 0 4 3.5 5 -v=0 3 0 3 2.5 4 : 77:<LineList>
1 A1 5	1 A2 4	15484.8470	15484.8502	-0.0032 1	.00016	0 : qR0,3(3)2.5,1,1.5,1 : 12CH4---65Cu35Cl v=0 4 0 4 2.5 1 -v=0 3 0 3 1.5 1 : 78:<LineList>
3 B1 10	3 B2 6	15693.2990	15693.3099	-0.0109 1	7.3e-5	0 : qR1,2(3)2.5,3,1.5,3 : 12CH4---65Cu35Cl v=0 4 1 3 2.5 3 -v=0 3 1 2 1.5 3 : 79:<LineList>
5 B1 4	4 B2 4	15694.2540	15694.2482	0.0058 1	.00056	0 : qR1,2(3)5.5,5,4.5,4 : 12CH4---65Cu35Cl v=0 4 1 3 5.5 5 -v=0 3 1 2 4.5 4 : 80:<LineList>
6 B1 2	5 B2 2	15694.2540	15694.2462	0.0078 1	.00067	0 : qR1,2(3)5.5,6,4.5,5 : 12CH4---65Cu35Cl v=0 4 1 3 5.5 6 -v=0 3 1 2 4.5 5 : 81:<LineList>
7 B1 1	6 B2 1	15694.8460	15694.8453	0.0007 1	.00082	0 : qR1,2(3)5.5,7,4.5,6 : 12CH4---65Cu35Cl v=0 4 1 3 5.5 7 -v=0 3 1 2 4.5 6 : 82:<LineList>
4 B1 8	3 B2 7	15694.8630	15694.8649	-0.0019 1	.00046	0 : qR1,2(3)5.5,4,4.5,3 : 12CH4---65Cu35Cl v=0 4 1 3 5.5 4 -v=0 3 1 2 4.5 3 : 83:<LineList>
2 B1 11	1 B2 7	15695.0330	15695.0347	-0.0017 1	.00015	0 : qR1,2(3)2.5,2,1.5,1 : 12CH4---65Cu35Cl v=0 4 1 3 2.5 2 -v=0 3 1 2 1.5 1 : 84:<LineList>
5 B1 4	5 B2 2	15695.1940	15695.1950	-0.0010 1	4.1e-5	0 : qR1,2(3)5.5,5,4.5,5 : 12CH4---65Cu35Cl v=0 4 1 3 5.5 5 -v=0 3 1 2 4.5 5 : 85:<LineList>
3 B1 10	2 B2 8	15695.3890	15695.3950	-0.0060 1	.00027	0 : qR1,2(3)2.5,3,1.5,2 : 12CH4---65Cu35Cl v=0 4 1 3 2.5 3 -v=0 3 1 2 1.5 2 : 86:<LineList>
4 B1 10	3 B2 9	15695.5740	15695.5659	0.0081 1	.00039	0 : qR1,2(3)4.5,4,3.5,3 : 12CH4---65Cu35Cl v=0 4 1 3 4.5 4 -v=0 3 1 2 3.5 3 : 87:<LineList>
5 B1 6	4 B2 6	15695.6680	15695.6647	0.0033 1	.00054	0 : qR1,2(3)4.5,5,3.5,4 : 12CH4---65Cu35Cl v=0 4 1 3 4.5 5 -v=0 3 1 2 3.5 4 : 88:<LineList>
4 B1 7	3 B2 6	15696.3720	15696.3769	-0.0049 1	.00041	0 : qR1,2(3)2.5,4,1.5,3 : 12CH4---65Cu35Cl v=0 4 1 3 2.5 4 -v=0 3 1 2 1.5 3 : 89:<LineList>
6 B1 3	5 B2 3	15696.3870	15696.3817	0.0053 1	.00066	0 : qR1,2(3)4.5,6,3.5,5 : 12CH4---65Cu35Cl v=0 4 1 3 4.5 6 -v=0 3 1 2 3.5 5 : 90:<LineList>
4 B1 9	3 B2 8	15696.7860	15696.7821	0.0039 1	.0004	0 : qR1,2(3)3.5,4,2.5,3 : 12CH4---65Cu35Cl v=0 4 1 3 3.5 4 -v=0 3 1 2 2.5 3 : 91:<LineList>
3 B1 11	2 B2 9	15696.8960	15696.8968	-0.0008 1	.00028	0 : qR1,2(3)3.5,3,2.5,2 : 12CH4---65Cu35Cl v=0 4 1 3 3.5 3 -v=0 3 1 2 2.5 2 : 92:<LineList>
5 B1 5	4 B2 5	15697.6630	15697.6667	-0.0037 1	.00049	0 : qR1,2(3)3.5,5,2.5,4 : 12CH4---65Cu35Cl v=0 4 1 3 3.5 5 -v=0 3 1 2 2.5 4 : 93:<LineList>
2 A1 7	1 A2 5	15481.8120	15481.8209	-0.0089 1	.00055	0 : qR0,3(3)3.5,2,2.5,1 : 12CH4---65Cu35Cl v=0 4 0 4 3.5 2 -v=0 3 0 3 2.5 1 : 94:<LineList>

94 Observations, 9 Parameters

Initial Average Error: 0.00798180028363219

Predicted New Error: 0.00797968367640912

Parameters:

# Old	New	Std Dev	Change/Std Sens	Summary	Name
1 24219.592950298	24219.6051174984	60.415262	0.0002 1.08326	24220(60)	C2H4-Cu-Cl 12CH4---65Cu35Cl v=0 A
2 1988.62175773136	1988.62175797756	.0006434	0.0004 2.34e-5	1988.62176(64)	C2H4-Cu-Cl 12CH4---65Cu35Cl v=0 B
3 1882.41547839413	1882.41547867808	.00064803	0.0004 2.56e-5	1882.41548(65)	C2H4-Cu-Cl 12CH4---65Cu35Cl v=0 C
4 .0155903168771076	.0155902064081683	.00089214	-0.0001 1.34e-5	0.01559(89)	C2H4-Cu-Cl 12CH4---65Cu35Cl v=0 DJK
5 .000385929835526979	.000385946441957684	3.171e-5	0.0005 3.5e-7	3.86(32)e-4	C2H4-Cu-Cl 12CH4---65Cu35Cl v=0 DJ
6 59.056998856698	59.0580597759377	.03745492	0.0283 .001202	59.058(37)	C2H4-Cu-Cl 12CH4---65Cu35Cl Copper CHlzz
7 -41.3918067112445	-41.3858289102993	.20030064	0.0298 .006183	-41.39(20)	C2H4-Cu-Cl 12CH4---65Cu35Cl Copper CHlxxmyy
8 -20.992112373059	-20.9918687740641	.01884036	0.0129 .001383	-20.992(19)	C2H4-Cu-Cl 12CH4---65Cu35Cl Chlorine CHlzz
9 -4.99384595601583	-4.97188762551006	.32608434	0.0673 .008748	-4.97(33)	C2H4-Cu-Cl 12CH4---65Cu35Cl Chlorine CHlxxmyy

Correlation Matrix

1	2	3	4	5	6	7	8	9
1 1.000								
2 -0.522	1.000							
3 -0.447	0.438	1.000						
4 -0.959	0.561	0.444	1.000					
5 0.863	-0.150	-0.046	-0.845	1.000				
6 -0.387	-0.323	-0.423	0.320	-0.732	1.000			
7 -0.383	-0.330	-0.446	0.305	-0.734	0.905	1.000		
8 -0.308	-0.235	-0.244	0.270	-0.537	0.715	0.647	1.000	
9 -0.383	-0.332	-0.435	0.302	-0.731	0.942	0.943	0.674	1.000

¹²C,¹H₄---⁶³Cu¹⁷Cl (Page 1 of 2)

Pgopher 8.0.102 08 Dec 2013 16:55 32 bit (Delphi 18.5/18)

Mixture: 12C2 H4 --- 65Cu 35Cl Chirped-Pulse.pgo

Units MHz
PrintLevel Detail
Precision 4
BasisOrder boDefault
QuantumNumberFormat J
FitCycles 1
FitDetails False
AutoReplot True
AllowComplex False
NoLineList False
ShowEstUnc False
ShowDerivatives False
SVDlimit 5
SVDThresh 1E-15
ScaleChanges 1
Species: C2H4-Cu-Cl
Jmax 30
Concentration 1
AsymmetricMolecule: C2H4-Cu-Cl 12CH4---63Cu37Cl
nNuclei 2
Jmax 30
Colour Blue
JAdjustSym False
BlockMatrix True
PointGroup C2v
Representation Ir
SReduction False
eeWt 1
eoWt 1
oeWt 1
ooWt 1
C2zAxis a
C2xAxis c
PseudoC2v False
FakeSym False
PhaseAdjust False
Abundance 1
AsymmetricManifold: C2H4-Cu-Cl 12CH4---63Cu37Cl Ground

Residuals before fit for 12CH4---63Cu37Cl for the Ground manifold

J'S'	#'	J"S"	#"	Observed	Calculated	Obs-Calc	StdDev	
5 A1	1	4 A2	1	7532.3340	7532.3292	0.0048	1	.00116 0 : qR0,1(1)3.5,5,2,5,4 : 12CH4---63Cu37Cl v=0 2 0 2 3.5 5 - v=0 1 0 1 2.5 4 : 1:<LineList>
6 B1	1	5 B2	1	11148.3320	11148.3429	-0.0109	1	.00064 0 : qR1,2(2)4.5,6,3,5,5 : 12CH4---63Cu37Cl v=0 3 1 3 4.5 6 - v=0 2 1 2 3.5 5 : 2:<LineList>
4 B1	6	3 B2	5	11151.2590	11151.2754	-0.0164	1	.00039 0 : qR1,2(2)3.5,4,2,5,3 : 12CH4---63Cu37Cl v=0 3 1 3 3.5 4 - v=0 2 1 2 2.5 3 : 3:<LineList>
2 A2	4	3 A1	3	11284.3040	11284.3033	0.0007	1	6.1e-5 0 : qR0,2(2)1.5,2,1,5,3 : 12CH4---63Cu37Cl v=0 3 0 3 1.5 2 - v=0 2 0 2 1.5 3 : 4:<LineList>
2 A2	4	1 A1	3	11284.3040	11284.3033	0.0007	1	5.2e-5 0 : qR0,2(2)1.5,2,1,5,1 : 12CH4---63Cu37Cl v=0 3 0 3 1.5 2 - v=0 2 0 2 1.5 1 : 5:<LineList>
2 A2	4	2 A1	4	11284.3040	11284.2942	0.0098	1	5.2e-5 0 : qR0,2(2)1.5,2,1,5,2 : 12CH4---63Cu37Cl v=0 3 0 3 1.5 2 - v=0 2 0 2 1.5 2 : 6:<LineList>
3 A2	3	3 A1	3	11286.8890	11286.8896	-0.0006	1	.00027 0 : qR0,2(2)1.5,3,1,5,3 : 12CH4---63Cu37Cl v=0 3 0 3 1.5 3 - v=0 2 0 2 1.5 3 : 7:<LineList>
2 A2	5	1 A1	4	11288.7620	11288.7682	-0.0062	1	4.8e-5 0 : qR0,2(2)2.5,2,2,5,1 : 12CH4---63Cu37Cl v=0 3 0 3 2.5 2 - v=0 2 0 2 2.5 1 : 8:<LineList>
4 A2	3	4 A1	2	11290.6480	11290.6639	-0.0159	1	.0004 0 : qR0,2(2)2.5,4,2,5,4 : 12CH4---63Cu37Cl v=0 3 0 3 2.5 4 - v=0 2 0 2 2.5 4 : 9:<LineList>
3 A2	6	2 A1	5	11297.5790	11297.5807	-0.0017	1	.00073 0 : qR0,2(2)3.5,3,2,5,2 : 12CH4---63Cu37Cl v=0 3 0 3 3.5 3 - v=0 2 0 2 2.5 2 : 10:<LineList>
4 A2	4	3 A1	4	11297.7180	11297.7068	0.0112	1	.0012 0 : qR0,2(2)3.5,4,2,5,3 : 12CH4---63Cu37Cl v=0 3 0 3 3.5 4 - v=0 2 0 2 2.5 3 : 11:<LineList>
6 A2	1	5 A1	1	11298.5860	11298.5781	0.0079	1	.00213 0 : qR0,2(2)4.5,6,3,5,5 : 12CH4---63Cu37Cl v=0 3 0 3 4.5 6 - v=0 2 0 2 3.5 5 : 12:<LineList>
5 A2	2	4 A1	2	11298.7930	11298.7893	0.0037	1	.00157 0 : qR0,2(2)3.5,5,2,5,4 : 12CH4---63Cu37Cl v=0 3 0 3 3.5 5 - v=0 2 0 2 2.5 4 : 13:<LineList>
2 A2	6	1 A1	4	11299.0830	11299.1013	-0.0183	1	.0005 0 : qR0,2(2)3.5,2,2,5,1 : 12CH4---63Cu37Cl v=0 3 0 3 3.5 2 - v=0 2 0 2 2.5 1 : 14:<LineList>
2 A2	6	2 A1	5	11300.3090	11300.2947	0.0143	1	.00022 0 : qR0,2(2)3.5,2,2,5,2 : 12CH4---63Cu37Cl v=0 3 0 3 3.5 2 - v=0 2 0 2 2.5 2 : 15:<LineList>
2 A2	4	2 A1	2	11300.4500	11300.4309	0.0191	1	.00031 0 : qR0,2(2)1.5,2,0,5,2 : 12CH4---63Cu37Cl v=0 3 0 3 1.5 2 - v=0 2 0 2 0.5 2 : 16:<LineList>
2 A2	4	1 A1	2	11300.6700	11300.6798	-0.0098	1	.00033 0 : qR0,2(2)1.5,2,0,5,1 : 12CH4---63Cu37Cl v=0 3 0 3 1.5 2 - v=0 2 0 2 0.5 1 : 17:<LineList>
3 A2	5	2 A1	4	11300.9300	11300.9247	0.0053	1	.00078 0 : qR0,2(2)2.5,3,1,5,2 : 12CH4---63Cu37Cl v=0 3 0 3 2.5 3 - v=0 2 0 2 1.5 2 : 18:<LineList>
2 A2	5	2 A1	4	11301.7340	11301.7330	0.0010	1	.00016 0 : qR0,2(2)2.5,2,1,5,2 : 12CH4---63Cu37Cl v=0 3 0 3 2.5 2 - v=0 2 0 2 1.5 2 : 19:<LineList>
2 A2	5	1 A1	3	11301.7430	11301.7421	0.0009	1	.00041 0 : qR0,2(2)2.5,2,1,5,1 : 12CH4---63Cu37Cl v=0 3 0 3 2.5 2 - v=0 2 0 2 1.5 1 : 20:<LineList>
4 A2	3	3 A1	3	11302.5790	11302.5865	-0.0075	1	.001 0 : qR0,2(2)2.5,4,1,5,3 : 12CH4---63Cu37Cl v=0 3 0 3 2.5 4 - v=0 2 0 2 1.5 3 : 21:<LineList>
3 A2	3	2 A1	2	11303.0200	11303.0172	0.0028	1	.00077 0 : qR0,2(2)1.5,3,0,5,2 : 12CH4---63Cu37Cl v=0 3 0 3 1.5 3 - v=0 2 0 2 0.5 2 : 22:<LineList>
1 A2	4	1 A1	2	11303.1900	11303.2030	-0.0130	1	.00026 0 : qR0,2(2)1.5,1,0,5,1 : 12CH4---63Cu37Cl v=0 3 0 3 1.5 1 - v=0 2 0 2 0.5 1 : 23:<LineList>
5 B2	2	4 B1	2	11448.4610	11448.4537	0.0073	1	.00052 0 : qR1,1(2)4.5,5,3,5,4 : 12CH4---63Cu37Cl v=0 3 1 2 4.5 5 - v=0 2 1 1 3.5 4 : 24:<LineList>
4 B2	4	3 B1	3	11448.7030	11448.6995	0.0035	1	.00041 0 : qR1,1(2)4.5,4,3,5,3 : 12CH4---63Cu37Cl v=0 3 1 2 4.5 4 - v=0 2 1 1 3.5 3 : 25:<LineList>
6 B2	1	5 B1	1	11449.5010	11449.4942	0.0068	1	.00066 0 : qR1,1(2)4.5,6,3,5,5 : 12CH4---63Cu37Cl v=0 3 1 2 4.5 6 - v=0 2 1 1 3.5 5 : 26:<LineList>
3 B2	7	2 B1	5	11449.6870	11449.6984	-0.0114	1	.00032 0 : qR1,1(2)4.5,3,3,5,2 : 12CH4---63Cu37Cl v=0 3 1 2 4.5 3 - v=0 2 1 1 3.5 2 : 27:<LineList>
6 B2	2	5 B1	2	14864.3390	14864.3401	-0.0011	1	.00063 0 : qR1,3(3)5.5,6,4,5,5 : 12CH4---63Cu37Cl v=0 4 1 4 5.5 6 - v=0 3 1 3 4.5 5 : 28:<LineList>
5 B2	4	4 B1	4	14864.3220	14864.3208	0.0012	1	.00053 0 : qR1,3(3)5.5,4,5,4 : 12CH4---63Cu37Cl v=0 4 1 4 5.5 5 - v=0 3 1 3 4.5 4 : 29:<LineList>
3 B2	10	2 B1	8	14864.3170	14864.3122	0.0048	1	.00026 0 : qR1,3(3)2.5,3,1,5,2 : 12CH4---63Cu37Cl v=0 4 1 4 2.5 3 - v=0 3 1 3 1.5 2 : 30:<LineList>
7 B2	1	6 B1	1	14864.8140	14864.8162	-0.0022	1	.00077 0 : qR1,3(3)5.5,7,4,5,6 : 12CH4---63Cu37Cl v=0 4 1 4 5.5 7 - v=0 3 1 3 4.5 6 : 31:<LineList>
4 B2	8	3 B1	7	14864.9310	14864.9367	-0.0057	1	.00044 0 : qR1,3(3)5.5,4,4,5,3 : 12CH4---63Cu37Cl v=0 4 1 4 5.5 4 - v=0 3 1 3 4.5 3 : 32:<LineList>
4 B2	7	3 B1	6	14865.2520	14865.2640	-0.0120	1	.00037 0 : qR1,3(3)2.5,4,1,5,3 : 12CH4---63Cu37Cl v=0 4 1 4 2.5 4 - v=0 3 1 3 1.5 3 : 33:<LineList>
4 B2	10	3 B1	9	14865.4920	14865.4870	0.0050	1	.00035 0 : qR1,3(3)4.5,4,3,5,3 : 12CH4---63Cu37Cl v=0 4 1 4 4.5 4 - v=0 3 1 3 3.5 3 : 34:<LineList>
4 B2	9	3 B1	8	14865.7150	14865.7109	0.0041	1	.0004 0 : qR1,3(3)3.5,4,2,5,3 : 12CH4---63Cu37Cl v=0 4 1 4 3.5 4 - v=0 3 1 3 2.5 3 : 35:<LineList>
3 B2	11	2 B1	9	14865.8890	14865.8793	0.0097	1	.00027 0 : qR1,3(3)3.5,3,2,5,2 : 12CH4---63Cu37Cl v=0 4 1 4 3.5 3 - v=0 3 1 3 2.5 2 : 36:<LineList>
5 B2	6	4 B1	6	14866.0910	14866.0963	-0.0053	1	.00052 0 : qR1,3(3)3.5,5,3,5,4 : 12CH4---63Cu37Cl v=0 4 1 4 3.5 5 - v=0 3 1 3 3.5 4 : 37:<LineList>
5 B2	5	4 B1	5	14866.2700	14866.2660	0.0040	1	.00042 0 : qR1,3(3)4.5,5,2,5,4 : 12CH4---63Cu37Cl v=0 4 1 4 4.5 5 - v=0 3 1 3 2.5 4 : 38:<LineList>
3 B2	12	2 B1	10	14866.4000	14866.3950	0.0050	1	.00027 0 : qR1,3(3)4.5,3,3,5,2 : 12CH4---63Cu37Cl v=0 4 1 4 4.5 3 - v=0 3 1 3 3.5 2 : 39:<LineList>
6 B2	3	5 B1	3	14866.4600	14866.4573	0.0027	1	.00062 0 : qR1,3(3)4.5,6,3,5,5 : 12CH4---63Cu37Cl v=0 4 1 4 4.5 6 - v=0 3 1 3 3.5 5 : 40:<LineList>
4 A1	3	4 A2	3	15049.9990	15050.0084	-0.0094	1	.00019 0 : qR0,3(3)2.5,4,2,5,4 : 12CH4---63Cu37Cl v=0 4 0 4 2.5 4 - v=0 3 0 3 2.5 4 : 41:<LineList>

Jmax 30
Initial True
EigenSearch True
LimitSearch True
AutoQConverge True
UsePopParams False
AsymmetricTop: C2H4-Cu-Cl 12CH4---63Cu37Cl v=0
Symmetry A1
Kmin 0
Kmax 10
A 24032.6442429726 Float
B 1933.70910163346 Float
C 1833.13166350826 Float
DJK 0.0168387172122373 Float
DJ 0.00026472474669823 Float
AsymmetricTopNucleus: C2H4-Cu-Cl 12CH4---63Cu37Cl Copper
Spin 1.5
AsNext False
CHlzz 63.8529338158731 Float
CHlxxmyy -44.684284181583 Float
AsymmetricTopNucleus: C2H4-Cu-Cl 12CH4---63Cu37Cl Chlorine
Spin 1.5
AsNext False
CHlzz -16.5659160263603 Float
CHlxxmyy -4.2 Float
<N ,K |A|N,K> = K^2
<N ,K-2|B|N,K> = sqrt((N*(N+1)+(-K+1)*(K-2))*(N*(N+1)-K*(K-1)))/4
<N ,K |B|N,K> = (N*(N+1)-K^2)/2
<N ,K+2|B|N,K> = sqrt((N*(N+1)+(-K-1)*(K+2))*(N*(N+1)-K*(K+1)))/4
<N ,K-2|C|N,K> = (-sqrt((N*(N+1)+(-K+1)*(K-2))*(N*(N+1)-K*(K-1)))/4
<N ,K |C|N,K> = (N*(N+1)-K^2)/2
<N ,K+2|C|N,K> = (-sqrt((N*(N+1)+(-K-1)*(K+2))*(N*(N+1)-K*(K+1)))/4
<N ,K |DJK|N,K> = -N*(N+1)*K^2
<N ,K |DJ|N,K> = -N^2*(N+1)^2
TransitionMoments: C2H4-Cu-Cl 12CH4---63Cu37Cl <Ground|mu|Ground>
CartesianTransitionMoment: C2H4-Cu-Cl 12CH4---63Cu37Cl <v=0|a|v=0>
Axis a
Strength 1
Symbolic Matrix Elements not available for <v=0|a|v=0>

5 A1 3	5 A2 2	15057.2940	15057.3020	-0.0080 1	.00031	0 : qR0,3(3)3.5,5,3.5,5 : 12CH4---63Cu37Cl v=0 4 0 4 3.5 5 - v=0 3 0 3 3.5 5 : 42:<LineList>
4 A1 6	3 A2 6	15062.9040	15062.8898	0.0142 1	.00114	0 : qR0,3(3)4.5,4,3.5,3 : 12CH4---63Cu37Cl v=0 4 0 4 4.5 4 - v=0 3 0 3 3.5 3 : 43:<LineList>
5 A1 4	4 A2 4	15063.1870	15063.1969	-0.0099 1	.00161	0 : qR0,3(3)4.5,5,3.5,4 : 12CH4---63Cu37Cl v=0 4 0 4 4.5 5 - v=0 3 0 3 3.5 4 : 44:<LineList>
6 A1 1	5 A2 1	15063.4040	15063.4064	-0.0024 1	.00199	0 : qR0,3(3)5.5,6,4.5,5 : 12CH4---63Cu37Cl v=0 4 0 4 5.5 6 - v=0 3 0 3 4.5 5 : 45:<LineList>
7 A1 1	6 A2 1	15063.5410	15063.5356	0.0054 1	.00242	0 : qR0,3(3)5.5,7,4.5,6 : 12CH4---63Cu37Cl v=0 4 0 4 5.5 7 - v=0 3 0 3 4.5 6 : 46:<LineList>
6 A1 2	5 A2 2	15063.6020	15063.6085	-0.0065 1	.00194	0 : qR0,3(3)4.5,6,3.5,5 : 12CH4---63Cu37Cl v=0 4 0 4 4.5 6 - v=0 3 0 3 3.5 5 : 47:<LineList>
2 A1 6	1 A2 4	15064.2700	15064.2728	-0.0028 1	.00046	0 : qR0,3(3)2.5,2,1.5,1 : 12CH4---63Cu37Cl v=0 4 0 4 2.5 2 - v=0 3 0 3 1.5 1 : 48:<LineList>
4 A1 5	3 A2 5	15064.7500	15064.7449	0.0051 1	.00118	0 : qR0,3(3)3.5,4,2.5,3 : 12CH4---63Cu37Cl v=0 4 0 4 3.5 4 - v=0 3 0 3 2.5 3 : 49:<LineList>
3 A1 6	2 A2 5	15064.7750	15064.7723	0.0027 1	.00083	0 : qR0,3(3)3.5,3,2.5,2 : 12CH4---63Cu37Cl v=0 4 0 4 3.5 3 - v=0 3 0 3 2.5 2 : 50:<LineList>
3 A1 5	2 A2 4	15065.0000	15064.9953	0.0047 1	.0008	0 : qR0,3(3)2.5,3,1.5,2 : 12CH4---63Cu37Cl v=0 4 0 4 2.5 3 - v=0 3 0 3 1.5 2 : 51:<LineList>
5 A1 3	4 A2 3	15065.4350	15065.4274	0.0076 1	.00142	0 : qR0,3(3)3.5,5,2.5,4 : 12CH4---63Cu37Cl v=0 4 0 4 3.5 5 - v=0 3 0 3 2.5 4 : 52:<LineList>
2 A1 7	1 A2 5	15065.5020	15065.5035	-0.0015 1	.00054	0 : qR0,3(3)3.5,2,2.5,1 : 12CH4---63Cu37Cl v=0 4 0 4 3.5 2 - v=0 3 0 3 2.5 1 : 53:<LineList>
4 A1 3	3 A2 3	15065.7100	15065.7053	0.0047 1	.00121	0 : qR0,3(3)2.5,4,1.5,3 : 12CH4---63Cu37Cl v=0 4 0 4 2.5 4 - v=0 3 0 3 1.5 3 : 54:<LineList>
3 A1 7	3 A2 6	15066.1970	15066.1986	-0.0016 1	.00018	0 : qR0,3(3)4.5,3,3.5,3 : 12CH4---63Cu37Cl v=0 4 0 4 4.5 3 - v=0 3 0 3 3.5 3 : 55:<LineList>
5 B1 4	4 B2 4	15266.2780	15266.2792	-0.0012 1	.00054	0 : qR1,2(3)5.5,5,4.5,4 : 12CH4---63Cu37Cl v=0 4 1 3 5.5 5 - v=0 3 1 2 4.5 4 : 56:<LineList>
6 B1 2	5 B2 2	15266.2780	15266.2785	-0.0005 1	.00065	0 : qR1,2(3)5.5,6,4.5,5 : 12CH4---63Cu37Cl v=0 4 1 3 5.5 6 - v=0 3 1 2 4.5 5 : 57:<LineList>
4 B1 8	3 B2 7	15266.7640	15266.7627	0.0013 1	.00044	0 : qR1,2(3)5.5,4,4.5,3 : 12CH4---63Cu37Cl v=0 4 1 3 5.5 4 - v=0 3 1 2 4.5 3 : 58:<LineList>
7 B1 1	6 B2 1	15266.7500	15266.7521	-0.0021 1	.00079	0 : qR1,2(3)5.5,7,4.5,6 : 12CH4---63Cu37Cl v=0 4 1 3 5.5 7 - v=0 3 1 2 4.5 6 : 59:<LineList>
3 B1 10	2 B2 8	15267.5770	15267.5791	-0.0021 1	.00026	0 : qR0,2(3)2.5,3,1.5,2 : 12CH4---63Cu37Cl v=0 4 1 3 2.5 3 - v=0 3 1 2 1.5 2 : 60:<LineList>
4 B1 10	3 B2 9	15267.7620	15267.7633	-0.0013 1	.00038	0 : qR1,2(3)4.5,4,3.5,3 : 12CH4---63Cu37Cl v=0 4 1 3 4.5 4 - v=0 3 1 2 3.5 3 : 61:<LineList>
5 B1 6	4 B2 6	15267.7750	15267.7802	-0.0052 1	.00051	0 : qR1,2(3)4.5,5,3.5,4 : 12CH4---63Cu37Cl v=0 4 1 3 4.5 5 - v=0 3 1 2 3.5 4 : 62:<LineList>
6 B1 3	5 B2 3	15268.3940	15268.3929	0.0011 1	.00063	0 : qR1,2(3)3.5,5,6,3.5,5 : 12CH4---63Cu37Cl v=0 4 1 3 4.5 6 - v=0 3 1 2 3.5 5 : 63:<LineList>
3 B1 12	2 B2 10	15268.4590	15268.4599	-0.0009 1	.00029	0 : qR1,2(3)4.5,3,3.5,2 : 12CH4---63Cu37Cl v=0 4 1 3 4.5 3 - v=0 3 1 2 3.5 2 : 64:<LineList>
3 A2 4	3 A1 2	11301.8020	11301.8059	-0.0039 1	9.4e-5	0 : qR0,2(2)4.5,3,3.5,3 : 12CH4---63Cu37Cl v=0 3 0 3 4.5 3 - v=0 2 0 2 3.5 3 : 65:<LineList>
5 B1 5	4 B2 5	15269.8500	15269.8570	-0.0070 1	.00048	0 : qR1,2(3)3.5,5,2.5,4 : 12CH4---63Cu37Cl v=0 4 1 3 3.5 5 - v=0 3 1 2 2.5 4 : 66:<LineList>
2 B2 12	1 B1 8	14866.7150	14866.7044	0.0106 1	.00017	0 : qR1,3(3)3.5,2,2.5,1 : 12CH4---63Cu37Cl v=0 4 1 4 3.5 2 - v=0 3 1 3 2.5 1 : 67:<LineList>
4 A1 1	3 A2 1	7531.6920	7531.6881	0.0039 1	.00082	0 : qR0,1(1)3.5,4,2.5,3 : 12CH4---63Cu37Cl v=0 2 0 2 3.5 4 - v=0 1 0 1 2.5 3 : 68:<LineList>
4 B1 4	3 B2 3	11147.8520	11147.8523	-0.0003 1	.00032	0 : qR1,2(2)4.5,4,3.5,3 : 12CH4---63Cu37Cl v=0 3 1 3 4.5 4 - v=0 2 1 2 3.5 3 : 69:<LineList>
4 B2 5	3 B1 4	11454.8680	11454.8518	0.0162 1	.00033	0 : qR1,1(2)2.5,4,1.5,3 : 12CH4---63Cu37Cl v=0 3 1 2 2.5 4 - v=0 2 1 1 1.5 3 : 70:<LineList>
4 B2 6	3 B1 5	11452.4140	11452.4155	-0.0015 1	.00036	0 : qR1,1(2)3.5,4,2.5,3 : 12CH4---63Cu37Cl v=0 3 1 2 3.5 4 - v=0 2 1 1 2.5 3 : 71:<LineList>
3 B2 8	2 B1 6	11453.6750	11453.6870	-0.0120 1	.00023	0 : qR1,1(2)2.5,3,1.5,2 : 12CH4---63Cu37Cl v=0 3 1 2 2.5 3 - v=0 2 1 1 1.5 2 : 72:<LineList>
3 A2 5	3 A1 4	11290.2480	11290.2347	0.0133 1	.00011	0 : qR0,2(2)2.5,3,2.5,3 : 12CH4---63Cu37Cl v=0 3 0 3 2.5 3 - v=0 2 0 2 2.5 3 : 73:<LineList>
2 A2 5	2 A1 5	11289.9400	11289.9617	-0.0217 1	8.8e-5	0 : qR0,2(2)2.5,2,2.5,2 : 12CH4---63Cu37Cl v=0 3 0 3 2.5 2 - v=0 2 0 2 2.5 2 : 74:<LineList>
0 A2 2	1 A1 3	11289.7210	11289.7076	0.0134 1	6.2e-5	0 : qR0,2(2)1.5,0,1.5,1 : 12CH4---63Cu37Cl v=0 3 0 3 1.5 0 - v=0 2 0 2 1.5 1 : 75:<LineList>
5 A2 1	4 A1 1	11298.3110	11298.3238	-0.0128 1	.00165	0 : qR0,2(2)4.5,5,3.5,4 : 12CH4---63Cu37Cl v=0 3 0 3 4.5 5 - v=0 2 0 2 3.5 4 : 76:<LineList>
4 A2 2	3 A1 2	11298.2750	11298.2855	-0.0105 1	.00129	0 : qR0,2(2)4.5,4,3.5,3 : 12CH4---63Cu37Cl v=0 3 0 3 4.5 4 - v=0 2 0 2 3.5 3 : 77:<LineList>

77 Observations, 9 Parameters

Initial Average Error: 0.00887114265434008

Predicted New Error: 0.00855803004571731

Parameters:

# Old	New	Std Dev	Change/Std Sens	Summary	Name
1 24032.6442429726	24033.9821843774	98.672006	0.0136 1.20356	24034(99)	C2H4-Cu-Cl 12CH4---63Cu37Cl v=0 A
2 1933.70910163346	1933.70910238716	.00077458	0.0010 2.6e-5	1933.70910(77)	C2H4-Cu-Cl 12CH4---63Cu37Cl v=0 B
3 1833.13166350826	1833.13166716525	.00079211	0.0046 2.5e-5	1833.13167(79)	C2H4-Cu-Cl 12CH4---63Cu37Cl v=0 C
4 .0168387172122373	.0168199021493017	.00137226	-0.0137 1.92e-5	0.0168(14)	C2H4-Cu-Cl 12CH4---63Cu37Cl v=0 DJK
5 .00026472474669823	.000265597282924526	5.3098e-5	0.0164 4.84e-7	2.656(531)e-4	C2H4-Cu-Cl 12CH4---63Cu37Cl v=0 DJ
6 63.8529338158731	63.8592019138942	.01572993	0.3985 .001391	63.859(16)	C2H4-Cu-Cl 12CH4---63Cu37Cl Copper CHlzz
7 -44.684284181583	-44.6935309276147	.16853963	-0.0549 .013986	-44.69(17)	C2H4-Cu-Cl 12CH4---63Cu37Cl Copper CHlxxmyy
8 -16.5659160263603	-16.5670249654437	.01604454	-0.0691 .001533	-16.567(16)	C2H4-Cu-Cl 12CH4---63Cu37Cl Chlorine CHlzz
9 -4.2	-3.94822862047448	.13317461	1.8905 .011027	-3.95(13)	C2H4-Cu-Cl 12CH4---63Cu37Cl Chlorine CHlxxmyy

Correlation Matrix

1	2	3	4	5	6	7	8	9
1 1.000								
2 -0.437	1.000							
3 -0.251	0.464	1.000						
4 -0.976	0.420	0.237	1.000					
5 0.904	-0.103	0.111	-0.909	1.000				
6 -0.167	0.277	0.259	0.203	-0.077	1.000			
7 0.166	0.022	0.064	-0.158	0.207	-0.034	1.000		
8 0.037	-0.122	-0.095	-0.035	-0.011	0.085	-0.009	1.000	
9 0.147	0.040	-0.023	-0.171	0.169	-0.035	-0.432	-0.040	1.000

¹²C₂H₄---⁶⁵Cu³⁷Cl (Page 1 of 2)

Pgopher 8.0.102 08 Dec 2013 16:55 32 bit (Delphi 18.5/18)

Mixture: 12C2 H4 --- 65Cu 37Cl Chirped-Pulse.pgo

Units MHz
PrintLevel Detail
Precision 4
BasisOrder boDefault
QuantumNumberFormat J
FitCycles 1
FitDetails False
AutoReplot True
AllowComplex False
NoLineList False
ShowEstUnc False
ShowDerivatives False
SVDlimit 5
SVDThresh 1E-15
ScaleChanges 1
Species: C2H4-Cu-Cl
Jmax 30
Concentration 1
AsymmetricMolecule: C2H4-Cu-Cl 12CH4---65Cu37Cl
nNuclei 2
Jmax 30
Colour \$FF8000
JAdjustSym False
BlockMatrix True
PointGroup C2v
Representation Ir
SReduction False
eeWt 1
eoWt 1
oeWt 1
ooWt 1
C2zAxis a
C2xAxis c
PseudoC2v False
FakeSym False
PhaseAdjust False
Abundance 1
AsymmetricManifold: C2H4-Cu-Cl 12CH4---65Cu37Cl Ground
Jmax 30
Initial True
EigenSearch True
LimitSearch True
AutoQConverge True
UsePopParams False
AsymmetricTop: C2H4-Cu-Cl 12CH4---65Cu37Cl v=0
Symmetry A1
Kmin 0
Kmax 10
A 23792.4752432385 Float
B 1933.2819531312 Float
C 1832.74662640056 Float
DJK 0.0223298445854635 Float
DJ 0.000174866784340803 Float
AsymmetricTopNucleus: C2H4-Cu-Cl 12CH4---65Cu37Cl Copper
Spin 1.5
AsNext False
CHlzz 59.1711925895412 Float
CHlxxmyy -41.6014296858364 Float
AsymmetricTopNucleus: C2H4-Cu-Cl 12CH4---65Cu37Cl Chlorine
Spin 1.5
AsNext False
CHlzz -16.58 Float
CHlxxmyy -3.99 Float
<N ,K |A|N,K> = K^2
<N ,K-2|B|N,K> = sqrt(((N*(N+1)+(-K+1)*(K-2))*(N*(N+1)-K*(K+1))))/4
<N ,K |B|N,K> = (N*(N+1)-K^2)/2
<N ,K+2|B|N,K> = sqrt(((N*(N+1)+(-K-1)*(K+2))*(N*(N+1)-K*(K+1))))/4
<N ,K-2|C|N,K> = (-sqrt(((N*(N+1)+(-K+1)*(K-2))*(N*(N+1)-K*(K+1))))/4
<N ,K |C|N,K> = (N*(N+1)-K^2)/2
<N ,K+2|C|N,K> = (-sqrt(((N*(N+1)+(-K-1)*(K+2))*(N*(N+1)-K*(K+1))))/4
<N ,K |DJK|N,K> = -N*(N+1)*K^2
<N ,K |DJ|N,K> = -N^2*(N+1)^2
TransitionMoments: C2H4-Cu-Cl 12CH4---65Cu37Cl <Ground|mu|Ground>
CartesianTransitionMoment: C2H4-Cu-Cl 12CH4---65Cu37Cl <v=0|a|v=0>
Axis a
Strength 1
Symbolic Matrix Elements not available for <v=0|a|v=0>

¹²C₆H₆---⁶⁵Cu³⁷Cl continued (Page 2 of 2)

Residuals before fit for 12CH4---65Cu37Cl for the Ground manifold

J"S" #	J"S" #	Observed	Calculated	Obs-Calc	StdDev	
6 B1 1	5 B2 1	11146.0440	11146.0497	-0.0057 1	.00064	0 : qR1,2(2)4.5,6,3,5,5 : 12CH4---65Cu37Cl v=0 3 1 3 4.5 6 -v=0 2 1 2 3.5 5 : 1:<LineList>
5 B1 3	4 B2 3	11149.7100	11149.7066	0.0034 1	.00048	0 : qR1,2(2)3.5,5,2,5,4 : 12CH4---65Cu37Cl v=0 3 1 3 3.5 5 -v=0 2 1 2 2.5 4 : 2:<LineList>
3 A2 6	2 A1 5	11295.1620	11295.1747	-0.0127 1	.00072	0 : qR0,2(2)3.5,3,2,5,2 : 12CH4---65Cu37Cl v=0 3 0 3 3.5 3 -v=0 2 0 2 2.5 2 : 3:<LineList>
4 A2 4	3 A1 4	11295.3390	11295.3434	-0.0044 1	.0012	0 : qR0,2(2)3.5,4,2,5,3 : 12CH4---65Cu37Cl v=0 3 0 3 3.5 4 -v=0 2 0 2 2.5 3 : 4:<LineList>
4 A2 2	3 A1 2	11295.9200	11295.9158	0.0042 1	.00129	0 : qR0,2(2)4.5,4,3,5,3 : 12CH4---65Cu37Cl v=0 3 0 3 4.5 4 -v=0 2 0 2 3.5 3 : 5:<LineList>
5 A2 1	4 A1 1	11295.9500	11295.9412	0.0088 1	.00165	0 : qR0,2(2)4.5,5,3,5,4 : 12CH4---65Cu37Cl v=0 3 0 3 4.5 5 -v=0 2 0 2 3.5 4 : 6:<LineList>
6 A2 1	5 A1 1	11296.1930	11296.1921	0.0009 1	.00212	0 : qR0,2(2)4.5,6,3,5,5 : 12CH4---65Cu37Cl v=0 3 0 3 4.5 6 -v=0 2 0 2 3.5 5 : 7:<LineList>
3 A2 4	2 A1 3	11296.2100	11296.1967	0.0133 1	.00102	0 : qR0,2(2)4.5,3,3,5,2 : 12CH4---65Cu37Cl v=0 3 0 3 4.5 3 -v=0 2 0 2 3.5 2 : 8:<LineList>
5 A2 2	4 A1 2	11296.3920	11296.4026	-0.0106 1	.00157	0 : qR0,2(2)3.5,5,2,5,4 : 12CH4---65Cu37Cl v=0 3 0 3 3.5 5 -v=0 2 0 2 2.5 4 : 9:<LineList>
6 B2 1	5 B1 1	11447.1120	11447.1136	-0.0016 1	.00066	0 : qR1,1(2)4.5,6,3,5,5 : 12CH4---65Cu37Cl v=0 3 1 2 4.5 6 -v=0 2 1 1 3.5 5 : 10:<LineList>
3 B2 7	2 B1 5	11447.3180	11447.3167	0.0013 1	.00032	0 : qR1,1(2)4.5,3,3,5,2 : 12CH4---65Cu37Cl v=0 3 1 2 4.5 3 -v=0 2 1 1 3.5 2 : 11:<LineList>
3 B2 9	2 B1 7	11450.0460	11450.0433	0.0027 1	.00024	0 : qR1,1(2)3.5,3,2,5,2 : 12CH4---65Cu37Cl v=0 3 1 2 3.5 3 -v=0 2 1 1 2.5 2 : 12:<LineList>
3 B2 10	2 B1 8	14861.1750	14861.1687	0.0063 1	.00026	0 : qR1,3(3)2.5,3,1,5,2 : 12CH4---65Cu37Cl v=0 4 1 4 2.5 3 -v=0 3 1 3 1.5 2 : 13:<LineList>
6 B2 2	5 B1 2	14861.2110	14861.2063	0.0047 1	.00063	0 : qR1,3(3)5.5,6,4,5,5 : 12CH4---65Cu37Cl v=0 4 1 4 5.5 6 -v=0 3 1 3 4.5 5 : 14:<LineList>
5 B2 4	4 B1 4	14861.1960	14861.1918	0.0042 1	.00053	0 : qR1,3(3)5.5,5,4,5,4 : 12CH4---65Cu37Cl v=0 4 1 4 5.5 5 -v=0 3 1 3 4.5 4 : 15:<LineList>
7 B2 1	6 B1 1	14861.6830	14861.6802	0.0028 1	.00078	0 : qR1,3(3)5.5,7,4,5,6 : 12CH4---65Cu37Cl v=0 4 1 4 5.5 7 -v=0 3 1 3 4.5 6 : 16:<LineList>
4 B2 8	3 B1 7	14861.8050	14861.8115	-0.0065 1	.00044	0 : qR1,3(3)5.5,4,4,5,3 : 12CH4---65Cu37Cl v=0 4 1 4 5.5 4 -v=0 3 1 3 4.5 3 : 17:<LineList>
4 B2 7	3 B1 6	14862.1040	14862.1149	-0.0109 1	.00037	0 : qR1,3(3)2.5,4,1,5,3 : 12CH4---65Cu37Cl v=0 4 1 4 2.5 4 -v=0 3 1 3 1.5 3 : 18:<LineList>
4 B2 10	3 B1 9	14862.2240	14862.2239	0.0001 1	.00035	0 : qR1,3(3)4.5,4,3,5,3 : 12CH4---65Cu37Cl v=0 4 1 4 4.5 4 -v=0 3 1 3 3.5 3 : 19:<LineList>
4 B2 9	3 B1 8	14862.4360	14862.4471	-0.0111 1	.0004	0 : qR1,3(3)3.5,4,2,5,3 : 12CH4---65Cu37Cl v=0 4 1 4 3.5 4 -v=0 3 1 3 2.5 3 : 20:<LineList>
3 B2 11	2 B1 9	14862.6170	14862.6171	-0.0001 1	.00027	0 : qR1,3(3)3.5,3,2,5,2 : 12CH4---65Cu37Cl v=0 4 1 4 3.5 3 -v=0 3 1 3 2.5 2 : 21:<LineList>
5 B2 6	4 B1 6	14862.8800	14862.8804	-0.0004 1	.00053	0 : qR1,3(3)3.5,5,3,5,4 : 12CH4---65Cu37Cl v=0 4 1 4 3.5 5 -v=0 3 1 3 3.5 4 : 22:<LineList>
5 B2 5	4 B1 5	14862.9590	14862.9579	0.0011 1	.00042	0 : qR1,3(3)4.5,5,2,5,4 : 12CH4---65Cu37Cl v=0 4 1 4 4.5 5 -v=0 3 1 3 2.5 4 : 23:<LineList>
6 B2 3	5 B1 3	14863.2150	14863.2031	0.0119 1	.00062	0 : qR1,3(3)4.5,6,3,5,5 : 12CH4---65Cu37Cl v=0 4 1 4 4.5 6 -v=0 3 1 3 3.5 5 : 24:<LineList>
4 A1 6	3 A2 6	15059.6640	15059.6562	0.0078 1	.00113	0 : qR0,3(3)4.5,4,3,5,3 : 12CH4---65Cu37Cl v=0 4 0 4 4.5 4 -v=0 3 0 3 3.5 3 : 25:<LineList>
5 A1 4	4 A2 4	15059.9980	15060.0004	-0.0024 1	.0016	0 : qR0,3(3)4.5,5,3,5,4 : 12CH4---65Cu37Cl v=0 4 0 4 4.5 5 -v=0 3 0 3 3.5 4 : 26:<LineList>
5 A1 2	4 A2 2	15060.0290	15060.0247	0.0043 1	.00165	0 : qR0,3(3)5.5,5,4,5,4 : 12CH4---65Cu37Cl v=0 4 0 4 5.5 5 -v=0 3 0 3 4.5 4 : 27:<LineList>
6 A1 1	5 A2 1	15060.1750	15060.1821	-0.0071 1	.00199	0 : qR0,3(3)5.5,6,4,5,5 : 12CH4---65Cu37Cl v=0 4 0 4 5.5 6 -v=0 3 0 3 4.5 5 : 28:<LineList>
7 A1 1	6 A2 1	15060.3070	15060.3094	-0.0024 1	.00242	0 : qR0,3(3)5.5,7,4,5,6 : 12CH4---65Cu37Cl v=0 4 0 4 5.5 7 -v=0 3 0 3 4.5 6 : 29:<LineList>
6 A1 2	5 A2 2	15060.3830	15060.3836	-0.0006 1	.0019	0 : qR0,3(3)4.5,6,3,5,5 : 12CH4---65Cu37Cl v=0 4 0 4 4.5 6 -v=0 3 0 3 3.5 5 : 30:<LineList>
2 A1 6	1 A2 4	15060.9200	15060.9167	0.0033 1	.00046	0 : qR0,3(3)2.5,2,1,5,1 : 12CH4---65Cu37Cl v=0 4 0 4 2.5 2 -v=0 3 0 3 1.5 1 : 31:<LineList>
4 A1 5	3 A2 5	15061.3860	15061.3863	-0.0003 1	.00119	0 : qR0,3(3)3.5,4,2,5,3 : 12CH4---65Cu37Cl v=0 4 0 4 3.5 4 -v=0 3 0 3 2.5 3 : 32:<LineList>
3 A1 6	2 A2 5	15061.4250	15061.4170	0.0080 1	.00083	0 : qR0,3(3)3.5,3,2,5,2 : 12CH4---65Cu37Cl v=0 4 0 4 3.5 3 -v=0 3 0 3 2.5 2 : 33:<LineList>
3 A1 5	2 A2 4	15061.6310	15061.6374	-0.0064 1	.0008	0 : qR0,3(3)2.5,3,1,5,2 : 12CH4---65Cu37Cl v=0 4 0 4 2.5 3 -v=0 3 0 3 1.5 2 : 34:<LineList>
5 A1 3	4 A2 3	15062.0370	15062.0392	-0.0022 1	.0014	0 : qR0,3(3)3.5,5,2,5,4 : 12CH4---65Cu37Cl v=0 4 0 4 3.5 5 -v=0 3 0 3 2.5 4 : 35:<LineList>
4 A1 3	3 A2 3	15062.3450	15062.3461	-0.0011 1	.00121	0 : qR0,3(3)2.5,4,1,5,3 : 12CH4---65Cu37Cl v=0 4 0 4 2.5 4 -v=0 3 0 3 1.5 3 : 36:<LineList>
6 B1 2	5 B2 2	15263.0030	15262.9980	0.0050 1	.00065	0 : qR1,2(3)5.5,6,4,5,5 : 12CH4---65Cu37Cl v=0 4 1 3 5.5 6 -v=0 3 1 2 4.5 5 : 37:<LineList>
5 B1 4	4 B2 4	15263.0030	15262.9982	0.0048 1	.00054	0 : qR1,2(3)5.5,5,4,5,4 : 12CH4---65Cu37Cl v=0 4 1 3 5.5 5 -v=0 3 1 2 4.5 4 : 38:<LineList>
7 B1 1	6 B2 1	15263.4790	15263.4724	0.0066 1	.00079	0 : qR1,2(3)5.5,7,4,5,6 : 12CH4---65Cu37Cl v=0 4 1 3 5.5 7 -v=0 3 1 2 4.5 6 : 39:<LineList>
4 B1 8	3 B2 7	15263.4790	15263.4837	-0.0047 1	.00045	0 : qR1,2(3)5.5,4,4,5,3 : 12CH4---65Cu37Cl v=0 4 1 3 5.5 4 -v=0 3 1 2 4.5 3 : 40:<LineList>
3 B1 10	2 B2 8	15264.1810	15264.1929	-0.0119 1	.00026	0 : qR1,2(3)2.5,3,1,5,2 : 12CH4---65Cu37Cl v=0 4 1 3 2.5 3 -v=0 3 1 2 1.5 2 : 41:<LineList>
4 B1 10	3 B2 9	15264.3660	15264.3612	0.0048 1	.00037	0 : qR1,2(3)4.5,4,3,5,3 : 12CH4---65Cu37Cl v=0 4 1 3 4.5 4 -v=0 3 1 2 3.5 3 : 42:<LineList>
5 B1 6	4 B2 6	15264.3910	15264.3913	-0.0003 1	.00051	0 : qR1,2(3)4.5,5,3,5,4 : 12CH4---65Cu37Cl v=0 4 1 3 4.5 5 -v=0 3 1 2 3.5 4 : 43:<LineList>
3 B1 11	2 B2 9	15265.6970	15265.6959	0.0011 1	.00027	0 : qR1,2(3)3.5,3,2,5,2 : 12CH4---65Cu37Cl v=0 4 1 3 3.5 3 -v=0 3 1 2 2.5 2 : 44:<LineList>
6 B1 3	5 B2 3	15265.0000	15264.9977	0.0023 1	.00063	0 : qR1,2(3)4.5,6,3,5,5 : 12CH4---65Cu37Cl v=0 4 1 3 4.5 6 -v=0 3 1 2 3.5 5 : 45:<LineList>
3 B1 12	2 B2 10	15265.0530	15265.0627	-0.0097 1	.00029	0 : qR1,2(3)4.5,3,3,5,2 : 12CH4---65Cu37Cl v=0 4 1 3 4.5 3 -v=0 3 1 2 3.5 2 : 46:<LineList>

46 Observations, 9 Parameters

Initial Average Error: 0.00693098361842117

Predicted New Error: 0.00692981485159749

Parameters:

# Old	New	Std Dev	Change/Std Sens	Summary	Name
1 23792.4752432385	23792.6821550021	114.99377	0.0018 .883141	23793(115)	C2H4-Cu-Cl 12CH4---65Cu37Cl v=0 A
2 1933.2819531312	1933.28195308932	.00110688	0.0000 1.95e-5	1933.2820(11)	C2H4-Cu-Cl 12CH4---65Cu37Cl v=0 B
3 1832.74662640056	1832.74662654434	.00107201	0.0001 1.86e-5	1832.7466(11)	C2H4-Cu-Cl 12CH4---65Cu37Cl v=0 C
4 .0223298445854635	.0223267634492082	.00171588	-0.0018 1.31e-5	0.02233(172)	C2H4-Cu-Cl 12CH4---65Cu37Cl v=0 DJK
5 .000174866784340803	.000174995321767933	5.6908e-5	0.0023 3.39e-7	1.750(569)e-4	C2H4-Cu-Cl 12CH4---65Cu37Cl v=0 DJ
6 59.1711925895412	59.172700228163	.06849295	0.0220 .004205	59.173(68)	C2H4-Cu-Cl 12CH4---65Cu37Cl Copper CHlzz
7 -41.6014296858364	-41.6028019179244	.23292762	-0.0059 .014113	-41.60(23)	C2H4-Cu-Cl 12CH4---65Cu37Cl Copper CHlxxmyy
8 -16.58	-16.5770144747625	.04883242	0.0611 .003056	-16.577(49)	C2H4-Cu-Cl 12CH4---65Cu37Cl Chlorine CHlzz
9 -3.99	-3.98345526609938	.14542501	0.0450 .008987	-3.98(15)	C2H4-Cu-Cl 12CH4---65Cu37Cl Chlorine CHlxxmyy

Correlation Matrix

1	2	3	4	5	6	7	8	9
1 1.000								
2 -0.582 1.000								
3 -0.535 0.781 1.000								
4 -0.985 0.568 0.527 1.000								
5 0.868 -0.150 -0.092 -0.875 1.000								
6 -0.286 0.372 0.286 0.275 -0.140 1.000								
7 -0.043 -0.148 -0.056 0.082 -0.123 -0.249 1.000								
8 0.244 -0.127 -0.057 -0.261 0.266 -0.418 0.018 1.000								
9 0.070 0.123 -0.011 -0.095 0.120 0.124 -0.500 -0.196 1.000								

Pgopher 8.0.169 24 Jan 2014 9:23 32 bit (Delphi 18.5/18)
Mixture: 13C2 H4 --- 63Cu 35Cl Balle Flygare.pgo

Units MHz
PrintLevel Detail
Precision 4
BasisOrder boDefault
QuantumNumberFormat J
FitCycles 1
FitDetails False
AutoReplot True
AllowComplex False
NoLineList False
ShowEstUnc False
ShowDerivatives False
SVDlimit 5
SVDThresh 1E-15
ScaleChanges 1
Species: Species
Jmax 25
Concentration 1
AsymmetricMolecule: AsymmetricTop
nNuclei 2
JAdjustSym False
BlockMatrix True
PointGroup C2v
Representation Ir
SReduction False
eeWt 1
eoWt 1
oeWt 1
ooWt 1
C2zAxis a
C2xAxis c
PseudoC2v False
FakeSym False
PhaseAdjust False
Abundance 1
AsymmetricManifold: Ground

Initial True
EigenSearch True
LimitSearch True
AutoQConverge True
UsePopParams False
AsymmetricTop: v=0
Symmetry A1
Kmin all
Kmax all
A 23068
B 1925.88759576665 Float
C 1819.72162573762 Float
DJK 0.01802
DJ 0.0002498
AsymmetricTopNucleus: Copper
Spin 1.5
AsNext False
CHlzz 63.7777
CHlxxmyy -44.521
AsymmetricTopNucleus: Chlorine
Spin 1.5
AsNext False
CHlzz -20.992
CHlxxmyy -5.093
<N ,K |A|N,K> = K^2
<N ,K-2|B|N,K> = sqrt((N*(N+1)+(-K+1)*(K-2))*(N*(N+1)-K*(K-1)))/4
<N ,K |B|N,K> = (N*(N+1)-K^2)/2
<N ,K+2|B|N,K> = sqrt((N*(N+1)+(-K-1)*(K+2))*(N*(N+1)-K*(K+1)))/4
<N ,K-2|C|N,K> = (-sqrt((N*(N+1)+(-K+1)*(K-2))*(N*(N+1)-K*(K-1)))/4
<N ,K |C|N,K> = (N*(N+1)-K^2)/2
<N ,K+2|C|N,K> = (-sqrt((N*(N+1)+(-K-1)*(K+2))*(N*(N+1)-K*(K+1)))/4
<N ,K |DJK|N,K> = -N*(N+1)*K^2
<N ,K |DJ|N,K> = -N^2*(N+1)^2
TransitionMoments: <Ground|mu|Ground>
CartesianTransitionMoment: <v=0|a|v=0>
Axis a
Strength 1
Symbolic Matrix Elements not available for <v=0|a|v=0>

Residuals before fit for AsymmetricTop for the Ground manifold

J"S'	#'	J"S"	#"	Observed	Calculated	Obs-Calc	StdDev	
4 A1	1	3 A2	1	7489.1237	7489.1255	-0.0018	1	1.3e-6 0 : qR0,1(1)3.5,4,2.5,3 : v=0 2 0 2 3.5 4 - v=0 1 0 1 2.5 3 : 1:<LineList>
5 A1	1	4 A2	1	7489.9063	7489.9077	-0.0014	1	1.9e-6 0 : qR0,1(1)3.5,5,2.5,4 : v=0 2 0 2 3.5 5 - v=0 1 0 1 2.5 4 : 2:<LineList>
3 A2	6	2 A1	5	11233.3578	11233.3673	-0.0095	1	1.8e-6 0 : qR0,2(2)3.5,3,2.5,2 : v=0 3 0 3 3.5 3 - v=0 2 0 2 2.5 2 : 3:<LineList>
4 A2	4	3 A1	4	11233.7020	11233.7114	-0.0094	1	3e-6 0 : qR0,2(2)3.5,4,2.5,3 : v=0 3 0 3 3.5 4 - v=0 2 0 2 2.5 3 : 4:<LineList>
5 A2	1	4 A1	1	11234.4075	11234.4072	0.0003	1	4.1e-6 0 : qR0,2(2)4.5,5,3.5,4 : v=0 3 0 3 4.5 5 - v=0 2 0 2 3.5 4 : 5:<LineList>
4 A2	2	3 A1	2	11234.4125	11234.4125	-0.0000	1	3.2e-6 0 : qR0,2(2)4.5,4,3.5,3 : v=0 3 0 3 4.5 4 - v=0 2 0 2 3.5 3 : 6:<LineList>
6 A2	1	5 A1	1	11234.7112	11234.7153	-0.0041	1	5.3e-6 0 : qR0,2(2)4.5,6,3.5,5 : v=0 3 0 3 4.5 6 - v=0 2 0 2 3.5 5 : 7:<LineList>
5 A2	2	4 A1	2	11234.9653	11234.9755	-0.0102	1	3.9e-6 0 : qR0,2(2)3.5,5,2.5,4 : v=0 3 0 3 3.5 5 - v=0 2 0 2 2.5 4 : 8:<LineList>
3 A2	5	2 A1	4	11236.6605	11236.6755	-0.0150	1	2e-6 0 : qR0,2(2)2.5,3,1.5,2 : v=0 3 0 3 2.5 3 - v=0 2 0 2 1.5 2 : 9:<LineList>
4 A2	3	3 A1	3	11238.5764	11238.5796	-0.0032	1	2.4e-6 0 : qR0,2(2)2.5,4,1.5,3 : v=0 3 0 3 2.5 4 - v=0 2 0 2 1.5 3 : 10:<LineList>
5 A1	3	4 A2	3	14979.8497	14979.8619	-0.0122	1	5.9e-6 0 : qR0,3(3)3.5,5,2.5,4 : v=0 4 0 4 3.5 5 - v=0 3 0 3 2.5 4 : 11:<LineList>
4 A1	5	3 A2	5	14979.1158	14979.1330	-0.0172	1	5.2e-6 0 : qR0,3(3)3.5,4,2.5,3 : v=0 4 0 4 3.5 4 - v=0 3 0 3 2.5 3 : 12:<LineList>

12 Observations, 2 Parameters
Initial Average Error: 0.00991860080187013
Predicted New Error: 0.00466819195415297
Parameters:

#	Old	New	Std Dev	Change/Std Sens	Summary	Name
1	1925.88759576665	1925.97980032988	.04900845	1.8814	1925.9798(490)	v=0 B
2	1819.72162573762	1819.62918080478	.04783588	-1.9325	1819.6292(478)	v=0 C

Correlation Matrix

1	2
1	1.000
2	-1.000 1.000

Pgopher 8.0.169 24 Jan 2014 9:23 32 bit (Delphi 18.5/18)
Mixture: 13C2 H4 ---65Cu 35Cl Balle Flygare.pgo

Units MHz
PrintLevel Detail
Precision 4
BasisOrder boDefault
QuantumNumberFormat J
FitCycles 1
FitDetails False
AutoReplot True
AllowComplex False
NoLineList False
ShowEstUnc False
ShowDerivatives False
SVDlimit 5
SVDThresh 1E-15
ScaleChanges 1
Species: Species
Jmax 25
Concentration 1
AsymmetricMolecule: AsymmetricTop
nNuclei 2
JAdjustSym False
BlockMatrix True
PointGroup C2v
Representation lr
SReduction False
eeWt 1
eoWt 1
oeWt 1
ooWt 1
C2zAxis a
C2xAxis c
PseudoC2v False
FakeSym False
PhaseAdjust False

Abundance 1
AsymmetricManifold: Ground
Initial True
EigenSearch True
LimitSearch True
AutoQConverge True
UsePopParams False
AsymmetricTop: v=0
Symmetry A1
Kmin all
Kmax all
A 23068
BBar 1872.64648818493 Float
BDelta 106.30871
DJK 0.01804
DJ 0.0002498
AsymmetricTopNucleus: Copper
Spin 1.5
AsNext False
CHlzz 59.058
CHlxxmyy -41.39
AsymmetricTopNucleus: Chlorine
Spin 1.5
AsNext False
CHlzz -20.992
CHlxxmyy -4.97
<N ,K |A|N,K> = K^2
<N ,K |BBar|N,K> = N*(N+1)-K^2
<N ,K-2|BDelta|N,K> = sqrt(((N*(N+1)+(-K+1)*(K-2))*(N*(N+1)-K*(K-1))))/4
<N ,K+2|BDelta|N,K> = sqrt(((N*(N+1)+(-K-1)*(K+2))*(N*(N+1)-K*(K+1))))/4
<N ,K |DJK|N,K> = -N*(N+1)*K^2
<N ,K |DJ|N,K> = -N^2*(N+1)^2
TransitionMoments: <Ground|mu|Ground>
CartesianTransitionMoment: <v=0|a|v=0>
Axis a
Strength 1
Symbolic Matrix Elements not available for <v=0|a|v=0>

Residuals before fit for AsymmetricTop for the Ground manifold

J"S'	#'	J"S"	#"	Observed	Calculated	Obs-Calc	StdDev	
4 A2 4	3 A1 4	11232.8443	11232.8547	-0.0104	1	.00117	0 : qR0,2(2)4,5,4,2,5,3 : v=0	3 0 3 4.5 4 - v=0 2 0 2 2.5 3 : 3:<LineList>
5 A2 1	4 A1 1	11233.5122	11233.5142	-0.0020	1	.00159	0 : qR0,2(2)3,5,5,2,5,4 : v=0	3 0 3 3.5 5 - v=0 2 0 2 2.5 4 : 4:<LineList>
4 A2 2	3 A1 2	11233.5361	11233.5395	-0.0034	1	.00123	0 : qR0,2(2)2,5,4,1,5,3 : v=0	3 0 3 2.5 4 - v=0 2 0 2 1.5 3 : 5:<LineList>
6 A2 1	5 A1 1	11233.8140	11233.8171	-0.0031	1	.00205	0 : qR0,2(2)4,5,6,3,5,5 : v=0	3 0 3 4.5 6 - v=0 2 0 2 3.5 5 : 6:<LineList>
3 A2 4	2 A1 3	11233.8773	11233.8791	-0.0018	1	.00097	0 : qR0,2(2)1,5,3,1,5,2 : v=0	3 0 3 1.5 3 - v=0 2 0 2 1.5 2 : 7:<LineList>
5 A2 2	4 A1 2	11234.0660	11234.0752	-0.0092	1	.00154	0 : qR0,2(2)3,5,5,2,5,4 : v=0	3 0 3 3.5 5 - v=0 2 0 2 2.5 4 : 8:<LineList>
4 A2 3	3 A1 3	11237.3152	11237.3292	-0.0140	1	.00091	0 : qR0,2(2)3,5,4,3,5,3 : v=0	3 0 3 3.5 4 - v=0 2 0 2 3.5 3 : 9:<LineList>

7 Observations, 1 Parameters
Initial Average Error: 0.00834974842545383
Predicted New Error: 0.00486506254344094
Parameters:

#	Old	New	Std Dev	Change/Std	Sens	Summary	Name
1	1872.64648818493	1872.64544107301	.00030647	-3.4166	8.11e-5	1872.64544(31)	v=0 BBar