

Supplementary Data for:

Three Coordinate, Cyclic Bent Allene Fe Complexes

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X-ray Data Collection and Reduction. Crystals were coated in Paratone-N oil in the glovebox, mounted on a MiTegen Micromount, and placed under a N₂ stream, thus maintaining a dry, O₂-free environment for each crystal. The data were collected on a Bruker Apex II diffractometer using a graphite monochromator with Mo K α radiation ($\lambda = 0.71073$ Å). The data were collected at 150((2) K for all crystals. The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. Data were corrected for absorption effects using the empirical multiscan method (SADABS).

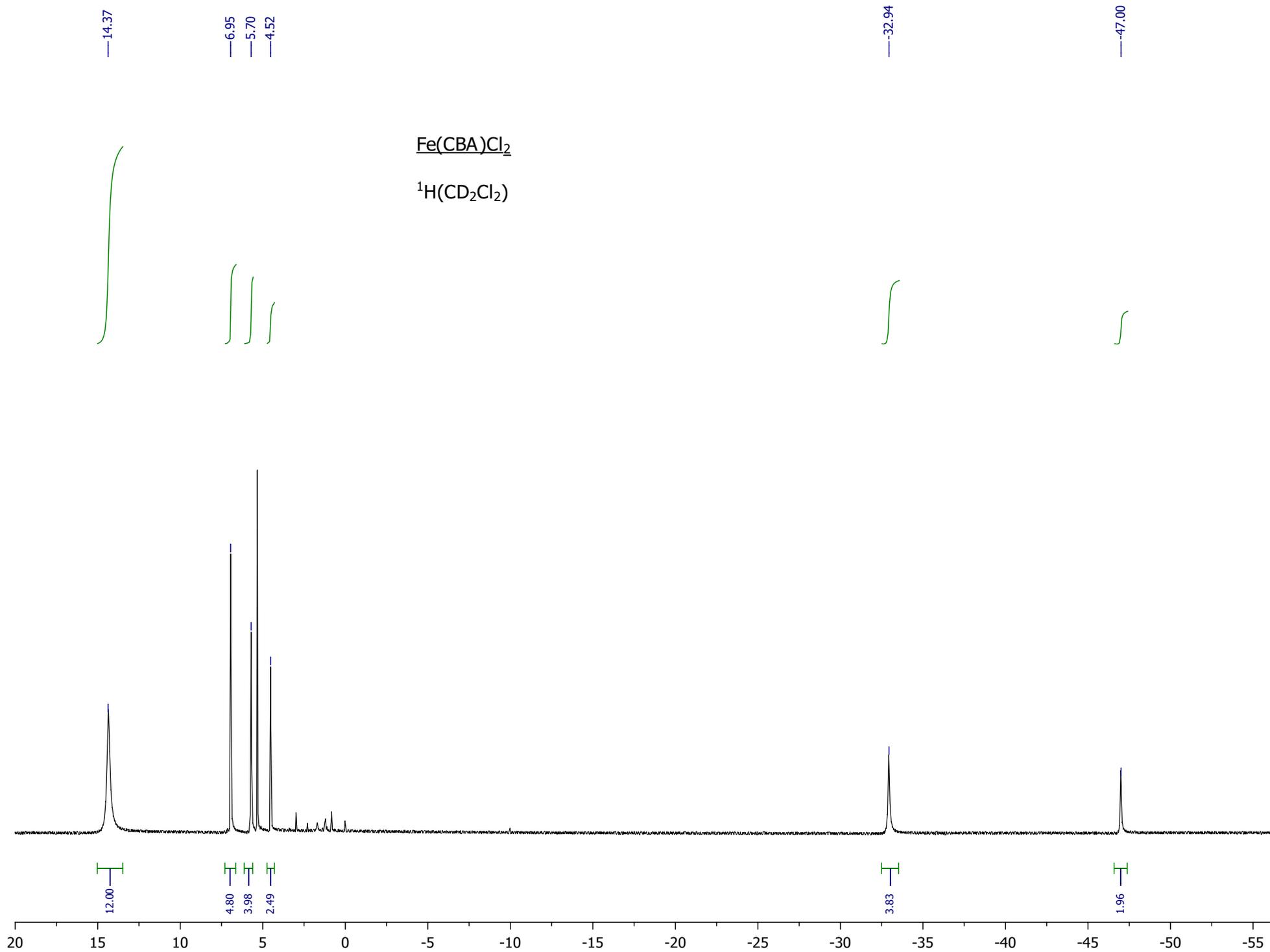
Structure Solution and Refinement. The structures were solved by direct methods using XS and refined by full-matrix least squares on F² using XL as implemented in the SHELXTL suite of programs. All non-hydrogen atoms were refined anisotropically. Carbon bound hydrogen atoms were placed in calculated positions using an appropriate riding model and coupled isotropic temperature factors.

Table 1 Crystallographic Data

	2•C₇H₈	3	4•C₆H₆
Formula	C ₃₈ H ₃₆ Cl ₂ FeN ₂ O ₂	C ₄₅ H ₄₂ FeN ₂ O ₂	C ₄₁ H ₃₄ FeN ₂ O ₆
wt	679.44	689.66	706.55
Cryst. syst.	monoclinic	orthorhombic	triclinic
Space group	P2 ₁ /c	Pbca	P-1
a(Å)	10.7373(12)	20.7197(11)	11.2843(8)
b(Å)	22.229(2)	17.4954(10)	12.3459(7)
c(Å)	16.1552(18)	20.3989(11)	14.570(1)
α (deg)	90.00	90.00	109.054(3)
β (deg)	116.914(7)	90.00	104.225(3)
γ (deg)	90.00	90.00	100.875(3)
V(Å ³)	3438.3(6)	7201.9(7)	1777.9(2)
Z	4	8	2
d(calc) gcm ⁻³	1.313	1.289	1.320
R(int)	0.149	0.0669	0.0255
μ , mm ⁻¹	0.629	0.460	0.474
Total data	35708	62770	29973
>2 σ (F _o ²)	6056	8290	8072
Variables	411	455	451
R (>2 σ)	0.0518	0.0384	0.0408
R _w	0.1084	0.0881	0.1185
GOF	0.950	1.007	1.054

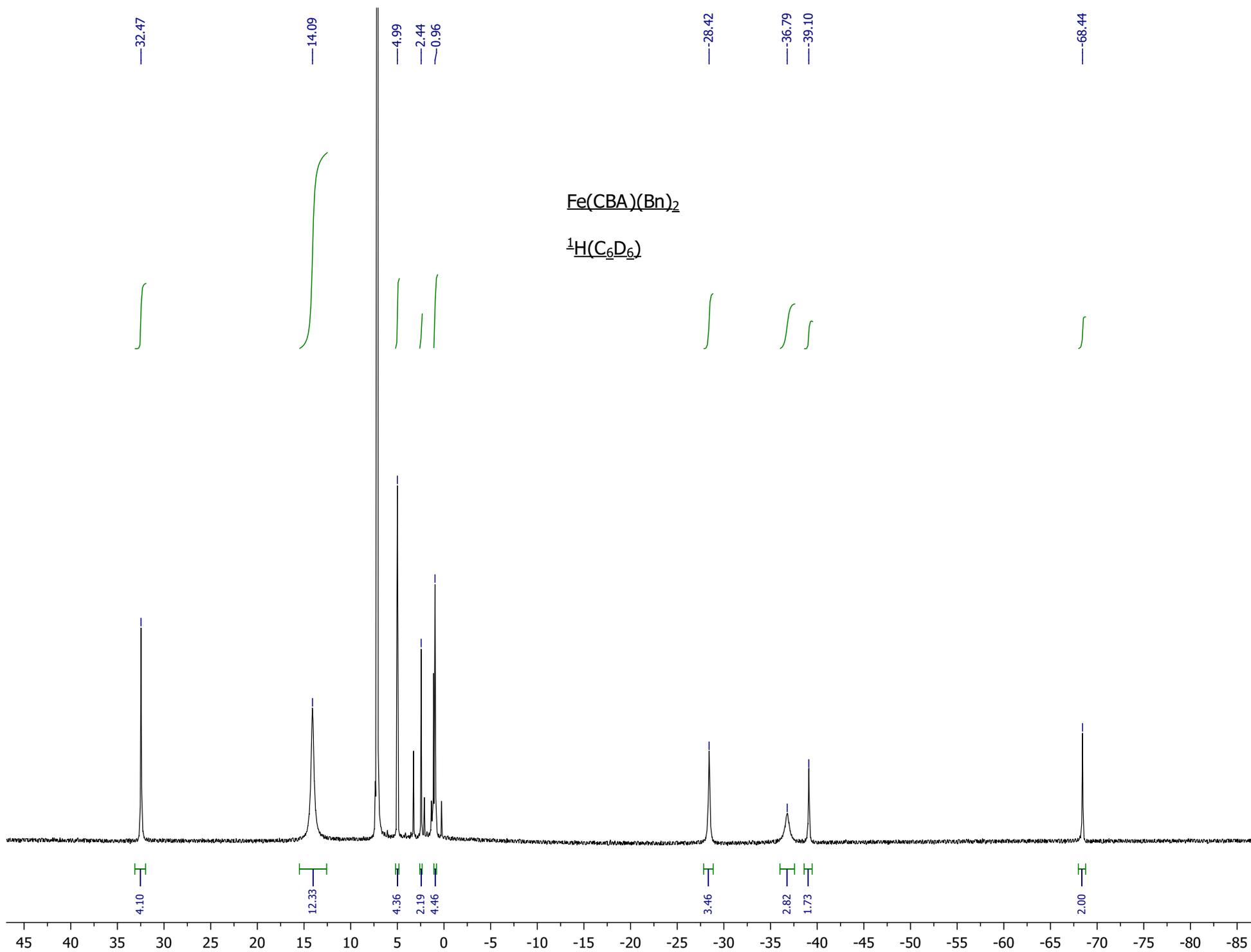
Fe(CBA)Cl₂

¹H(CD₂Cl₂)



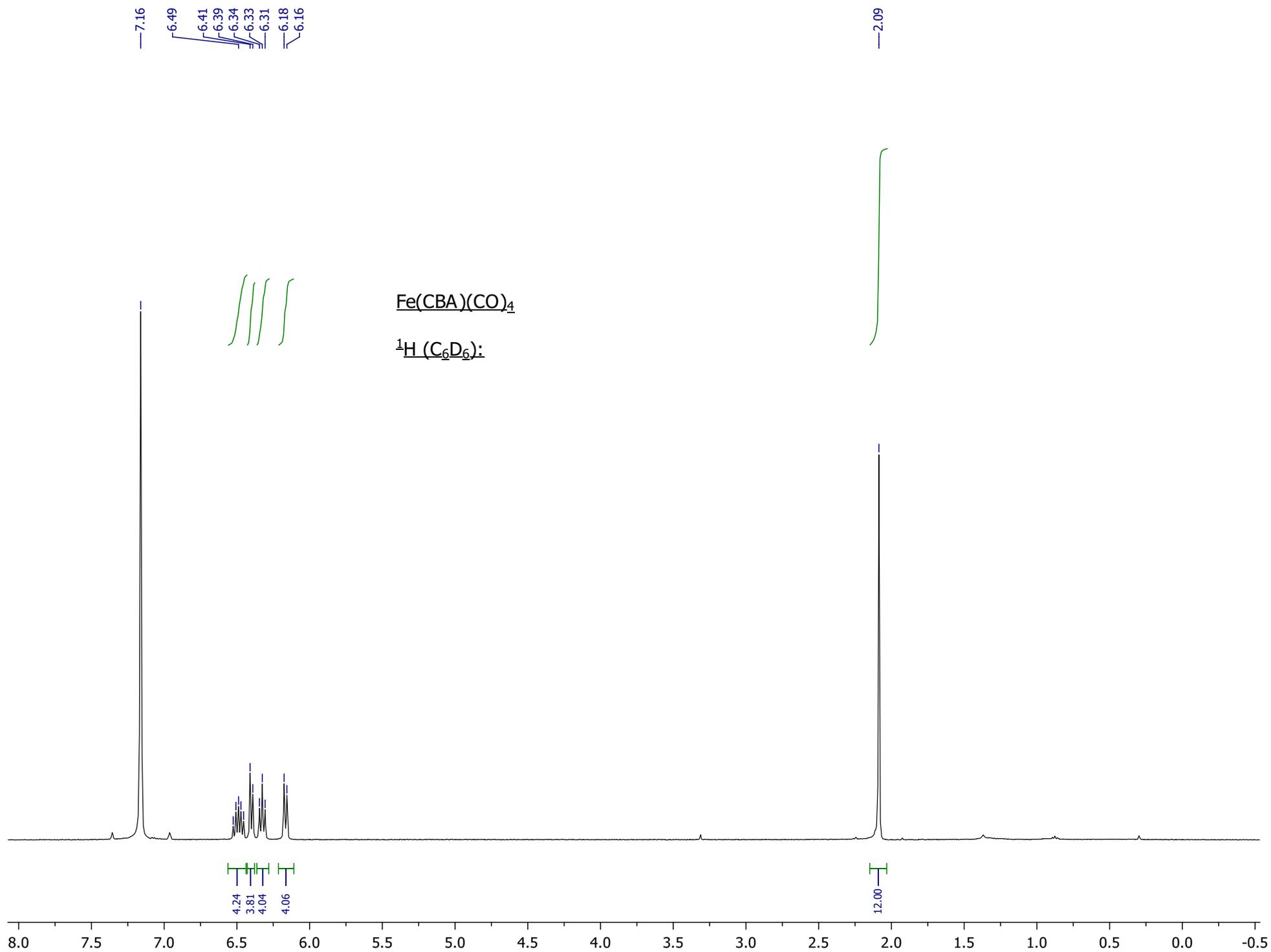
Fe(CBA)(Bn)₂

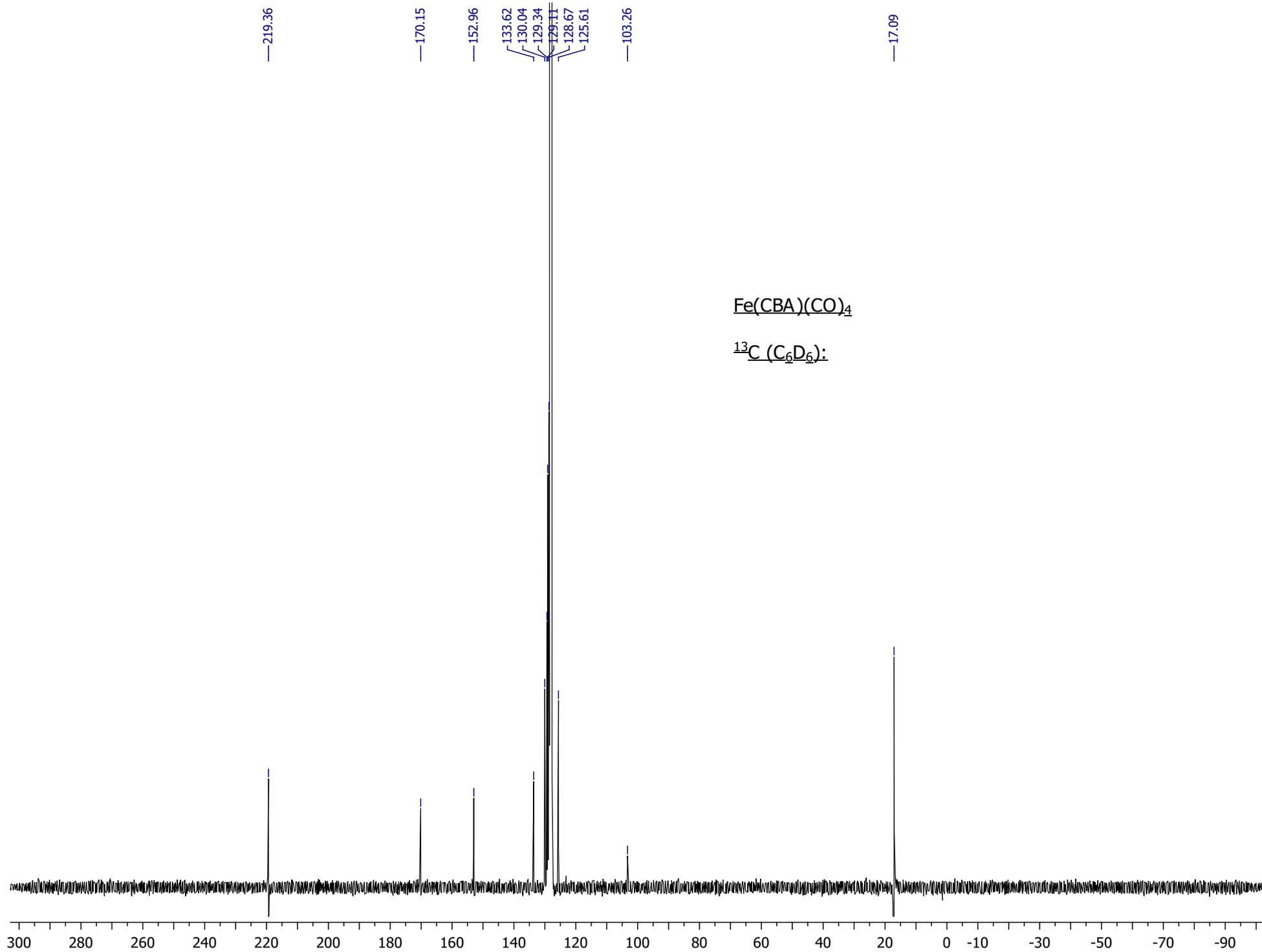
¹H(C₆D₆)

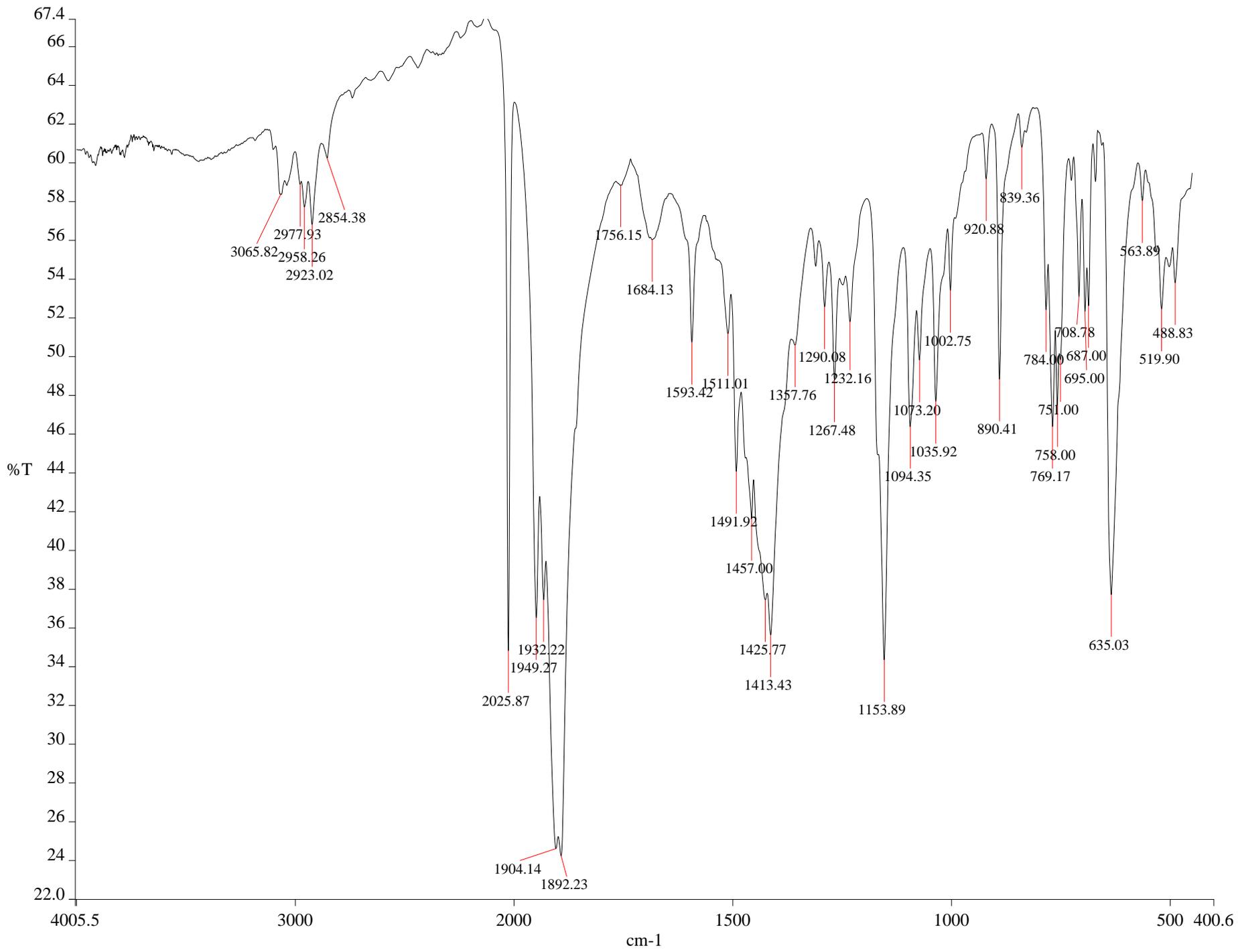


Fe(CBA)(CO)₄

¹H (C₆D₆)₂

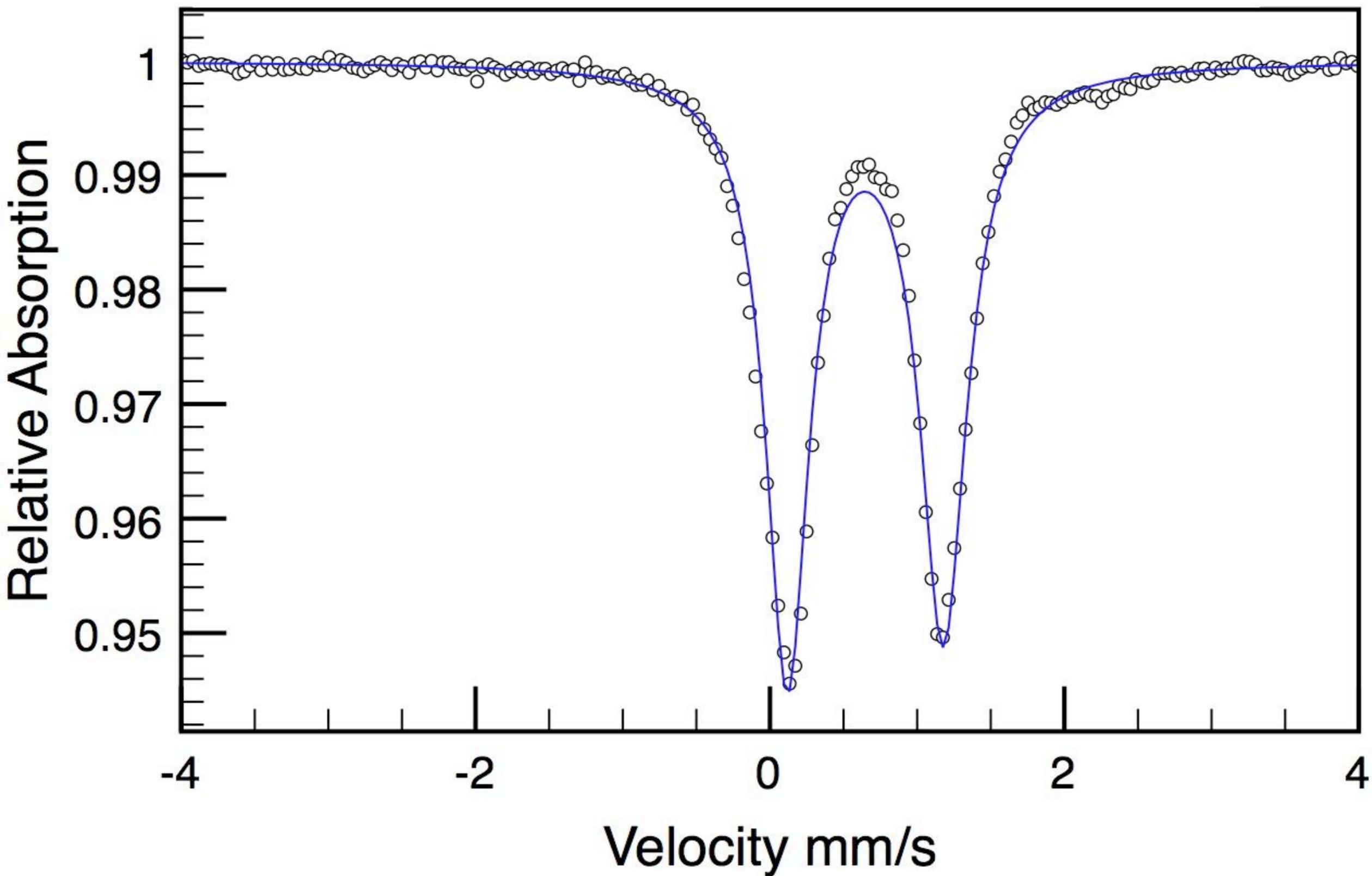






c:\pel_data\spectra\cp\fecbac04.sp

Mössbauer Spectrum of 4 recorded at 80K in zero field



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0.000000E+00	0.000000E+00	0.000000E+00									
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-9.592	0.016										
-9.553	-0.024										
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0.000000E+00	0.000000E+00	0.000000E+00									
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-5.385 -0.016
-5.347 -0.016
-5.308 -0.017
-5.269 -0.017
-5.231 -0.017
-5.192 -0.017
-5.154 -0.017
-5.115 -0.017
-5.077 -0.017
-5.038 -0.018
-4.999 -0.018
-4.961 -0.018
-4.922 -0.018
-4.884 -0.018

-4.845	-0.018
-4.806	-0.019
-4.768	-0.019
-4.729	-0.019
-4.691	-0.019
-4.652	-0.019
-4.613	-0.020
-4.575	-0.020
-4.536	-0.020
-4.498	-0.020
-4.459	-0.020
-4.420	-0.021
-4.382	-0.021
-4.343	-0.021
-4.305	-0.021
-4.266	-0.022
-4.228	-0.022
-4.189	-0.022
-4.150	-0.022
-4.112	-0.023
-4.073	-0.023
-4.035	-0.023
-3.996	-0.023
-3.957	-0.024
-3.919	-0.024
-3.880	-0.024
-3.842	-0.025
-3.803	-0.025
-3.764	-0.025
-3.726	-0.026
-3.687	-0.026
-3.649	-0.026
-3.610	-0.027
-3.572	-0.027
-3.533	-0.028
-3.494	-0.028
-3.456	-0.028
-3.417	-0.029
-3.379	-0.029
-3.340	-0.030
-3.301	-0.030
-3.263	-0.031
-3.224	-0.031
-3.186	-0.032
-3.147	-0.032
-3.108	-0.033
-3.070	-0.034

-3.031	-0.034
-2.993	-0.035
-2.954	-0.035
-2.915	-0.036
-2.877	-0.037
-2.838	-0.037
-2.800	-0.038
-2.761	-0.039
-2.723	-0.040
-2.684	-0.041
-2.645	-0.041
-2.607	-0.042
-2.568	-0.043
-2.530	-0.044
-2.491	-0.045
-2.452	-0.046
-2.414	-0.047
-2.375	-0.049
-2.337	-0.050
-2.298	-0.051
-2.259	-0.052
-2.221	-0.054
-2.182	-0.055
-2.144	-0.057
-2.105	-0.058
-2.066	-0.060
-2.028	-0.062
-1.989	-0.063
-1.951	-0.065
-1.912	-0.067
-1.874	-0.069
-1.835	-0.072
-1.796	-0.074
-1.758	-0.076
-1.719	-0.079
-1.681	-0.082
-1.642	-0.085
-1.603	-0.088
-1.565	-0.091
-1.526	-0.095
-1.488	-0.098
-1.449	-0.102
-1.410	-0.107
-1.372	-0.111
-1.333	-0.116
-1.295	-0.122

-1.256	-0.127
-1.218	-0.134
-1.179	-0.140
-1.140	-0.147
-1.102	-0.155
-1.063	-0.164
-1.025	-0.173
-0.986	-0.184
-0.947	-0.195
-0.909	-0.207
-0.870	-0.221
-0.832	-0.237
-0.793	-0.254
-0.754	-0.273
-0.716	-0.295
-0.677	-0.319
-0.639	-0.347
-0.600	-0.379
-0.561	-0.416
-0.523	-0.459
-0.484	-0.509
-0.446	-0.569
-0.407	-0.639
-0.369	-0.724
-0.330	-0.827
-0.291	-0.954
-0.253	-1.112
-0.214	-1.310
-0.176	-1.562
-0.137	-1.886
-0.098	-2.301
-0.060	-2.829
-0.021	-3.479
0.017	-4.222
0.056	-4.945
0.095	-5.443
0.133	-5.509
0.172	-5.118
0.210	-4.448
0.249	-3.721
0.287	-3.070
0.326	-2.541
0.365	-2.131
0.403	-1.820
0.442	-1.589
0.480	-1.419
0.519	-1.297

0.558 -1.214
0.596 -1.165
0.635 -1.145
0.673 -1.152
0.712 -1.188
0.751 -1.254
0.789 -1.354
0.828 -1.495
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0.905 -1.938
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1.021 -3.210
1.059 -3.812
1.098 -4.429
1.136 -4.923
1.175 -5.127
1.214 -4.954
1.252 -4.471
1.291 -3.840
1.329 -3.207
1.368 -2.648
1.407 -2.186
1.445 -1.815
1.484 -1.521
1.522 -1.288
1.561 -1.101
1.600 -0.951
1.638 -0.829
1.677 -0.728
1.715 -0.645
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1.793 -0.517
1.831 -0.467
1.870 -0.424
1.908 -0.387
1.947 -0.354
1.985 -0.326
2.024 -0.301
2.063 -0.279
2.101 -0.260
2.140 -0.242
2.178 -0.226
2.217 -0.212
2.256 -0.200
2.294 -0.188

2.333 -0.177
2.371 -0.168
2.410 -0.159
2.449 -0.151
2.487 -0.143
2.526 -0.137
2.564 -0.130
2.603 -0.124
2.641 -0.119
2.680 -0.114
2.719 -0.109
2.757 -0.105
2.796 -0.101
2.834 -0.097
2.873 -0.093
2.912 -0.090
2.950 -0.086
2.989 -0.083
3.027 -0.081
3.066 -0.078
3.105 -0.075
3.143 -0.073
3.182 -0.071
3.220 -0.068
3.259 -0.066
3.298 -0.064
3.336 -0.063
3.375 -0.061
3.413 -0.059
3.452 -0.058
3.490 -0.056
3.529 -0.055
3.568 -0.053
3.606 -0.052
3.645 -0.051
3.683 -0.049
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3.761 -0.047
3.799 -0.046
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3.876 -0.044
3.915 -0.043
3.954 -0.042
3.992 -0.041
4.031 -0.040
4.069 -0.040
4.108 -0.039

4.146	-0.038
4.185	-0.037
4.224	-0.037
4.262	-0.036
4.301	-0.035
4.339	-0.035
4.378	-0.034
4.417	-0.033
4.455	-0.033
4.494	-0.032
4.532	-0.032
4.571	-0.031
4.610	-0.031
4.648	-0.030
4.687	-0.030
4.725	-0.029
4.764	-0.029
4.803	-0.028
4.841	-0.028
4.880	-0.027
4.918	-0.027
4.957	-0.027
4.995	-0.026
5.034	-0.026
5.073	-0.026
5.111	-0.025
5.150	-0.025
5.188	-0.025
5.227	-0.024
5.266	-0.024
5.304	-0.024
5.343	-0.023
5.381	-0.023
5.420	-0.023
5.459	-0.022
5.497	-0.022
5.536	-0.022
5.574	-0.022
5.613	-0.021
5.652	-0.021
5.690	-0.021
5.729	-0.021
5.767	-0.021
5.806	-0.020
5.844	-0.020
5.883	-0.020

5.922	-0.020
5.960	-0.019
5.999	-0.019
6.037	-0.019
6.076	-0.019
6.115	-0.019
6.153	-0.019
6.192	-0.018
6.230	-0.018
6.269	-0.018
6.308	-0.018
6.346	-0.018
6.385	-0.018
6.423	-0.017
6.462	-0.017
6.500	-0.017
6.539	-0.017
6.578	-0.017
6.616	-0.017
6.655	-0.017
6.693	-0.016
6.732	-0.016
6.771	-0.016
6.809	-0.016
6.848	-0.016
6.886	-0.016
6.925	-0.016
6.964	-0.016
7.002	-0.015
7.041	-0.015
7.079	-0.015
7.118	-0.015
7.157	-0.015
7.195	-0.015
7.234	-0.015
7.272	-0.015
7.311	-0.015
7.349	-0.014
7.388	-0.014
7.427	-0.014
7.465	-0.014
7.504	-0.014
7.542	-0.014
7.581	-0.014
7.620	-0.014
7.658	-0.014
7.697	-0.014

7.735 -0.014
7.774 -0.013
7.813 -0.013
7.851 -0.013
7.890 -0.013
7.928 -0.013
7.967 -0.013
8.005 -0.013
8.044 -0.013
8.083 -0.013
8.121 -0.013
8.160 -0.013
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8.237 -0.013
8.276 -0.013
8.314 -0.012
8.353 -0.012
8.391 -0.012
8.430 -0.012
8.469 -0.012
8.507 -0.012
8.546 -0.012
8.584 -0.012
8.623 -0.012
8.662 -0.012
8.700 -0.012
8.739 -0.012
8.777 -0.012
8.816 -0.012
8.854 -0.012
8.893 -0.012
8.932 -0.012
8.970 -0.012
9.009 -0.011
9.047 -0.011
9.086 -0.011
9.125 -0.011
9.163 -0.011
9.202 -0.011
9.240 -0.011
9.279 -0.011
9.318 -0.011
9.356 -0.011
9.395 -0.011
9.433 -0.011
9.472 -0.011

9.511	-0.011
9.549	-0.011
9.588	-0.011
9.626	-0.011
9.665	-0.011
9.703	-0.011
9.742	-0.011
9.781	-0.011
9.819	-0.011
9.858	-0.011
9.896	-0.011
9.935	-0.010

WMOSS Program, WEB Research Co., 612-942-6276

'output.po

'Example parameter input file for quadrupole doublets

'-----Comment Line 2-----

'Reduced Chi squared = 2.882 for fit to data:

' 12100401

Fit Controls

#	name	value
1	'Nfipar	12
2	'Version #	-6
3	'Report>Prn'	0
4	'Maxit Glob'	0
5	'Maxit Locl'	999
6	'Maxit Area'	0
7	'Report Glo'	1
8	'Report Loc'	3
9	'N Anneal	0
10	'Perturb	0
11	'Theor.Modl'	3
12	'Fit Method'	5

Parameter Output File

'output.po

Global Integer Parameters

#	name	value
101	'Ngipar	3
102	'Ngpar	0
103	'N Sites	1

Global Nonlinear Parameters

#	name	value	kon	lb	ub
---	------	-------	-----	----	----

Local 1 Local 1 Local 1 Local 1 Local 1 Local 1

Local Integer Parameters

#	name	value
101	'NLIPAR	3
102	'NLPAR	4
103	'Nlnpar	1

Local Linear Parameters

#	name	value	kon	wt
---	------	-------	-----	----

101 'Rel. Area ' 0.9799179 101 1.000000

Local Nonlinear Parameters

#	name	value	kon	lb	ub
101	'Shift	' 0.6480341	101	-.5000000	2.000000
102	'dEq	' 1.059656	102	0.0000000E+00	4.000000
103	'Gamma L	' 0.3582211	103	0.2000000	0.5000000
104	'Gamma R	' 0.3876445	104	0.2000000	0.5000000