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

Calculations on ferrocene the H/Mu adducts of ferrocene

All calculations were performed with the Gaussian 09 package of programs along with the UB3LYP functional and the 6-311++g(2d,p) basis set. Frequency calculations were performed on the optimized structures and the reported energies are the sum of electronic and zero-point energies.

Ferrocene with eclipsed Cp rings

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.690393	0.539183	1.084476
2	6	0	-1.690820	1.197951	-0.177552
3	6	0	-1.691573	0.201186	-1.194004
4	6	0	-1.691467	-1.073572	-0.560185
5	6	0	-1.690802	-0.864695	0.848017
6	1	0	-1.672327	1.019435	2.050226
7	1	0	-1.673030	2.264906	-0.335705
8	1	0	-1.674775	0.380537	-2.257562
9	1	0	-1.674357	-2.029735	-1.059454
10	1	0	-1.673018	-1.634861	1.603153
11	26	0	-0.000089	-0.000126	-0.000517
12	6	0	1.690238	0.535249	1.086566
13	6	0	1.690845	1.198642	-0.173023
14	6	0	1.691684	0.205643	-1.193144
15	6	0	1.691694	-1.071406	-0.564078
16	6	0	1.690769	-0.867752	0.844893
17	1	0	1.672071	1.011896	2.054107
18	1	0	1.673078	2.266159	-0.327355
19	1	0	1.675185	0.388876	-2.256045
20	1	0	1.675364	-2.025753	-1.066851
21	1	0	1.673068	-1.640744	1.597132

Sum of electronic and zero-point Energies= -1650.743848

H/Mu addition at Cp ring with staggered Cp rings

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.016354	1.074848	0.006117
2	6	0	-1.858529	0.262262	-1.140428
3	6	0	-1.674845	-1.088874	-0.716254
4	6	0	-1.675679	-1.096834	0.704564
5	6	0	-1.859569	0.249363	1.143581
6	1	0	-2.154678	2.145132	0.012200
7	1	0	-1.889481	0.600660	-2.164892
8	1	0	-1.575060	-1.945405	-1.364466
9	1	0	-1.576448	-1.960563	1.343250
10	1	0	-1.891447	0.576429	2.171692
11	26	0	-0.013413	0.013880	0.000545
12	6	0	1.550881	1.109814	0.713247
13	6	0	1.550474	1.109760	-0.713083
14	6	0	1.682186	-0.235748	-1.142389
15	6	0	2.267770	-1.060474	-0.000037
16	6	0	1.682807	-0.235745	1.142660
17	1	0	1.398689	1.973068	1.344557
18	1	0	1.397816	1.973018	-1.344265
19	1	0	1.724345	-0.534374	-2.180515
20	1	0	1.921127	-2.096927	0.000015
21	1	0	1.726152	-0.534140	2.180804
22	1	0	3.372852	-1.088017	-0.000421

Exo Mu (H22) adduct: Sum of electronic and zero-point Energies = -1651.273089 Hartrees. There are no imaginary frequencies, which indicate this is a minimum energy geometry.

Endo Mu (H20) adduct: Sum of electronic and zero-point Energies = -1651.272054 Hartrees. There are no imaginary frequencies, which indicate this is a minimum energy geometry.

Isotropic Fermi Contact Couplings

Atom	a.u.	MegaHertz	Gauss	10(-4) cm-1
1 C(13)	0.00344	3.86640	1.37963	1.28969
2 C(13)	0.00121	1.36188	0.48595	0.45427
3 C(13)	-0.00007	-0.07884	-0.02813	-0.02630
4 C(13)	0.00002	0.01959	0.00699	0.00653
5 C(13)	0.00118	1.32734	0.47363	0.44275

6 H(1)	0.00006	0.26430	0.09431	0.08816
7 H(1)	-0.00008	-0.36858	-0.13152	-0.12294
8 H(1)	0.00034	1.50703	0.53774	0.50269
9 H(1)	0.00034	1.51639	0.54109	0.50581
10 H(1)	-0.00008	-0.35063	-0.12511	-0.11696
11 Fe(57)	-0.07019	-10.18013	-3.63252	-3.39573
12 C(13)	0.00213	2.39382	0.85417	0.79849
13 C(13)	0.00214	2.40422	0.85789	0.80196
14 C(13)	-0.00824	-9.26864	-3.30728	-3.09169
15 C(13)	0.01817	20.42309	7.28747	6.81241
16 C(13)	-0.00825	-9.27881	-3.31091	-3.09508
17 H(1)	0.00052	2.32480	0.82955	0.77547
18 H(1)	0.00052	2.31517	0.82611	0.77226
19 H(1)	0.00058	2.59470	0.92585	0.86550
20 H(1)	-0.00023	-1.02444	-0.36555	-0.34172
21 H(1)	0.00058	2.58662	0.92297	0.86280
22 H(1)	0.00145	6.46758	2.30779	2.15735

Anisotropic Spin Dipole Couplings in Principal Axis System

Atom	a.u.	MegaHertz	Gauss	10(-4) cm-1	Axes		
	Baa	-0.0179	-2.396	-0.855	-0.799	0.6433	0.7656	0.0078
1 C(13)	Bbb	-0.0079	-1.065	-0.380	-0.355	-0.0012	-0.0093	1.0000
	Bcc	0.0258	3.461	1.235	1.155	0.7656	-0.6433	-0.0051
	Baa	-0.0220	-2.947	-1.051	-0.983	-0.6852	0.1043	0.7209
2 C(13)	Bbb	-0.0040	-0.531	-0.190	-0.177	-0.0299	0.9848	-0.1709
	Bcc	0.0259	3.478	1.241	1.160	0.7278	0.1387	0.6716
	Baa	-0.0231	-3.095	-1.104	-1.032	0.8047	-0.3838	-0.4529
3 C(13)	Bbb	-0.0041	-0.551	-0.196	-0.184	0.1438	-0.6141	0.7760
	Bcc	0.0272	3.646	1.301	1.216	0.5760	0.6896	0.4390
	Baa	-0.0229	-3.072	-1.096	-1.025	0.7964	-0.4005	0.4531
4 C(13)	Bbb	-0.0046	-0.622	-0.222	-0.208	-0.1435	0.6027	0.7849
	Bcc	0.0275	3.694	1.318	1.232	0.5875	0.6902	-0.4225
	Baa	-0.0218	-2.932	-1.046	-0.978	0.6859	-0.1104	0.7193
5 C(13)	Bbb	-0.0039	-0.529	-0.189	-0.176	-0.0270	0.9839	0.1767
	Bcc	0.0258	3.461	1.235	1.154	0.7272	0.1406	-0.6719
	Baa	-0.0068	-3.628	-1.295	-1.210	0.6877	0.7260	0.0036
6 H(1)	Bbb	-0.0055	-2.909	-1.038	-0.970	0.0005	-0.0055	1.0000
	Bcc	0.0123	6.537	2.333	2.181	0.7260	-0.6876	-0.0041
	Baa	-0.0071	-3.794	-1.354	-1.265	0.7687	0.0681	-0.6360
7 H(1)	Bbb	-0.0059	-3.167	-1.130	-1.056	0.0681	0.9799	0.1873
	Bcc	0.0130	6.961	2.484	2.322	0.6360	-0.1873	0.7486

	Baa	-0.0073	-3.882	-1.385	-1.295	0.7774	-0.6115	-0.1473
8 H(1)	Bbb	-0.0063	-3.373	-1.204	-1.125	-0.2119	-0.4752	0.8540
	Bcc	0.0136	7.255	2.589	2.420	0.5922	0.6327	0.4990
	Baa	-0.0072	-3.864	-1.379	-1.289	0.7661	-0.6352	0.0979
9 H(1)	Bbb	-0.0064	-3.403	-1.214	-1.135	0.2496	0.4344	0.8654
	Bcc	0.0136	7.268	2.593	2.424	0.5923	0.6386	-0.4913
	Baa	-0.0071	-3.794	-1.354	-1.266	0.7683	0.0674	0.6366
10 H(1)	Bbb	-0.0059	-3.159	-1.127	-1.054	0.0636	0.9815	-0.1806
	Bcc	0.0130	6.953	2.481	2.319	-0.6370	0.1793	0.7498
	Baa	-1.6793	-29.074	-10.374	-9.698	0.9390	0.3438	0.0003
11 Fe(57)	Bbb	-0.2309	-3.997	-1.426	-1.333	-0.0001	-0.0006	1.0000
	Bcc	1.9102	33.071	11.801	11.031	-0.3438	0.9390	0.0005
	Baa	-0.0402	-5.398	-1.926	-1.800	0.9481	0.0452	-0.3147
12 C(13)	Bbb	0.0122	1.632	0.582	0.544	-0.2487	0.7221	-0.6455
	Bcc	0.0281	3.766	1.344	1.256	0.1981	0.6903	0.6959
	Baa	-0.0402	-5.391	-1.924	-1.798	0.9481	0.0451	0.3146
13 C(13)	Bbb	0.0121	1.628	0.581	0.543	-0.2485	0.7223	0.6454
	Bcc	0.0280	3.762	1.343	1.255	-0.1981	-0.6901	0.6961
	Baa	-0.0741	-9.940	-3.547	-3.316	0.9114	0.4115	-0.0052
14 C(13)	Bbb	0.0310	4.156	1.483	1.386	0.2115	-0.4576	0.8636
	Bcc	0.0431	5.784	2.064	1.929	-0.3530	0.7882	0.5041
	Baa	-0.0147	-1.972	-0.703	-0.658	-0.0001	-0.0002	1.0000
15 C(13)	Bbb	-0.0130	-1.744	-0.622	-0.582	0.3457	0.9383	0.0002
	Bcc	0.0277	3.716	1.326	1.239	0.9383	-0.3457	0.0000
	Baa	-0.0741	-9.948	-3.550	-3.318	0.9115	0.4112	0.0045
16 C(13)	Bbb	0.0310	4.162	1.485	1.388	-0.2112	0.4589	0.8630
	Bcc	0.0431	5.786	2.065	1.930	-0.3528	0.7876	-0.5051
	Baa	-0.0096	-5.146	-1.836	-1.716	0.7879	-0.3810	-0.4838
17 H(1)	Bbb	-0.0044	-2.343	-0.836	-0.782	0.1441	-0.6498	0.7464
	Bcc	0.0140	7.489	2.672	2.498	0.5987	0.6578	0.4570
	Baa	-0.0096	-5.145	-1.836	-1.716	0.7882	-0.3809	0.4834
18 H(1)	Bbb	-0.0044	-2.345	-0.837	-0.782	-0.1438	0.6498	0.7464
	Bcc	0.0140	7.491	2.673	2.499	0.5984	0.6578	-0.4574
	Baa	-0.0099	-5.279	-1.884	-1.761	0.6711	0.4214	0.6099
19 H(1)	Bbb	-0.0018	-0.935	-0.334	-0.312	-0.2006	0.8953	-0.3978
	Bcc	0.0116	6.214	2.217	2.073	0.7137	-0.1446	-0.6854
	Baa	-0.0089	-4.770	-1.702	-1.591	0.0009	0.0007	1.0000
20 H(1)	Bbb	-0.0071	-3.805	-1.358	-1.269	0.7053	0.7089	-0.0011
	Bcc	0.0161	8.575	3.060	2.860	0.7089	-0.7053	-0.000
	Baa	-0.0099	-5.277	-1.883	-1.760	0.6707	0.4210	-0.6107
21 H(1)	Bbb	-0.0017	-0.932	-0.333	-0.311	-0.2000	0.8954	0.3977
	Bcc	0.0116	6.209	2.215	2.071	0.7143	-0.1446	0.6847

	Baa	-0.0040	-2.133	-0.761	-0.712	0.0004	0.0006	1.0000
22 H(1)	Bbb	-0.0034	-1.793	-0.640	-0.598	0.1727	0.9850	-0.0006
	Bcc	0.0074	3.926	1.401	1.310	0.9850	-0.1727	-0.0003

H/Mu addition at Cp ring with eclipsed Cp rings

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.895039	0.883370	0.702849
2	6	0	-1.893160	0.877961	-0.710986
3	6	0	-1.775534	-0.476286	-1.145086
4	6	0	-1.734747	-1.304938	0.004443
5	6	0	-1.777773	-0.467283	1.147355
6	1	0	-1.963773	1.753090	1.337628
7	1	0	-1.960842	1.742795	-1.352524
8	1	0	-1.746229	-0.811772	-2.170027
9	1	0	-1.645016	-2.380744	0.008858
10	1	0	-1.749586	-0.794893	2.174883
11	26	0	-0.012333	0.008019	-0.000083
12	6	0	1.552524	1.093170	0.715179
13	6	0	1.552808	1.094533	-0.712690
14	6	0	1.680051	-0.250070	-1.143653
15	6	0	2.255957	-1.081202	-0.000686
16	6	0	1.679585	-0.252276	1.143626
17	1	0	1.406540	1.957213	1.346703
18	1	0	1.407052	1.959770	-1.342628
19	1	0	1.722539	-0.547972	-2.181947
20	1	0	1.899551	-2.114611	-0.001731
21	1	0	1.721717	-0.552148	2.181366
22	1	0	3.360661	-1.121102	-0.000541

Exo Mu (H22) adduct: Sum of electronic and zero-point Energies = -1651.272162 Hartrees. There is one imaginary frequency, which indicates it is a saddle point.

Endo Mu (H20) adduct: Sum of electronic and zero-point Energies = -1651.271126 Hartrees. There is one imaginary frequency, which indicates it is a saddle point.

Isotropic Fermi Contact Couplings

Atom	a.u.	MegaHertz	Gauss	10(-4) cm-1
1 C(13)	0.00238	2.67374	0.95406	0.89187
2 C(13)	0.00237	2.66396	0.95057	0.88860
3 C(13)	-0.00208	-2.33479	-0.83311	-0.77880
4 C(13)	0.00444	4.99657	1.78290	1.66668
5 C(13)	-0.00204	-2.28796	-0.81640	-0.76318
6 H(1)	-0.00008	-0.36364	-0.12975	-0.12130

7 H(1)	-0.00009	-0.38921	-0.13888	-0.12983
8 H(1)	0.00026	1.14429	0.40831	0.38169
9 H(1)	0.00017	0.74183	0.26470	0.24745
10 H(1)	0.00025	1.13117	0.40363	0.37732
11 Fe(57)	-0.07592	-11.01210	-3.92939	-3.67324
12 C(13)	0.00192	2.15999	0.77074	0.72050
13 C(13)	0.00193	2.16489	0.77249	0.72213
14 C(13)	-0.00704	-7.91429	-2.82401	-2.63992
15 C(13)	0.01942	21.83212	7.79024	7.28241
16 C(13)	-0.00704	-7.91560	-2.82448	-2.64036
17 H(1)	0.00050	2.21404	0.79003	0.73853
18 H(1)	0.00049	2.20229	0.78583	0.73460
19 H(1)	0.00043	1.91720	0.68411	0.63951
20 H(1)	0.00030	1.36307	0.48638	0.45467
21 H(1)	0.00043	1.91678	0.68395	0.63937
22 H(1)	0.00355	15.88590	5.66849	5.29897

Anisotropic Spin Dipole Couplings in Principal Axis System

	Atom	a.u.	MegaHertz	Gauss	10(-4) cm-1	Axes		
	Baa	-0.0226	-3.035	-1.083	-1.012	0.6665	0.3543	0.6559
1 C(13)	Bbb	-0.0042	-0.557	-0.199	-0.186	-0.0187	0.8875	-0.4604
	Bcc	0.0268	3.592	1.282	1.198	0.7453	-0.2946	-0.5981
	Baa	-0.0227	-3.044	-1.086	-1.015	0.6648	0.3475	-0.6613
2 C(13)	Bbb	-0.0042	-0.564	-0.201	-0.188	-0.0211	0.8936	0.4483
	Bcc	0.0269	3.608	1.287	1.204	0.7467	-0.2841	0.6014
	Baa	-0.0285	-3.822	-1.364	-1.275	0.9227	0.0511	-0.3821
3 C(13)	Bbb	0.0051	0.682	0.243	0.227	-0.1099	0.9849	-0.1337
	Bcc	0.0234	3.140	1.120	1.047	0.3695	0.1654	0.9144
	Baa	-0.0345	-4.624	-1.650	-1.543	-0.0023	0.0047	1.0000
4 C(13)	Bbb	-0.0318	-4.272	-1.524	-1.425	-0.4301	0.9028	-0.0052
	Bcc	0.0663	8.896	3.174	2.968	0.9028	0.4301	0.0000
	Baa	-0.0282	-3.778	-1.348	-1.260	0.9211	0.0502	0.3860
5 C(13)	Bbb	0.0049	0.652	0.233	0.217	-0.1079	0.9857	0.1291
	Bcc	0.0233	3.126	1.115	1.043	-0.3740	-0.1606	0.9134
	Baa	-0.0069	-3.667	-1.308	-1.223	0.7513	0.4715	0.4618
6 H(1)	Bbb	-0.0058	-3.096	-1.105	-1.033	-0.0398	-0.6660	0.7449
	Bcc	0.0127	6.763	2.413	2.256	0.6587	-0.5780	-0.4816
	Baa	-0.0069	-3.666	-1.308	-1.223	0.7521	0.4615	-0.4706
7 H(1)	Bbb	-0.0058	-3.107	-1.109	-1.036	0.0459	0.6757	0.7358
	Bcc	0.0127	6.772	2.417	2.259	0.6575	-0.5749	0.4870
	Baa	-0.0081	-4.295	-1.533	-1.433	0.7692	-0.1316	-0.6253
8 H(1)	Bbb	-0.0041	-2.178	-0.777	-0.727	-0.0507	0.9629	-0.2651
	Bcc	0.0121	6.473	2.310	2.159	0.6370	0.2356	0.7340

	Baa	-0.0104	-5.535	-1.975	-1.846	-0.0014	0.0053	1.0000
9 H(1)	Bbb	-0.0042	-2.241	-0.800	-0.748	0.8068	-0.5909	0.0043
	Bcc	0.0146	7.776	2.775	2.594	0.5909	0.8068	-0.0035
	Baa	-0.0080	-4.287	-1.530	-1.430	0.7689	-0.1267	0.6266
10 H(1)	Bbb	-0.0041	-2.187	-0.781	-0.730	-0.0514	0.9647	0.2582
	Bcc	0.0121	6.474	2.310	2.160	-0.6373	-0.2307	0.7353
	Baa	-1.6155	-27.969	-9.980	-9.329	0.9383	0.3459	0.0009
11 Fe(57)	Bbb	-0.2666	-4.615	-1.647	-1.539	-0.0004	-0.0015	1.0000
	Bcc	1.8821	32.584	11.627	10.869	-0.3459	0.9383	0.0013
	Baa	-0.0400	-5.367	-1.915	-1.790	0.9534	0.0403	-0.2988
12 C(13)	Bbb	0.0120	1.606	0.573	0.536	-0.2411	0.6971	-0.6753
	Bcc	0.0280	3.761	1.342	1.255	0.1811	0.7159	0.6743
	Baa	-0.0399	-5.359	-1.912	-1.788	0.9532	0.0398	0.2998
13 C(13)	Bbb	0.0119	1.602	0.572	0.534	-0.2417	0.6961	0.6760
	Bcc	0.0280	3.757	1.341	1.253	0.1818	0.7168	-0.6731
	Baa	-0.0621	-8.329	-2.972	-2.778	0.8858	0.4640	0.0095
14 C(13)	Bbb	0.0245	3.283	1.171	1.095	0.2068	-0.4129	0.8870
	Bcc	0.0376	5.046	1.800	1.683	-0.4155	0.7837	0.4617
	Baa	-0.0149	-2.000	-0.714	-0.667	-0.0007	-0.0012	1.0000
15 C(13)	Bbb	-0.0132	-1.766	-0.630	-0.589	0.3453	0.9385	0.0013
	Bcc	0.0281	3.766	1.344	1.256	0.9385	-0.3453	0.0002
	Baa	-0.0621	-8.336	-2.974	-2.781	0.8860	0.4636	-0.0080
16 C(13)	Bbb	0.0245	3.289	1.174	1.097	-0.2074	0.4115	0.8875
	Bcc	0.0376	5.047	1.801	1.684	-0.4148	0.7846	-0.4608
	Baa	-0.0094	-5.008	-1.787	-1.671	0.7896	-0.3757	-0.4853
17 H(1)	Bbb	-0.0042	-2.247	-0.802	-0.750	0.1500	-0.6486	0.7462
	Bcc	0.0136	7.255	2.589	2.420	0.5951	0.6620	0.4557
	Baa	-0.0094	-5.007	-1.787	-1.670	0.7893	-0.3763	0.4851
18 H(1)	Bbb	-0.0042	-2.250	-0.803	-0.750	-0.1506	0.6472	0.7473
	Bcc	0.0136	7.257	2.589	2.421	0.5952	0.6629	-0.4542
	Baa	-0.0094	-5.022	-1.792	-1.675	0.6804	0.4496	0.5787
19 H(1)	Bbb	-0.0024	-1.280	-0.457	-0.427	-0.2429	0.8834	-0.4007
	Bcc	0.0118	6.301	2.248	2.102	-0.6914	0.1320	0.7103
	Baa	-0.0091	-4.860	-1.734	-1.621	0.0006	-0.0001	1.0000
20 H(1)	Bbb	-0.0069	-3.689	-1.316	-1.231	0.7187	0.6953	-0.0004
	Bcc	0.0160	8.549	3.050	2.852	-0.6953	0.7187	0.0005
	Baa	-0.0094	-5.022	-1.792	-1.675	0.6806	0.4504	-0.5779
21 H(1)	Bbb	-0.0024	-1.278	-0.456	-0.426	-0.2427	0.8828	0.4022
	Bcc	0.0118	6.300	2.248	2.101	0.6913	-0.1334	0.7101
	Baa	-0.0040	-2.131	-0.760	-0.711	0.0000	0.0003	1.0000
22 H(1)	Bbb	-0.0034	-1.823	-0.651	-0.608	0.1780	0.9840	-0.0003
	Bcc	0.0074	3.954	1.411	1.319	0.9840	-0.1780	0.0000

H/Mu addition at Cp ring with planar C_5H_5Mu ring and eclipsed Cp rings

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.839562	0.924148	0.703590
2	6	0	-1.838687	0.922128	-0.706605
3	6	0	-1.767001	-0.438011	-1.145811
4	6	0	-1.769244	-1.271094	0.001543
5	6	0	-1.767710	-0.434660	1.146503
6	1	0	-1.870656	1.794492	1.340585
7	1	0	-1.869278	1.790682	-1.346074
8	1	0	-1.758780	-0.770304	-2.172402
9	1	0	-1.732668	-2.350169	0.003194
10	1	0	-1.759739	-0.764142	2.174008
11	26	0	-0.002786	-0.013024	-0.000049
12	6	0	1.555322	1.081982	0.719333
13	6	0	1.555243	1.084814	-0.715248
14	6	0	1.802948	-0.218668	-1.162090
15	6	0	1.985130	-1.179817	-0.001791
16	6	0	1.803074	-0.223244	1.161058
17	1	0	1.439570	1.948093	1.353010
18	1	0	1.439415	1.953414	-1.345494
19	1	0	1.826082	-0.522483	-2.198381
20	1	0	1.249147	-2.003511	-0.003460
21	1	0	1.826064	-0.530777	2.196272
22	1	0	2.966191	-1.692131	-0.002899

Exo Mu (H22) adduct: Sum of electronic and zero-point Energies = -1651.257767 Hartrees.

Endo Mu (H20) adduct: Sum of electronic and zero-point Energies = -1651.257413 Hartrees.

Isotropic Fermi Contact Couplings

Atom	a.u.	MegaHertz	Gauss	10(-4) cm-1
1 C(13)	0.00377	4.23520	1.51122	1.41271
2 C(13)	0.00377	4.23472	1.51105	1.41255
3 C(13)	-0.00341	-3.83320	-1.36778	-1.27862
4 C(13)	0.00772	8.67933	3.09700	2.89511
5 C(13)	-0.00339	-3.81355	-1.36077	-1.27206
6 H(1)	-0.00022	-0.99988	-0.35678	-0.33352

7 H(1)	-0.00023	-1.01782	-0.36318	-0.33951
8 H(1)	0.00039	1.73792	0.62013	0.57971
9 H(1)	-0.00043	-1.92601	-0.68725	-0.64245
10 H(1)	0.00039	1.72663	0.61610	0.57594
11 Fe(57)	-0.07142	-10.35926	-3.69644	-3.45548
12 C(13)	0.00123	1.37720	0.49142	0.45938
13 C(13)	0.00122	1.37708	0.49138	0.45935
14 C(13)	0.00081	0.91595	0.32683	0.30553
15 C(13)	0.01719	19.32179	6.89450	6.44506
16 C(13)	0.00081	0.91279	0.32571	0.30448
17 H(1)	0.00045	2.01883	0.72037	0.67341
18 H(1)	0.00045	2.01779	0.72000	0.67306
19 H(1)	0.00005	0.23088	0.08239	0.07701
20 H(1)	0.00997	44.58226	15.90806	14.87104
21 H(1)	0.00005	0.23282	0.08308	0.07766
22 H(1)	0.01621	72.44558	25.85038	24.16524

Anisotropic Spin Dipole Couplings in Principal Axis System

Atom	a.u.	MegaHertz	Gauss	10(-4) cm-1	Axes		
	Baa	-0.0252	-3.385	-1.208	-1.129	0.6104	0.1179	0.7833
1 C(13)	Bbb	-0.0086	-1.155	-0.412	-0.385	0.0465	0.9818	-0.1840
	Bcc	0.0338	4.540	1.620	1.514	0.7908	-0.1487	-0.5938
	Baa	-0.0253	-3.392	-1.210	-1.131	-0.6091	-0.1157	0.7846
2 C(13)	Bbb	-0.0087	-1.167	-0.417	-0.389	0.0447	0.9827	0.1796
	Bcc	0.0340	4.559	1.627	1.521	0.7919	-0.1445	0.5934
	Baa	-0.0390	-5.236	-1.868	-1.747	0.9709	0.0160	-0.2389
3 C(13)	Bbb	0.0127	1.706	0.609	0.569	-0.0473	0.9909	-0.1261
	Bcc	0.0263	3.530	1.260	1.178	0.2347	0.1337	0.9628
	Baa	-0.0462	-6.198	-2.212	-2.068	-0.0002	0.0008	1.0000
4 C(13)	Bbb	-0.0403	-5.403	-1.928	-1.802	-0.2806	0.9598	-0.0008
	Bcc	0.0865	11.602	4.140	3.870	0.9598	0.2806	0.0000
	Baa	-0.0388	-5.213	-1.860	-1.739	0.9707	0.0152	0.2398
5 C(13)	Bbb	0.0126	1.696	0.605	0.566	-0.0463	0.9912	0.1244
	Bcc	0.0262	3.517	1.255	1.173	-0.2358	-0.1318	0.9628
	Baa	-0.0063	-3.344	-1.193	-1.115	0.5778	-0.0794	0.8123
6 H(1)	Bbb	-0.0058	-3.072	-1.096	-1.025	0.5275	0.7959	-0.2974
	Bcc	0.0120	6.416	2.289	2.140	0.6229	-0.6003	-0.5017
	Baa	-0.0063	-3.349	-1.195	-1.117	-0.5659	0.1005	0.8183
7 H(1)	Bbb	-0.0058	-3.074	-1.097	-1.025	0.5410	0.7942	0.2765
	Bcc	0.0120	6.423	2.292	2.143	0.6221	-0.5992	0.5038
	Baa	-0.0077	-4.105	-1.465	-1.369	0.7524	-0.1949	-0.6292

8 H(1)	Bbb	-0.0028	-1.478	-0.527	-0.493	0.0241	0.9627	-0.2694
	Bcc	0.0105	5.583	1.992	1.862	0.6583	0.1875	0.7291
	Baa	-0.0111	-5.905	-2.107	-1.970	-0.0005	0.0021	1.0000
9 H(1)	Bbb	-0.0033	-1.741	-0.621	-0.581	0.8093	-0.5873	0.0017
	Bcc	0.0143	7.646	2.728	2.550	0.5873	0.8093	-0.0014
	Baa	-0.0077	-4.104	-1.464	-1.369	0.7526	-0.1923	0.6298
10 H(1)	Bbb	-0.0028	-1.482	-0.529	-0.494	0.0230	0.9635	0.2667
	Bcc	0.0105	5.586	1.993	1.863	-0.6581	-0.1862	0.7296
	Baa	-1.0140	-17.555	-6.264	-5.856	0.0029	-0.0007	1.0000
11 Fe(57)	Bbb	-0.9722	-16.832	-6.006	-5.614	0.9035	0.4286	-0.0023
	Bcc	1.9862	34.387	12.270	11.470	-0.4286	0.9035	0.0018
	Baa	-0.0355	-4.762	-1.699	-1.588	0.9470	0.0355	-0.3192
12 C(13)	Bbb	0.0080	1.070	0.382	0.357	-0.2499	0.7057	-0.6630
	Bcc	0.0275	3.691	1.317	1.231	0.2017	0.7077	0.6771
	Baa	-0.0355	-4.760	-1.698	-1.588	0.9471	0.0342	0.3192
13 C(13)	Bbb	0.0080	1.070	0.382	0.357	-0.2498	0.7028	0.6660
	Bcc	0.0275	3.690	1.317	1.231	0.2016	0.7105	-0.6742
	Baa	-0.0325	-4.367	-1.558	-1.457	0.5953	0.7858	0.1677
14 C(13)	Bbb	0.0026	0.348	0.124	0.116	0.0454	-0.2413	0.9694
	Bcc	0.0300	4.019	1.434	1.341	0.8022	-0.5695	-0.1793
	Baa	-0.0190	-2.554	-0.912	-0.852	-0.0004	-0.0023	1.0000
15 C(13)	Bbb	-0.0105	-1.407	-0.502	-0.469	0.0900	0.9959	0.0023
	Bcc	0.0295	3.961	1.414	1.321	0.9959	-0.0900	0.0002
	Baa	-0.0325	-4.363	-1.557	-1.455	0.5956	0.7862	-0.1651
16 C(13)	Bbb	0.0026	0.348	0.124	0.116	-0.0461	0.2386	0.9700
	Bcc	0.0299	4.015	1.433	1.339	0.8020	-0.5701	0.1784
	Baa	-0.0081	-4.302	-1.535	-1.435	0.7898	-0.3120	-0.5281
17 H(1)	Bbb	-0.0039	-2.073	-0.740	-0.691	0.2210	-0.6584	0.7195
	Bcc	0.0119	6.375	2.275	2.127	0.5722	0.6850	0.4510
	Baa	-0.0081	-4.302	-1.535	-1.435	0.7898	-0.3141	0.5268
18 H(1)	Bbb	-0.0039	-2.074	-0.740	-0.692	-0.2209	0.6555	0.7221
	Bcc	0.0119	6.376	2.275	2.127	0.5721	0.6868	-0.4484
	Baa	-0.0076	-4.080	-1.456	-1.361	0.6318	0.6623	0.4027
19 H(1)	Bbb	-0.0042	-2.259	-0.806	-0.754	-0.4680	0.7401	-0.4829
	Bcc	0.0119	6.339	2.262	2.114	-0.6179	0.1167	0.7776
	Baa	-0.0164	-8.745	-3.120	-2.917	0.0001	-0.0016	1.0000
20 H(1)	Bbb	-0.0073	-3.874	-1.382	-1.292	0.8539	0.5204	0.0007
	Bcc	0.0237	12.619	4.503	4.209	-0.5204	0.8539	0.0015
	Baa	-0.0076	-4.080	-1.456	-1.361	0.6321	0.6632	-0.4007
21 H(1)	Bbb	-0.0042	-2.260	-0.806	-0.754	-0.4674	0.7388	0.4854
	Bcc	0.0119	6.339	2.262	2.115	0.6180	-0.1195	0.7770
	Baa	-0.0042	-2.245	-0.801	-0.749	-0.0008	-0.0031	1.0000

22 H(1)	Bbb	-0.0040	-2.125	-0.758	-0.709	0.4684	0.8835	0.0031
	Bcc	0.0082	4.370	1.559	1.458	0.8835	-0.4684	-0.0008

H/Mu addition at Cp ring with planar C_5H_5Mu ring and staggered Cp rings

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.922362	1.136098	0.007573
2	6	0	-1.812028	0.311972	-1.138602
3	6	0	-1.730793	-1.050291	-0.715453
4	6	0	-1.731049	-1.059478	0.702340
5	6	0	-1.811966	0.296887	1.143075
6	1	0	-1.992701	2.212597	0.014645
7	1	0	-1.818650	0.650300	-2.163689
8	1	0	-1.691347	-1.911050	-1.365212
9	1	0	-1.692260	-1.928686	1.340825
10	1	0	-1.817811	0.622081	2.172411
11	26	0	-0.003015	-0.016063	-0.000133
12	6	0	1.546759	1.094284	0.718989
13	6	0	1.546825	1.097076	-0.714658
14	6	0	1.811726	-0.203139	-1.162030
15	6	0	2.006391	-1.161796	-0.001770
16	6	0	1.811632	-0.207740	1.161357
17	1	0	1.418078	1.958916	1.352339
18	1	0	1.418376	1.964188	-1.344654
19	1	0	1.839004	-0.506244	-2.198414
20	1	0	1.288262	-1.999136	-0.003608
21	1	0	1.838407	-0.514638	2.196648
22	1	0	2.998234	-1.653924	-0.002760

Exo Mu (H22) adduct: Sum of electronic and zero-point Energies = -1651.257669 Hartrees.

Endo Mu (H20) adduct: Sum of electronic and zero-point Energies = -1651.257215 Hartrees.

Isotropic Fermi Contact Couplings

Atom	a.u.	MegaHertz	Gauss	10(-4) cm-1
1 C(13)	0.00412	4.63599	1.65424	1.54640
2 C(13)	0.00144	1.61525	0.57636	0.53879
3 C(13)	0.00144	1.61456	0.57612	0.53856
4 C(13)	0.00157	1.76196	0.62871	0.58773
5 C(13)	0.00137	1.54234	0.55034	0.51447
6 H(1)	0.00002	0.10088	0.03600	0.03365
7 H(1)	-0.00010	-0.46055	-0.16433	-0.15362

8 H(1)	0.00021	0.93784	0.33465	0.31283
9 H(1)	0.00020	0.90494	0.32291	0.30186
10 H(1)	-0.00010	-0.42619	-0.15208	-0.14216
11 Fe(57)	-0.06054	-8.78084	-3.13322	-2.92897
12 C(13)	0.00150	1.69008	0.60306	0.56375
13 C(13)	0.00150	1.68583	0.60155	0.56233
14 C(13)	-0.00027	-0.30693	-0.10952	-0.10238
15 C(13)	0.01815	20.40870	7.28233	6.80761
16 C(13)	-0.00028	-0.31035	-0.11074	-0.10352
17 H(1)	0.00049	2.20646	0.78732	0.73600
18 H(1)	0.00049	2.20115	0.78543	0.73422
19 H(1)	0.00030	1.34020	0.47822	0.44704
20 H(1)	0.00802	35.83231	12.78586	11.95237
21 H(1)	0.00030	1.34617	0.48035	0.44904
22 H(1)	0.01372	61.31742	21.87958	20.45329

Anisotropic Spin Dipole Couplings in Principal Axis System

Atom	a.u.	MegaHertz	Gauss	10(-4) cm-1	Axes			
	Baa	-0.0183	-2.452	-0.875	-0.818	0.6795	0.7336	0.0145
1 C(13)	Bbb	-0.0083	-1.120	-0.400	-0.374	-0.0038	-0.0162	0.9999
	Bcc	0.0266	3.572	1.275	1.192	0.7337	-0.6794	-0.0083
	Baa	-0.0218	-2.925	-1.044	-0.976	-0.6934	0.1617	0.7022
2 C(13)	Bbb	-0.0037	-0.492	-0.176	-0.164	0.0053	0.9756	-0.2194
	Bcc	0.0255	3.417	1.219	1.140	0.7205	0.1484	0.6773
	Baa	-0.0195	-2.617	-0.934	-0.873	0.6814	-0.4133	-0.6040
3 C(13)	Bbb	-0.0093	-1.254	-0.447	-0.418	-0.1473	0.7309	-0.6664
	Bcc	0.0288	3.871	1.381	1.291	0.7169	0.5431	0.4372
	Baa	-0.0195	-2.612	-0.932	-0.871	0.6665	-0.4265	0.6115
4 C(13)	Bbb	-0.0100	-1.343	-0.479	-0.448	-0.1508	0.7261	0.6708
	Bcc	0.0295	3.955	1.411	1.319	0.7301	0.5393	-0.4196
	Baa	-0.0217	-2.911	-1.039	-0.971	0.6985	-0.1646	0.6964
5 C(13)	Bbb	-0.0034	-0.461	-0.165	-0.154	0.0070	0.9747	0.2234
	Bcc	0.0251	3.372	1.203	1.125	0.7155	0.1512	-0.6820
	Baa	-0.0065	-3.453	-1.232	-1.152	0.7366	0.6763	0.0054
6 H(1)	Bbb	-0.0051	-2.746	-0.980	-0.916	-0.0003	-0.0077	1.0000
	Bcc	0.0116	6.199	2.212	2.068	-0.6763	0.7366	0.0054
	Baa	-0.0067	-3.549	-1.266	-1.184	0.7876	0.1445	-0.5990
7 H(1)	Bbb	-0.0056	-2.987	-1.066	-0.996	0.0172	0.9666	0.2557
	Bcc	0.0122	6.535	2.332	2.180	0.6159	-0.2117	0.7589
	Baa	-0.0066	-3.535	-1.261	-1.179	-0.4559	0.8010	-0.3879
8 H(1)	Bbb	-0.0058	-3.095	-1.104	-1.032	-0.6315	0.0159	0.7752

	Bcc	0.0124	6.630	2.366	2.212	0.6271	0.5984	0.4986
	Baa	-0.0067	-3.560	-1.270	-1.187	-0.4070	0.7910	0.4567
9 H(1)	Bbb	-0.0058	-3.089	-1.102	-1.030	0.6647	-0.0864	0.7421
	Bcc	0.0125	6.648	2.372	2.218	0.6265	0.6056	-0.4906
	Baa	-0.0067	-3.559	-1.270	-1.187	0.7874	0.1452	0.5991
10 H(1)	Bbb	-0.0056	-2.968	-1.059	-0.990	0.0107	0.9685	-0.2489
	Bcc	0.0122	6.527	2.329	2.177	-0.6163	0.2024	0.7610
	Baa	-1.0475	-18.134	-6.471	-6.049	0.9050	0.4253	0.0051
11 Fe(57)	Bbb	-0.9939	-17.207	-6.140	-5.740	-0.0038	-0.0039	1.0000
	Bcc	2.0413	35.341	12.611	11.789	-0.4253	0.9050	0.0019
	Baa	-0.0363	-4.871	-1.738	-1.625	0.9294	0.0627	-0.3636
12 C(13)	Bbb	0.0079	1.064	0.380	0.355	-0.2884	0.7383	-0.6098
	Bcc	0.0284	3.807	1.359	1.270	0.2302	0.6716	0.7042
	Baa	-0.0363	-4.869	-1.737	-1.624	0.9294	0.0610	0.3640
13 C(13)	Bbb	0.0079	1.063	0.379	0.355	-0.2883	0.7356	0.6130
	Bcc	0.0284	3.806	1.358	1.269	-0.2303	-0.6747	0.7013
	Baa	-0.0403	-5.401	-1.927	-1.802	0.7578	0.6359	0.1459
14 C(13)	Bbb	0.0123	1.651	0.589	0.551	0.0697	-0.3012	0.9510
	Bcc	0.0279	3.750	1.338	1.251	-0.6487	0.7105	0.2726
	Baa	-0.0186	-2.495	-0.890	-0.832	-0.0005	-0.0023	1.0000
15 C(13)	Bbb	-0.0104	-1.401	-0.500	-0.467	0.1209	0.9927	0.0023
	Bcc	0.0290	3.896	1.390	1.300	0.9927	-0.1209	0.0003
	Baa	-0.0403	-5.404	-1.928	-1.803	0.7585	0.6357	-0.1432
16 C(13)	Bbb	0.0123	1.656	0.591	0.552	-0.0706	0.2987	0.9517
	Bcc	0.0279	3.748	1.338	1.250	-0.6478	0.7118	-0.2714
	Baa	-0.0084	-4.500	-1.606	-1.501	0.7887	-0.3133	-0.5289
17 H(1)	Bbb	-0.0041	-2.180	-0.778	-0.727	0.2198	-0.6597	0.7187
	Bcc	0.0125	6.680	2.384	2.228	0.5741	0.6831	0.4515
	Baa	-0.0084	-4.499	-1.605	-1.501	0.7886	-0.3154	0.5279
18 H(1)	Bbb	-0.0041	-2.181	-0.778	-0.728	-0.2200	0.6569	0.7212
	Bcc	0.0125	6.680	2.384	2.228	0.5742	0.6849	-0.4486
	Baa	-0.0080	-4.293	-1.532	-1.432	0.6669	0.5513	0.5013
19 H(1)	Bbb	-0.0034	-1.814	-0.647	-0.605	-0.3588	0.8272	-0.4324
	Bcc	0.0114	6.107	2.179	2.037	-0.6531	0.1085	0.7495
	Baa	-0.0163	-8.712	-3.109	-2.906	0.0001	-0.0016	1.0000
20 H(1)	Bbb	-0.0082	-4.354	-1.554	-1.452	0.8407	0.5415	0.0008
	Bcc	0.0245	13.067	4.662	4.359	-0.5415	0.8407	0.0015
	Baa	-0.0080	-4.293	-1.532	-1.432	0.6672	0.5524	-0.4996
21 H(1)	Bbb	-0.0034	-1.813	-0.647	-0.605	-0.3582	0.8261	0.4350
	Bcc	0.0114	6.106	2.179	2.037	0.6531	-0.1113	0.7491
	Baa	-0.0043	-2.283	-0.815	-0.761	-0.0002	-0.0019	1.0000
22 H(1)	Bbb	-0.0040	-2.121	-0.757	-0.708	0.4392	0.8984	0.0018

Bcc	0.0083	4.404	1.572	1.469	0.8984	-0.4392	-0.0007

H/Mu addition at the iron with eclipsed Cp rings

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.659978	1.084100	0.708329
2	6	0	1.842357	-0.262826	1.143743
3	6	0	2.017585	-1.071624	-0.011917
4	6	0	1.831886	-0.244727	-1.152672
5	6	0	1.654675	1.095439	-0.694451
6	1	0	1.498940	1.934506	1.352385
7	1	0	1.909904	-0.597178	2.166878
8	1	0	2.237674	-2.126564	-0.021286
9	1	0	1.888578	-0.563191	-2.181547
10	1	0	1.487461	1.955886	-1.323365
11	26	0	0.000158	-0.256596	0.003607
12	6	0	-1.660208	1.084515	0.707636
13	6	0	-1.842348	-0.262145	1.143927
14	6	0	-2.017519	-1.071756	-0.011130
15	6	0	-1.832012	-0.245592	-1.152432
16	6	0	-1.654918	1.094892	-0.695134
17	1	0	-1.499254	1.935383	1.351103
18	1	0	-1.909845	-0.595838	2.167283
19	1	0	-2.237588	-2.126706	-0.019799
20	1	0	-1.888773	-0.564710	-2.181101
21	1	0	-1.487874	1.954944	-1.324635
22	1	0	-0.000200	-1.736698	0.004922

Mu (H22) adduct: Sum of electronic and zero-point Energies = -1651.255478 Hartrees.

Isotropic Fermi Contact Couplings

	Atom	a.u.	MegaHertz	Gauss	10(-4) cm-1
1	C(13)	0.01028	11.55749	4.12400	3.85517
2	C(13)	-0.00284	-3.18993	-1.13825	-1.06405
3	C(13)	0.00517	5.81017	2.07321	1.93806
4	C(13)	-0.00296	-3.32513	-1.18649	-1.10914
5	C(13)	0.01061	11.93259	4.25784	3.98028
6	H(1)	-0.00078	-3.48270	-1.24271	-1.16170
7	H(1)	0.00017	0.77530	0.27665	0.25861
8	H(1)	-0.00100	-4.46717	-1.59400	-1.49009
9	H(1)	0.00019	0.84881	0.30288	0.28313

10	H(1)	-0.00082	-3.68213	-1.31387	-1.22823
11	Fe(57)	-0.17152	-24.87756	-8.87693	-8.29826
12	C(13)	0.01029	11.56991	4.12843	3.85931
13	C(13)	-0.00285	-3.20263	-1.14278	-1.06828
14	C(13)	0.00518	5.82721	2.07929	1.94375
15	C(13)	-0.00296	-3.32448	-1.18626	-1.10893
16	C(13)	0.01060	11.91401	4.25121	3.97408
17	H(1)	-0.00078	-3.49647	-1.24763	-1.16630
18	H(1)	0.00017	0.78063	0.27855	0.26039
19	H(1)	-0.00100	-4.47732	-1.59762	-1.49347
20	H(1)	0.00019	0.84798	0.30258	0.28286
21	H(1)	-0.00082	-3.67757	-1.31225	-1.22671
22	H(1)	-0.02160	-96.57010	-34.45861	-32.21232

Anisotropic Spin Dipole Couplings in Principal Axis System

Atom	a.u.	MegaHertz	Gauss	10(-4) cm-1	Axes		
	Baa	-0.0396	-5.313	-1.896	-1.772	-0.1702	-0.3239	0.9306
1 C(13)	Bbb	-0.0353	-4.737	-1.690	-1.580	-0.3655	0.8978	0.2457
	Bcc	0.0749	10.050	3.586	3.352	0.9151	0.2983	0.2712
	Baa	-0.0303	-4.072	-1.453	-1.358	0.9261	0.0107	-0.3772
2 C(13)	Bbb	0.0100	1.340	0.478	0.447	-0.0482	0.9948	-0.0901
	Bcc	0.0204	2.731	0.975	0.911	0.3743	0.1016	0.9217
	Baa	-0.0381	-5.116	-1.825	-1.706	0.0089	0.0014	1.0000
3 C(13)	Bbb	-0.0304	-4.084	-1.457	-1.362	0.0498	0.9988	-0.0018
	Bcc	0.0686	9.200	3.283	3.069	0.9987	-0.0498	-0.0088
	Baa	-0.0309	-4.146	-1.479	-1.383	0.9342	0.0213	0.3560
4 C(13)	Bbb	0.0105	1.408	0.502	0.470	-0.0488	0.9965	0.0683
	Bcc	0.0204	2.738	0.977	0.913	-0.3533	-0.0812	0.9320
	Baa	-0.0413	-5.539	-1.976	-1.848	0.1540	0.3427	0.9267
5 C(13)	Bbb	-0.0369	-4.954	-1.768	-1.652	-0.3672	0.8906	-0.2683
	Bcc	0.0782	10.492	3.744	3.500	0.9173	0.2990	-0.2630
	Baa	-0.0091	-4.880	-1.741	-1.628	0.1852	-0.6761	0.7132
6 H(1)	Bbb	-0.0038	-2.043	-0.729	-0.682	0.8886	-0.1947	-0.4153
	Bcc	0.0130	6.924	2.471	2.310	0.4196	0.7106	0.5648
	Baa	-0.0063	-3.371	-1.203	-1.124	0.7507	0.2945	-0.5914
7 H(1)	Bbb	-0.0034	-1.836	-0.655	-0.612	-0.1547	0.9486	0.2759
	Bcc	0.0098	5.207	1.858	1.737	0.6422	-0.1156	0.7577
	Baa	-0.0084	-4.479	-1.598	-1.494	0.0047	-0.0088	1.0000
8 H(1)	Bbb	-0.0042	-2.217	-0.791	-0.739	0.7327	0.6805	0.0025
	Bcc	0.0125	6.695	2.389	2.233	-0.6805	0.7327	0.0097
	Baa	-0.0064	-3.390	-1.210	-1.131	0.7554	0.2823	0.5913

9 H(1)	Bbb	-0.0034	-1.797	-0.641	-0.599	-0.1525	0.9534	-0.2603
	Bcc	0.0097	5.187	1.851	1.730	-0.6372	0.1064	0.7633
	Baa	-0.0094	-4.998	-1.783	-1.667	-0.1712	0.6605	0.7311
10 H(1)	Bbb	-0.0038	-2.012	-0.718	-0.671	0.8953	-0.2054	0.3953
	Bcc	0.0131	7.009	2.501	2.338	0.4113	0.7222	-0.5561
	Baa	-2.1488	-37.202	-13.275	-12.409	0.0000	0.0005	1.0000
11 Fe(57)	Bbb	0.9743	16.868	6.019	5.627	1.0000	0.0032	0.0000
	Bcc	1.1745	20.334	7.256	6.783	-0.0032	1.0000	-0.0005
	Baa	-0.0397	-5.327	-1.901	-1.777	0.1688	-0.3256	0.9303
12 C(13)	Bbb	-0.0354	-4.750	-1.695	-1.584	0.3653	0.8973	0.2478
	Bcc	0.0751	10.077	3.596	3.361	0.9155	-0.2980	-0.2704
	Baa	-0.0304	-4.077	-1.455	-1.360	0.9264	-0.0109	0.3763
13 C(13)	Bbb	0.0100	1.345	0.480	0.449	0.0481	0.9948	-0.0896
	Bcc	0.0204	2.732	0.975	0.911	-0.3734	0.1011	0.9222
	Baa	-0.0382	-5.127	-1.829	-1.710	-0.0085	0.0014	1.0000
14 C(13)	Bbb	-0.0305	-4.093	-1.461	-1.365	-0.0491	0.9988	-0.0018
	Bcc	0.0687	9.220	3.290	3.075	0.9988	0.0491	0.0084
	Baa	-0.0309	-4.144	-1.479	-1.382	0.9341	-0.0207	-0.3564
15 C(13)	Bbb	0.0105	1.406	0.502	0.469	0.0486	0.9964	0.0695
	Bcc	0.0204	2.738	0.977	0.913	0.3536	-0.0822	0.9318
	Baa	-0.0412	-5.533	-1.974	-1.846	-0.1547	0.3425	0.9267
16 C(13)	Bbb	-0.0369	-4.947	-1.765	-1.650	0.3669	0.8908	-0.2680
	Bcc	0.0781	10.480	3.739	3.496	0.9173	-0.2986	0.2635
	Baa	-0.0092	-4.887	-1.744	-1.630	-0.1845	-0.6754	0.7140
17 H(1)	Bbb	-0.0038	-2.041	-0.728	-0.681	0.8889	0.1953	0.4144
	Bcc	0.0130	6.927	2.472	2.311	-0.4193	0.7111	0.5644
	Baa	-0.0063	-3.371	-1.203	-1.124	0.7507	-0.2942	0.5916
18 H(1)	Bbb	-0.0034	-1.833	-0.654	-0.611	0.1548	0.9488	0.2754
	Bcc	0.0098	5.203	1.857	1.736	-0.6423	-0.1152	0.7578
	Baa	-0.0084	-4.483	-1.600	-1.495	-0.0046	-0.0081	1.0000
19 H(1)	Bbb	-0.0042	-2.216	-0.791	-0.739	0.7330	-0.6802	-0.0021
	Bcc	0.0126	6.699	2.390	2.234	0.6802	0.7330	0.0091
	Baa	-0.0064	-3.389	-1.209	-1.131	0.7554	-0.2829	-0.5911
20 H(1)	Bbb	-0.0034	-1.798	-0.641	-0.600	0.1527	0.9532	-0.2610
	Bcc	0.0097	5.187	1.851	1.730	0.6373	0.1068	0.7632
	Baa	-0.0094	-4.994	-1.782	-1.666	0.1714	0.6611	0.7305
21 H(1)	Bbb	-0.0038	-2.012	-0.718	-0.671	0.8952	0.2052	-0.3957
	Bcc	0.0131	7.006	2.500	2.337	-0.4115	0.7217	-0.5566
	Baa	-0.0514	-27.435	-9.789	-9.151	0.0000	0.0009	1.0000
22 H(1)	Bbb	-0.0397	-21.191	-7.561	-7.069	1.0000	-0.0002	0.0000
	Bcc	0.0911	48.626	17.351	16.220	0.0002	1.0000	-0.0009
