Supporting Information for:

Axial Bonding in Alkylcobalamins: DFT Analysis of the Inverse vs Normal Trans Influence

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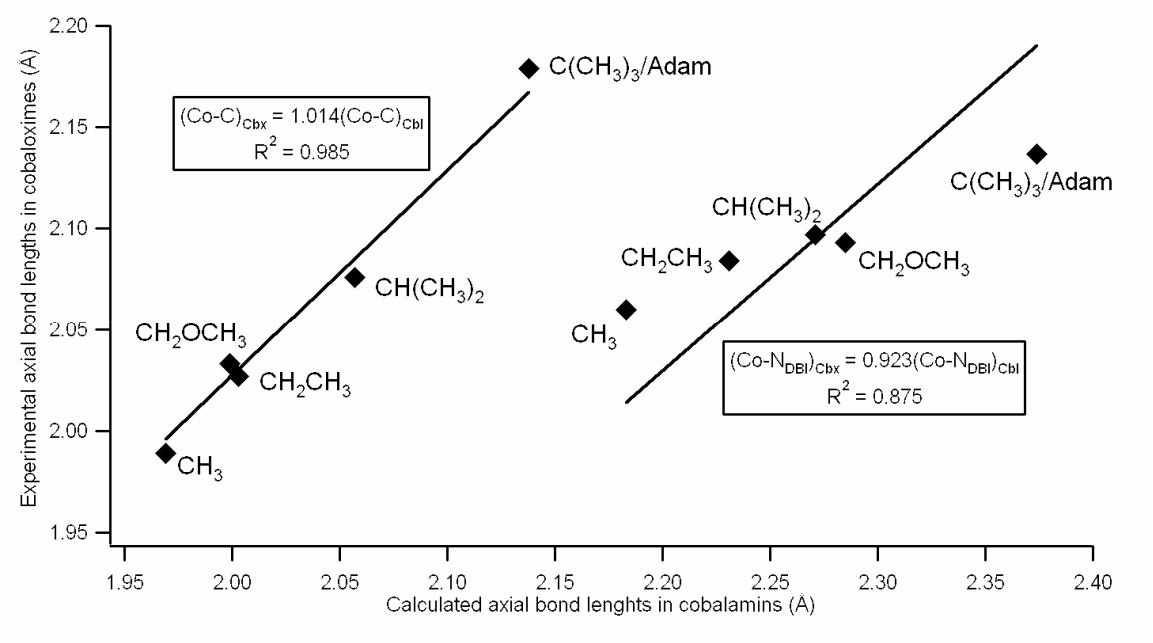
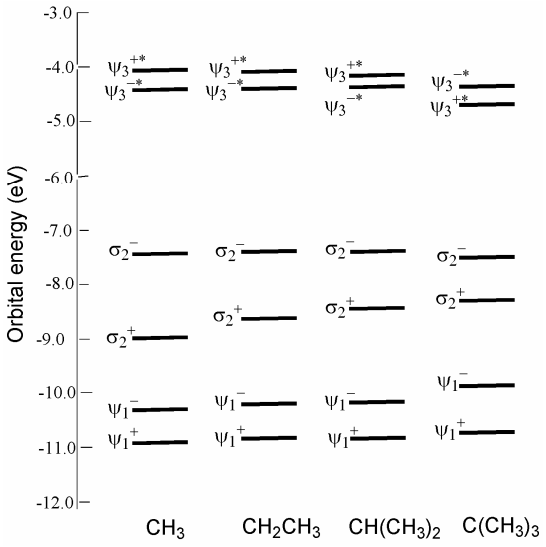
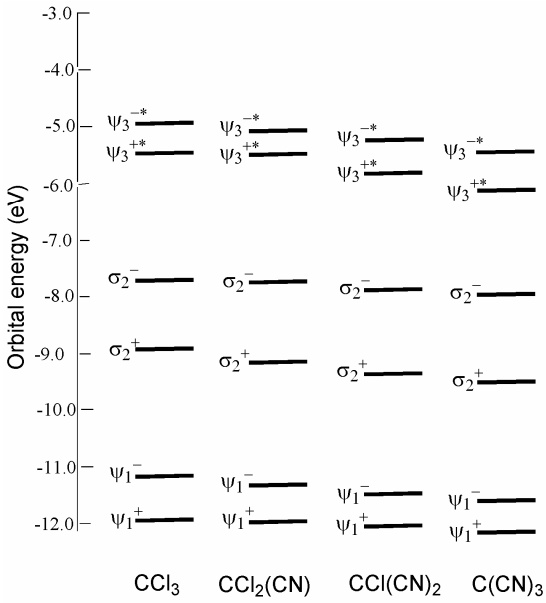


Figure S1. Comparison of calculated Co-C and Co-N_{DBl} axial bond lengths in selected cobalamins with experimental axial bond lengths in selected cobaloximes.



(a)

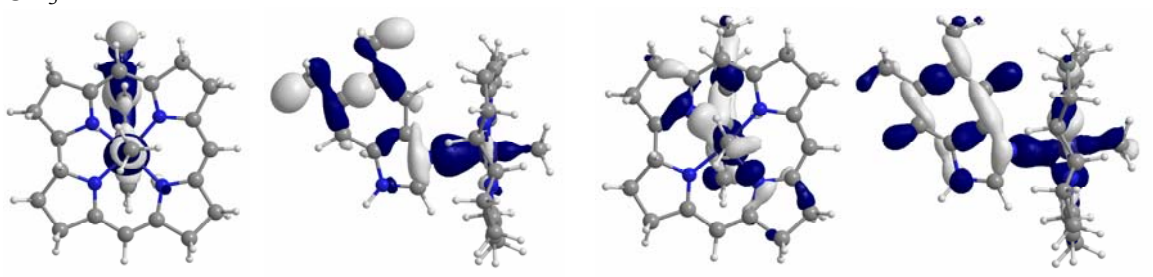


(b)

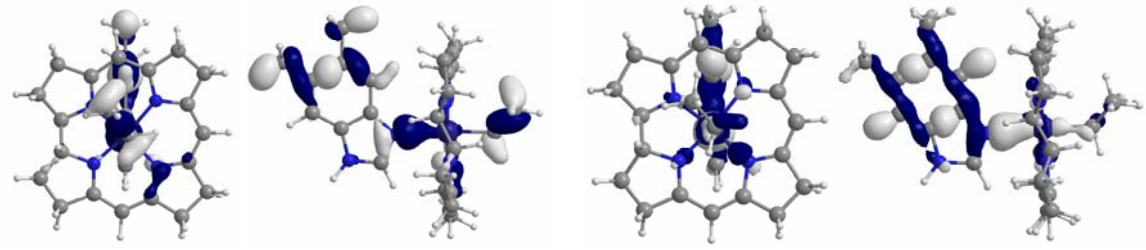
Figure S2. Orbital energy level diagram for the (a) Set 1 and (b) Set 2.

ψ_1^+ ψ_1^-

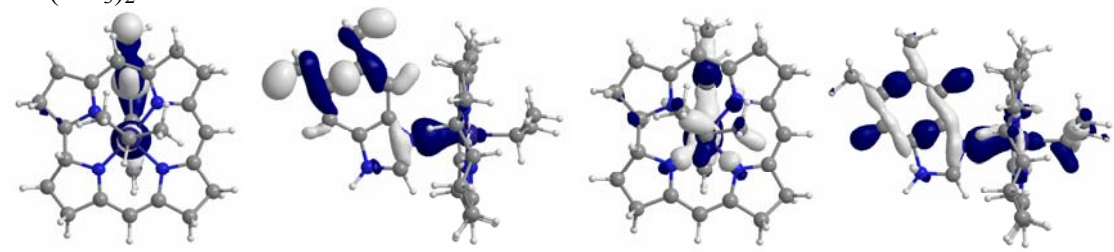
CH_3



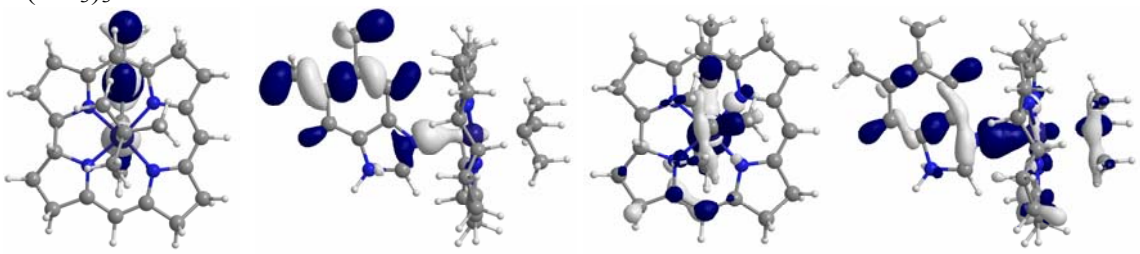
CH_2CH_3



$CH(CH_3)_2$

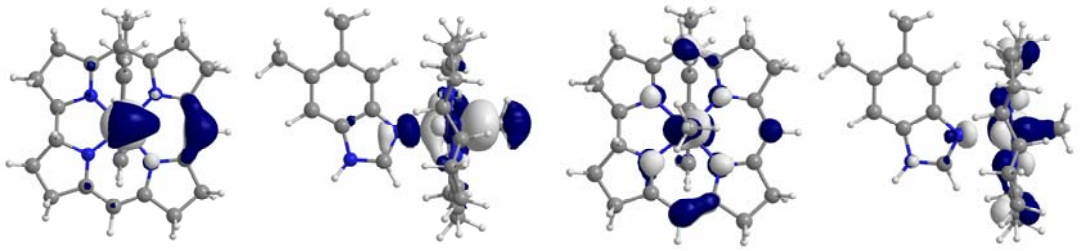


$C(CH_3)_3$



σ_2^+ σ_2^-

CH_3



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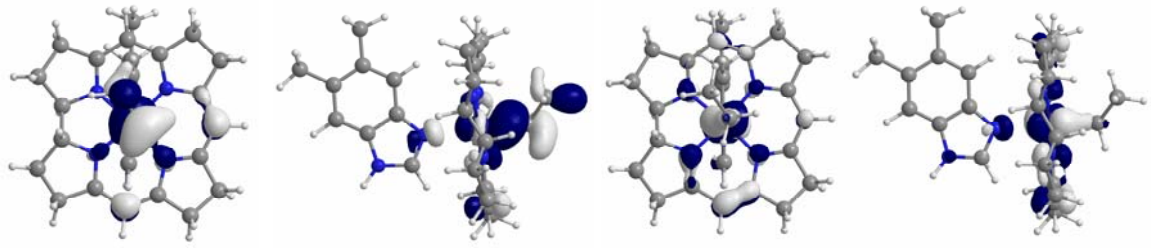

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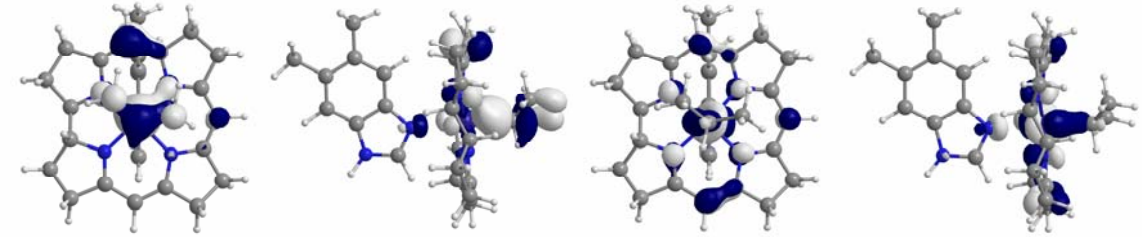

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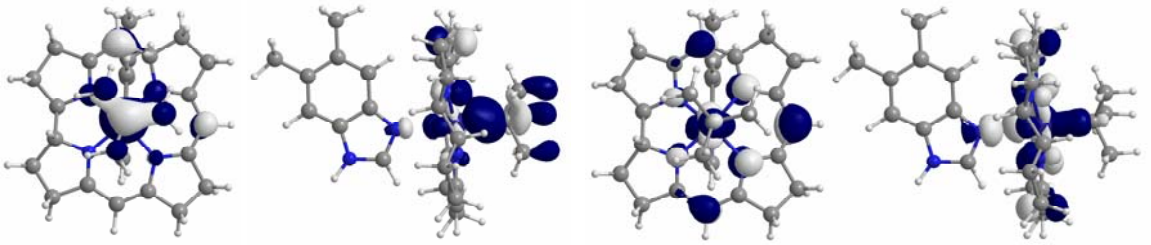
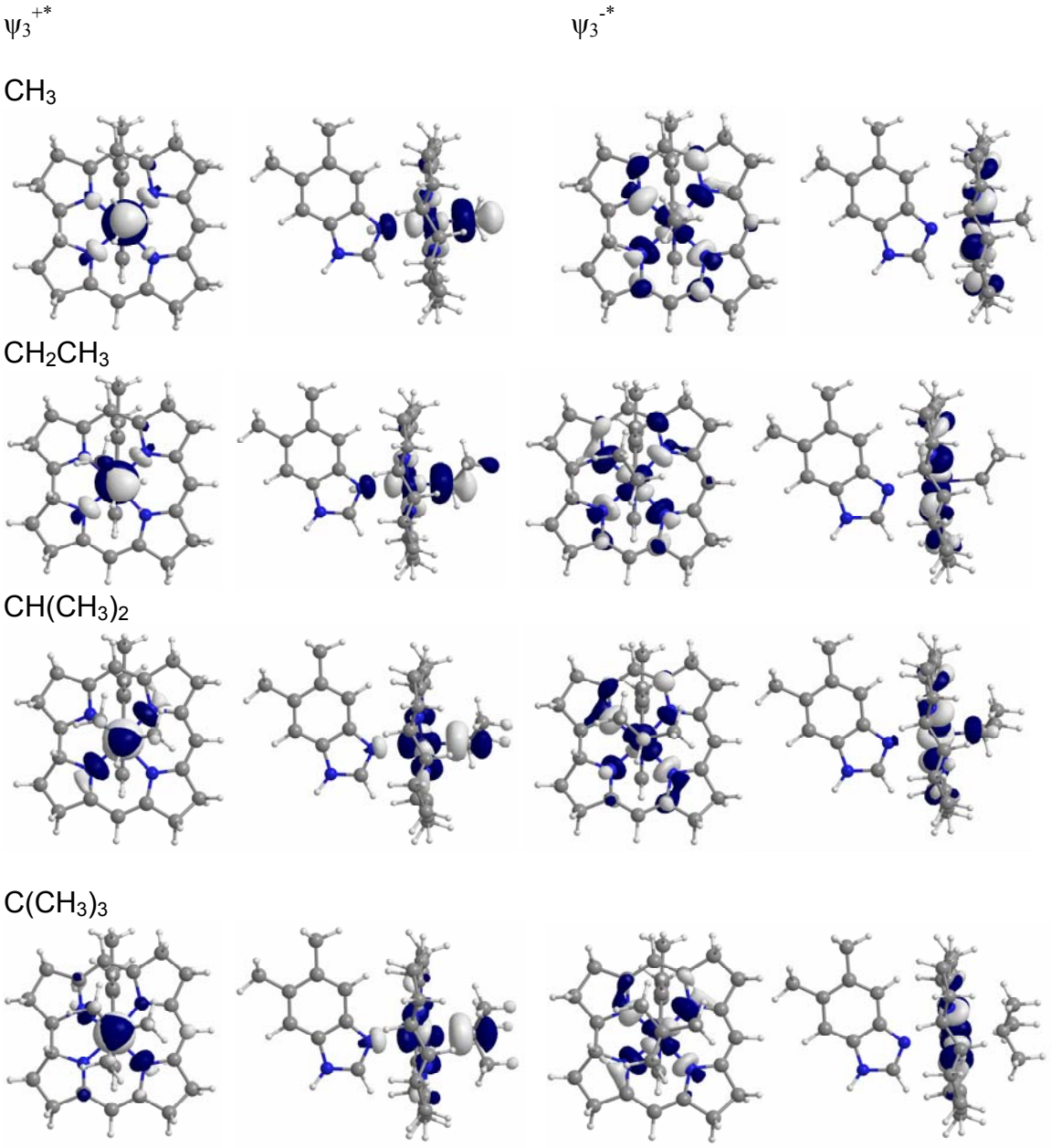
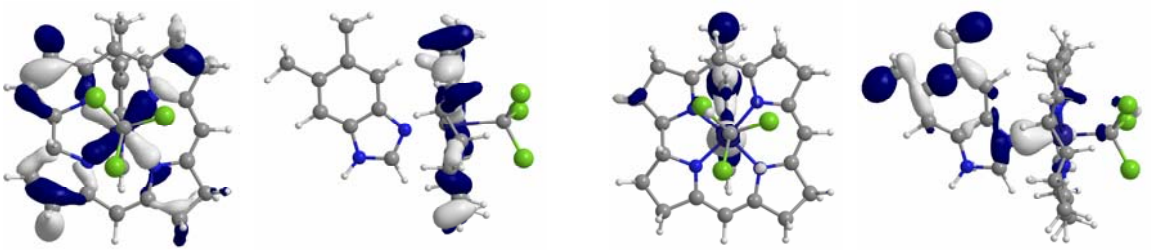




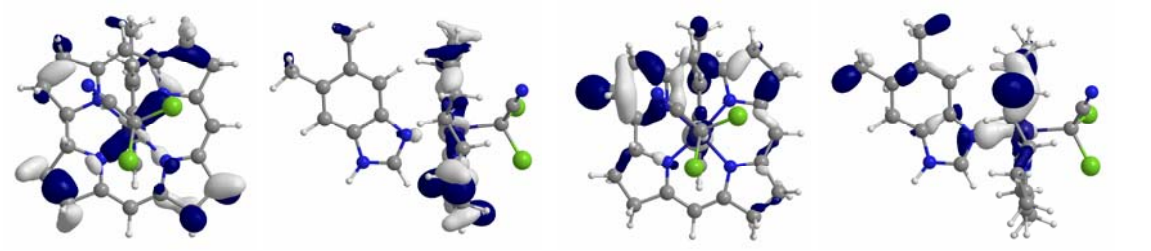
(a)

ψ_1^+ ψ_1^-

CCl_3



$CCl_2(CN)$



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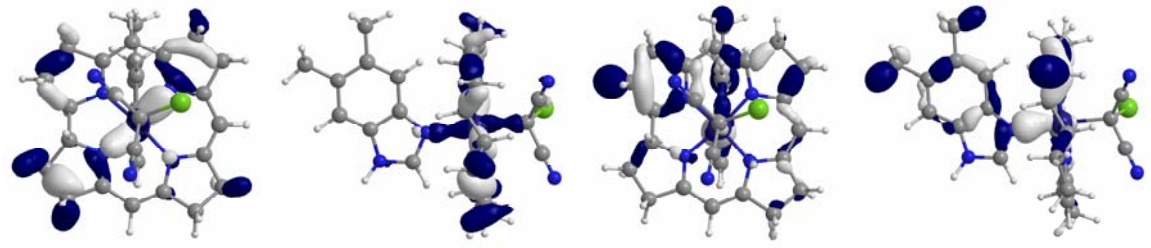
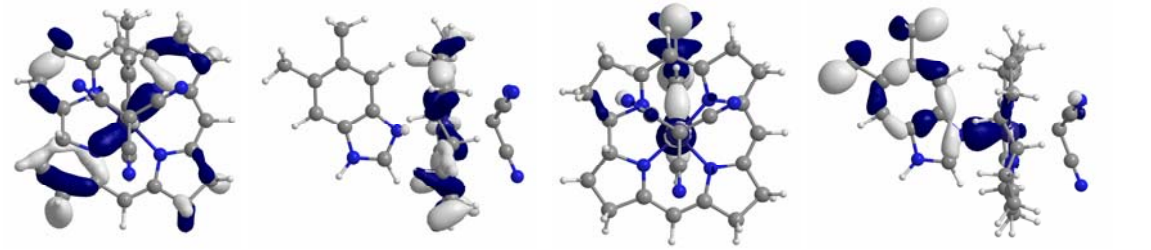
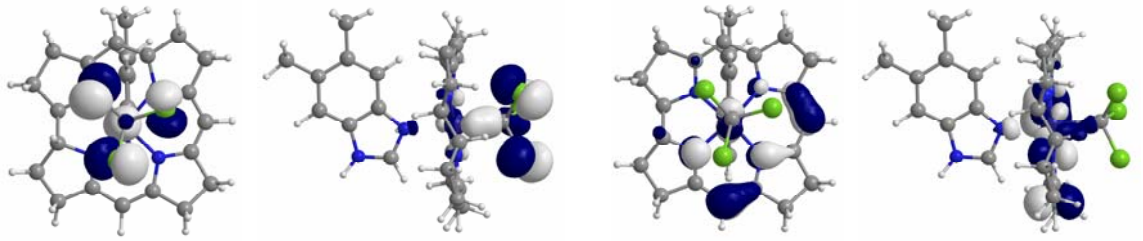


$C(CN)_3$

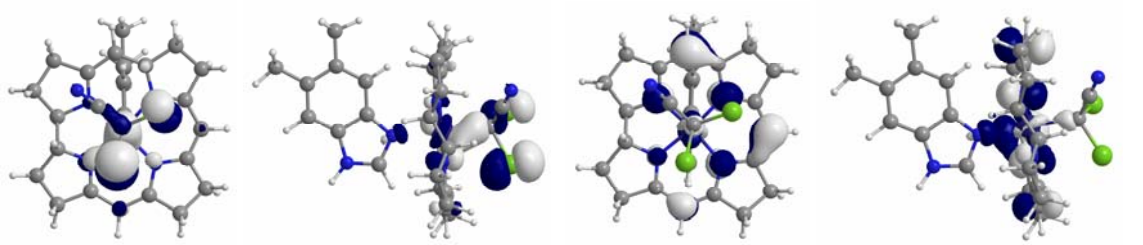


σ_2^+ σ_2^-

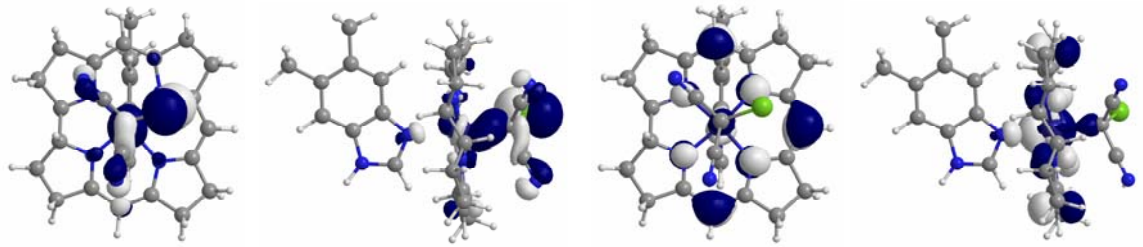
CCl_3



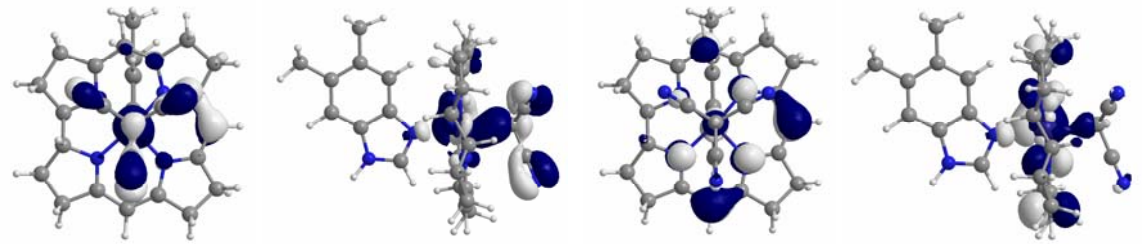
$CCl_2(CN)$

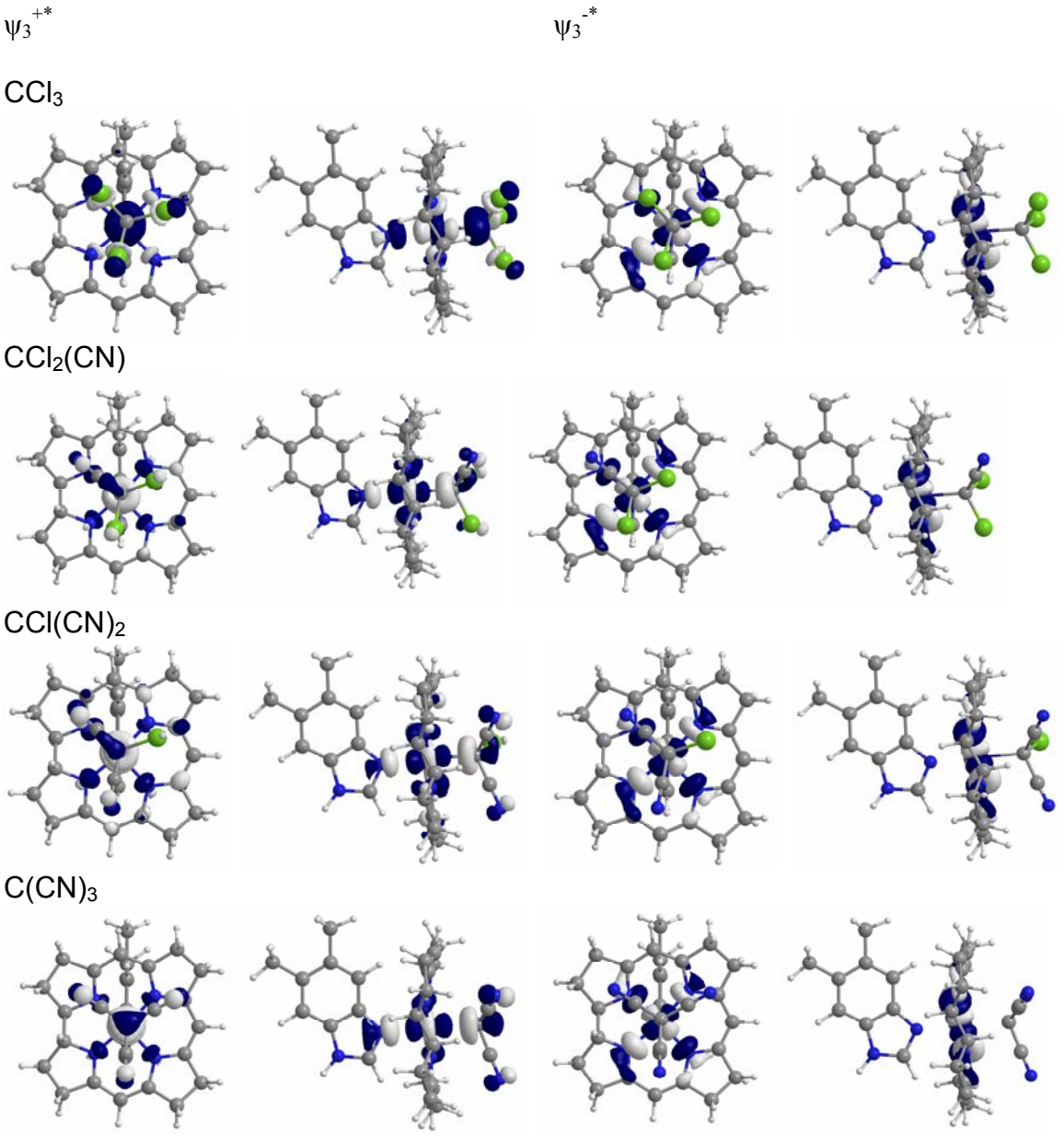


$CCl(CN)_2$



$C(CN)_3$





(b)

Figure S3. Pictures of the six molecular orbitals involved in interligand bonding for (a) Set 1 and (b) Set 2.

Table S1. Experimental coordination distances (Å) in alkylcobalamins with estimated standard deviations in parenthesis.

-R	Co-C	Co-N_{DBI}	Co-N_1	Co-N_2	Co-N_3	Co-N_4	Ref.
CN	1.858(12)	2.011(10)	1.875(8)	1.908(8)	1.917(9)	1.875(8)	[59]
CN(KCl)	1.868(8)	2.029(6)	1.864(5)	1.904(5)	1.906(5)	1.896(5)	[60]
CN(LiCl)	1.886(4)	2.041(3)	1.881(3)	1.911(3)	1.920(3)	1.883(3)	[60]
CF_3	1.878(10)	2.047(10)	1.870(9)	1.951(10)	1.887(10)	1.917(9)	[20]
$CH=CH_2$	1.911(7)	2.165(6)	1.877(5)	1.919(5)	1.910(6)	1.882(5)	[61]
CHF_2	1.949(8)	2.187(7)	1.894(7)	1.911(7)	1.891(7)	1.887(7)	[62]
cis-CH=CHCl	1.951(7)	2.144(5)	1.894(5)	1.922(5)	1.908(5)	1.893(5)	[61]
Adeninylpropyl	1.959(10)	2.212(8)	1.853(7)	1.885(7)	1.886(7)	1.850(7)	[63]
CH_3	1.979(4)	2.162(4)	1.877(4)	1.922(4)	1.918(4)	1.874(4)	[60]
Ado	2.033(4)	2.237(3)	1.880(3)	1.916(3)	1.914(3)	1.866(3)	[33]
i-Amyl	2.044(3)	2.277(2)	1.869(2)	1.914(2)	1.915(2)	1.889(2)	[64]

Table 2. DFT BP86/6-31g(d) 5d optimized coordination distances (Å) in cobalamins.

Alkyl group	Co-C	Co-N_{DBI}	Co-N_1	Co-N_2	Co-N_3	Co-N_4
CN	1.843	2.085	1.885	1.936	1.939	1.878
cis-CH=CHCl	1.920	2.164	1.867	1.927	1.941	1.870
trans-CH=CHCl	1.920	2.174	1.872	1.927	1.937	1.872
$CH{=}CH_2$	1.921	2.202	1.870	1.924	1.937	1.874
$CH{=}CCl_2$	1.928	2.144	1.869	1.928	1.942	1.872
CHF_2	1.942	2.188	1.875	1.931	1.931	1.867
CF_3	1.945	2.150	1.877	1.930	1.930	1.874
CH_2F	1.956	2.186	1.872	1.927	1.932	1.866
CF_2CF_3	1.966	2.203	1.877	1.928	1.930	1.877
CH_3	1.969	2.183	1.868	1.928	1.932	1.865
CH_2CHF_2	1.986	2.198	1.871	1.926	1.934	1.870
CH_2CF_3	1.990	2.174	1.870	1.929	1.938	1.871
CH_2CH_2F	1.990	2.208	1.869	1.928	1.930	1.867
Ado	1.994	2.208	1.872	1.926	1.927	1.867
CH_2OCH_3	1.999	2.285	1.864	1.928	1.930	1.863
CH_2CH_3	2.003	2.231	1.866	1.926	1.931	1.866
$CH_2CH_2CH(CH_3)_2$ (i-Amyl)	2.005	2.228	1.867	1.922	1.928	1.864
CH_2NH_2	2.039	2.330	1.864	1.924	1.926	1.861
$CCl_2(NO_2)$	2.044	2.138	1.880	1.931	1.934	1.876
CBr_3	2.053	2.129	1.877	1.926	1.934	1.875
CCl_3	2.057	2.128	1.878	1.926	1.932	1.874
$CH(CH_3)_2$ (i-Prop)	2.057	2.271	1.862	1.918	1.925	1.866
$CCl_2(CN)$	2.059	2.104	1.881	1.926	1.935	1.878
$CF(CF_3)_2$	2.064	2.286	1.874	1.938	1.937	1.875
$CCl(CN)_2$	2.075	2.097	1.880	1.924	1.938	1.881
$C(CH_3)_3$ (t-But)	2.138	2.374	1.866	1.925	1.926	1.862
$C(CN)_3$	2.161	2.051	1.877	1.925	1.941	1.884
$C(CF_3)_3$	2.315	2.150	1.876	1.929	1.941	1.881

Table S3. Corrin dihedral angles.

Alkyl group	ω_a	ω_b	ω_c	ω_d	ω_e	ω_f	ω_g	ω_h
CN	-15.8	-6.0	4.4	-0.9	-0.6	-12.7	-13.3	16.2
cis-CH=CHCl	-14.0	-4.9	3.3	-1.5	-2.1	-17.0	-9.0	16.6
trans-CH=CHCl	-11.1	-4.1	2.8	-0.8	-0.9	-14.2	-12.1	13.6
$CH=CH_2$	-9.6	-4.2	2.9	-1.9	-0.1	-14.1	-12.2	11.9
$CH=CCl_2$	-14.0	-4.9	3.2	-1.3	-2.3	-17.0	-8.8	16.6
CHF_2	-14.3	-5.4	3.7	-2.8	0.1	-13.8	-12.0	15.3
CF_3	-14.8	-5.9	4.5	-2.7	-0.7	-14.5	-10.9	16.4
CH_2F	-15.1	-6.6	5.0	-2.1	-0.3	-14.2	-11.3	15.2
CF_2CF_3	-14.4	-3.8	3.5	-4.6	-1.7	-17.1	-7.2	17.3
CH_3	-13.8	-4.6	3.4	-2.6	-0.1	-14.6	-11.1	14.1
CH_2CHF_2	-8.9	-3.0	1.7	-1.3	-1.8	-15.8	-9.6	12.1
CH_2CF_3	-10.1	-3.3	2.4	-1.3	-2.0	-14.8	-10.5	12.0
CH_2CH_2F	-10.0	-3.7	3.1	-1.8	-1.7	-15.7	-9.8	12.8
Ado	-14.9	-4.4	4.1	-3.8	-1.0	-14.4	-10.6	15.2
CH_2OCH_3	-15.7	-3.6	3.8	-4.9	-0.2	-13.9	-10.7	15.4
CH_2CH_3	-10.5	-3.3	2.9	-2.4	-0.8	-15.4	-10.1	12.5
$CH_2CH_2CH(CH_3)_2$ (i-Amyl)	-15.1	-7.4	6.2	-1.6	-1.6	-15.2	-10.0	15.6
CH_2NH_2	-11.4	-3.2	2.9	-2.8	-0.6	-15.9	-9.7	13.1
$CCl_2(NO_2)$	-13.3	-5.6	5.3	-2.0	-3.2	-13.8	-11.3	16.0
CBr_3	-16.3	-6.4	6.1	-3.6	-1.5	-12.9	-12.5	19.0
CCl_3	-15.5	-6.6	6.6	-3.8	-1.3	-13.2	-12.1	17.8
$CH(CH_3)_2$ (i-Prop)	-12.4	-8.6	6.3	-0.7	-4.1	-17.1	-7.3	15.6
$CCl_2(CN)$	-16.5	-5.9	6.3	-4.1	-0.5	-13.0	-11.9	17.2
$CF(CF_3)_2$	-6.4	2.4	-2.9	-6.2	3.8	-13.2	-12.3	10.0
$CCl(CN)_2$	-16.9	-5.8	5.8	-4.0	-0.4	-13.5	-11.4	18.0
$C(CH_3)_3$ (t-But)	-11.8	-5.6	4.4	-3.8	-1.6	-15.1	-9.9	15.4
$C(CN)_3$	-7.1	-6.5	5.7	-5.6	0.7	-15.2	-9.4	18.5
$C(CF_3)_3$	-12.2	-4.8	4.1	-4.1	-1.6	-16.0	-8.2	15.9

$\omega_a = \omega(N_{22}\text{-Co-}N_{21}\text{-}C_4)$
$\omega_b = \omega(N_{22}\text{-Co-}N_{23}\text{-}C_{11})$
$\omega_c = \omega(N_{23}\text{-Co-}N_{22}\text{-}C_9)$
$\omega_d = \omega(N_{23}\text{-Co-}N_{24}\text{-}C_{16})$
$\omega_e = \omega(N_{24}\text{-Co-}N_{23}\text{-}C_{14})$
$\omega_f = \omega(N_{24}\text{-Co-}N_{21}\text{-}C_1)$
$\omega_g = \omega(N_{21}\text{-Co-}N_{24}\text{-}C_{19})$
$\omega_h = \omega(N_{21}\text{-Co-}N_{22}\text{-}C_6)$

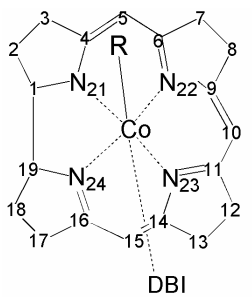


Table S4. Orbital energies (eV) and axial bond lengths (Å) of six molecular orbitals essential in interligand bonding for two sets.

	CH_3	CH_2CH_3	$CH(CH_3)_2$	$C(CH_3)_3$	CCl_3	$CCl_2(CN)$	$CCl(CN)_2$	$C(CN)_3$
Ψ_1^+	-10.93	-10.79	-10.78	-10.68	-11.96	-11.99	-12.06	-12.15
Ψ_1^-	-10.34	-10.19	-10.15	-9.87	-11.20	-11.35	-11.44	-11.57
σ_2^+	-8.96	-8.65	-8.39	-8.26	-8.92	-9.13	-9.32	-9.47
σ_2^-	-7.38	-7.33	-7.34	-7.45	-7.76	-7.80	-7.87	-7.94
Ψ_3^{*+}	-4.06	-4.10	-4.22	-4.65	-5.45	-5.50	-5.78	-6.11
Ψ_3^{*-}	-4.39	-4.37	-4.33	-4.31	-4.94	-5.06	-5.18	-5.29
Co-C	1.969	2.003	2.057	2.138	2.057	2.059	2.075	2.161
Co-N_{ax}	2.183	2.231	2.271	2.374	2.128	2.104	2.097	2.051

Table S5. Cartesian coordinates of all the structures optimized in current work.

DBI-[Co^{III}(corrin)]-CN^+

Co	-0.976882	0.014914	0.394303
N	-0.131426	1.594196	0.980320
N	0.034822	-1.042796	1.661057
N	-1.923612	-1.497212	-0.365839
N	-1.982615	1.220506	-0.636755
C	-0.412244	2.829152	0.200259
C	-0.087435	3.973887	1.186757
C	0.899727	3.319166	2.188923
C	0.568420	1.842462	2.066681
C	0.980451	0.815019	2.965794
C	0.723412	-0.522827	2.751649
C	1.150179	-1.638172	3.687672
C	0.874000	-2.913849	2.865661
C	0.005189	-2.399869	1.734613
C	-0.748243	-3.230171	0.901001
C	-1.674002	-2.798024	-0.050315
C	-2.538767	-3.746711	-0.858291
C	-3.498211	-2.799398	-1.607736
C	-2.943682	-1.418199	-1.304649
C	-3.403084	-0.255597	-1.894916
C	-2.934408	1.040198	-1.529301
C	-3.468488	2.374247	-2.029704
C	-2.401109	3.378262	-1.513356
C	-1.858718	2.654468	-0.268126
N	1.169190	-0.484135	-3.217654
C	0.090849	-0.385832	-2.386357
N	0.446990	-0.196236	-1.114312
C	2.795937	0.012612	-0.083545
C	4.164390	-0.000509	-0.391244
C	4.612942	-0.191175	-1.742293
C	3.680955	-0.364883	-2.775032

C	2.319017	-0.347623	-2.444270
C	1.854308	-0.163880	-1.115411
C	5.179096	0.188635	0.716752
C	6.092142	-0.206507	-2.059746
H	0.782426	3.683558	3.223684
H	0.371395	-3.710892	3.437959
H	-0.662793	-4.309086	1.060218
H	-4.531011	-2.872170	-1.220315
H	-1.596768	3.501152	-2.262466
H	-2.524261	2.822381	0.604877
H	-0.935388	-0.455767	-2.744050
H	2.474298	0.159959	0.950451
H	4.016140	-0.509023	-3.807969
H	4.683871	0.319776	1.693243
H	5.816778	1.075394	0.541500
H	5.862201	-0.677558	0.798750
H	6.582426	0.741101	-1.767945
H	6.269345	-0.358576	-3.137056
H	1.129109	-0.630236	-4.224945
H	-1.007663	4.282296	1.714875
H	1.956667	3.487423	1.903100
H	1.525650	1.102194	3.868820
H	2.198856	-1.531501	4.010365
H	0.522710	-1.606891	4.598279
H	1.804982	-3.347062	2.451938
H	-3.058907	-4.467212	-0.204323
H	-1.907346	-4.338736	-1.547167
H	-3.549318	-2.991051	-2.692969
H	-4.204602	-0.331003	-2.634869
H	-3.607995	2.391127	-3.124285
H	-4.459889	2.564508	-1.572824
H	-2.818221	4.371972	-1.286669
H	0.331745	4.860399	0.685575
H	0.261277	2.839885	-0.681794
C	-2.271357	0.176699	1.696119
N	-3.109744	0.293558	2.520284

DBI-[Co^{III}(corrin)]-CH=$CHCl^{+}$ cis

Co	0.907251	0.106344	0.246147
N	0.359097	-1.556535	-0.401883
N	-0.009956	-0.205867	1.912124
N	1.433457	1.923305	0.680356
N	1.835577	0.177930	-1.375949
C	0.543109	-1.778770	-1.860142
C	0.436903	-3.311383	-2.024721
C	-0.370201	-3.755393	-0.772930
C	-0.160148	-2.605652	0.195613
C	-0.515079	-2.590008	1.578612
C	-0.447826	-1.452775	2.354423
C	-0.858076	-1.379279	3.814160
C	-0.916868	0.138768	4.085306
C	-0.179250	0.718981	2.893577
C	0.279684	2.039145	2.834870
C	1.051603	2.586567	1.808054
C	1.569252	4.013772	1.821855

C	2.521100	4.054144	0.607902
C	2.254608	2.732365	-0.094911
C	2.758082	2.399107	-1.337927
C	2.530735	1.134139	-1.958433
C	3.043093	0.687868	-3.320209
C	2.171367	-0.565368	-3.605064
C	1.862182	-1.071629	-2.184502
N	-1.966349	2.419660	-1.979052
C	-0.754342	2.026587	-1.482710
N	-0.850008	0.969895	-0.675921
C	-2.932214	-0.367589	0.022089
C	-4.323261	-0.452383	-0.137734
C	-5.025456	0.481763	-0.972315
C	-4.323166	1.494633	-1.640886
C	-2.933748	1.559360	-1.466875
C	-2.219505	0.647014	-0.645681
C	-5.091052	-1.543004	0.579821
C	-6.525983	0.378656	-1.136394
H	-0.025404	-4.713787	-0.347896
H	-0.456413	0.438361	5.041425
H	0.057505	2.683780	3.690590
H	3.580820	4.100480	0.920508
H	1.235916	-0.270813	-4.116900
H	2.692601	-1.697738	-1.801466
H	0.174197	2.537199	-1.734079
H	-2.414265	-1.087289	0.661133
H	-4.853492	2.209875	-2.279197
H	-4.415002	-2.184593	1.169325
H	-5.638957	-2.193121	-0.127960
H	-5.847143	-1.125674	1.271321
H	-6.823215	-0.593626	-1.572650
H	-6.913053	1.173295	-1.795240
H	-7.049637	0.461572	-0.165599
H	-2.123913	3.203125	-2.610521
H	1.443468	-3.762663	-2.004898
H	-1.450366	-3.867268	-0.990989
H	-0.881162	-3.513529	2.035338
H	-1.808082	-1.904135	4.006830
H	-0.084622	-1.866150	4.438075
H	-1.958911	0.512711	4.095631
H	2.065323	4.256757	2.776942
H	0.724619	4.720252	1.713412
H	2.348316	4.916005	-0.058571
H	3.375202	3.133692	-1.862953
H	2.954514	1.477962	-4.085555
H	4.117629	0.426736	-3.246342
H	2.683591	-1.316144	-4.227309
H	-0.049733	-3.600070	-2.969624
H	-0.282922	-1.255102	-2.384979
C	2.485654	-0.510155	1.149479
C	3.267926	-1.596151	1.243207
H	2.849650	0.294545	1.809377
H	4.139164	-1.617618	1.907912
Cl	3.137090	-3.154530	0.411529

DBI-[Co^{III}(corrin)]-CH=$CHCl^{+}$ trans

Co	-0.841348	0.042763	-0.058067
N	-0.310369	-1.108145	1.320149
N	-0.112782	-1.152325	-1.382916
N	-1.356681	1.408824	-1.331077
N	-1.610475	0.999675	1.354853
C	-0.428271	-0.577890	2.706444
C	-0.415680	-1.844379	3.588116
C	0.369000	-2.865702	2.722191
C	0.142501	-2.344955	1.312839
C	0.403066	-3.048601	0.099248
C	0.275576	-2.466885	-1.147267
C	0.542474	-3.186817	-2.456272
C	0.576757	-2.038856	-3.484914
C	-0.030106	-0.882499	-2.714650
C	-0.451762	0.305827	-3.316525
C	-1.092161	1.362059	-2.666917
C	-1.581945	2.606024	-3.384434
C	-2.347380	3.370785	-2.284429
C	-2.060379	2.567333	-1.026205
C	-2.455936	2.954388	0.241569
C	-2.234041	2.160453	1.405483
C	-2.695124	2.473967	2.821143
C	-1.888163	1.451048	3.666413
C	-1.678538	0.300293	2.665677
N	2.310536	2.949258	0.411430
C	1.045005	2.438622	0.323526
N	1.036136	1.115296	0.163311
C	3.011877	-0.524310	0.029611
C	4.411844	-0.607036	0.054505
C	5.215575	0.573765	0.203853
C	4.604635	1.829267	0.332047
C	3.204360	1.887179	0.305521
C	2.390533	0.733476	0.151733
C	5.081507	-1.959045	-0.077119
C	6.724846	0.470254	0.226051
H	0.022476	-3.906290	2.844249
H	0.018140	-2.254706	-4.410798
H	-0.310971	0.395618	-4.397867
H	-3.435952	3.388884	-2.475819
H	-0.911937	1.882791	3.955729
H	-2.566562	-0.365424	2.637214
H	0.156734	3.066718	0.374368
H	2.416275	-1.434536	-0.080025
H	5.212041	2.733367	0.449829
H	4.335775	-2.766083	-0.170622
H	5.717675	-2.189104	0.798191
H	5.741003	-2.005760	-0.964211
H	7.078144	-0.170834	1.055465
H	7.193373	1.461006	0.345679
H	7.117003	0.023332	-0.706760
H	2.547659	3.931917	0.536267
H	-1.449616	-2.201286	3.746815
H	1.452769	-2.856365	2.952296
H	0.724537	-4.092211	0.157041
H	1.467664	-3.785287	-2.420816

H	-0.289789	-3.885175	-2.666114
H	1.612632	-1.784919	-3.781735
H	-2.211850	2.344783	-4.252142
H	-0.722606	3.180939	-3.777408
H	-2.026706	4.421249	-2.177655
H	-2.995102	3.899715	0.350120
H	-2.516742	3.525998	3.102766
H	-3.786233	2.297744	2.902466
H	-2.412890	1.137206	4.582501
H	0.042563	-1.673385	4.574951
H	0.458485	0.060946	2.901268
C	-2.572416	-0.755068	-0.287241
C	-2.921686	-2.039503	-0.146327
H	-3.342709	-0.021083	-0.564858
H	-2.258197	-2.866288	0.117626
Cl	-4.584179	-2.599725	-0.406026

DBI-[Co^{III}(corrin)]-$CH=CH_2^+$

Co	-1.043106	0.030240	0.393199
N	-0.214365	1.622459	0.917299
N	-0.075845	-0.961509	1.728228
N	-1.942839	-1.516362	-0.347988
N	-1.985506	1.178336	-0.749841
C	-0.422034	2.803076	0.035531
C	-0.072097	4.003105	0.938952
C	0.932034	3.392945	1.952857
C	0.551191	1.921813	1.946609
C	0.968630	0.938799	2.892007
C	0.660538	-0.401346	2.766287
C	1.078938	-1.467834	3.762228
C	0.756325	-2.782310	3.024178
C	-0.112206	-2.314414	1.872482
C	-0.852803	-3.184352	1.068327
C	-1.720738	-2.802913	0.044946
C	-2.532153	-3.793152	-0.770204
C	-3.430286	-2.885570	-1.635260
C	-2.899333	-1.488871	-1.354965
C	-3.327248	-0.355886	-2.022910
C	-2.872982	0.956350	-1.700021
C	-3.351958	2.259367	-2.323259
C	-2.300870	3.279431	-1.807627
C	-1.847854	2.635540	-0.485145
N	1.294935	-0.627838	-3.206795
C	0.198240	-0.503567	-2.397243
N	0.521786	-0.271143	-1.125807
C	2.842501	-0.034197	-0.052475
C	4.218743	-0.055039	-0.322763
C	4.701930	-0.285094	-1.655206
C	3.797427	-0.491565	-2.706907
C	2.426998	-0.465077	-2.413046
C	1.927761	-0.239880	-1.102803
C	5.204008	0.166146	0.806023
C	6.189289	-0.307578	-1.933244
H	0.865518	3.836983	2.961092
H	0.238623	-3.527395	3.651211

H	-0.775310	-4.253906	1.286127
H	-4.491892	-2.948964	-1.333285
H	-1.449269	3.338095	-2.510896
H	-2.548813	2.887646	0.338406
H	-0.819259	-0.586865	-2.777268
H	2.489968	0.140444	0.967960
H	4.161132	-0.667835	-3.725258
H	4.681791	0.343702	1.761035
H	5.859989	1.036145	0.614706
H	5.871794	-0.705070	0.945120
H	6.670578	0.651254	-1.663279
H	6.394727	-0.497079	-2.999708
H	6.702282	-1.093351	-1.347360
H	1.277167	-0.811515	-4.208419
H	-0.978720	4.348487	1.468543
h	1.981413	3.509266	1.616903
H	1.560063	1.259305	3.754251
H	2.136338	-1.368413	4.058145
H	0.472309	-1.367479	4.682069
H	1.669079	-3.268952	2.629921
H	-3.101621	-4.477709	-0.118177
H	-1.858307	-4.423554	-1.380265
H	-3.391473	-3.127361	-2.711153
H	-4.077674	-0.470091	-2.810350
H	-3.418059	2.203839	-3.423558
H	-4.367928	2.498073	-1.950249
H	-2.710366	4.293540	-1.676624
H	0.343517	4.855441	0.378600
H	0.286030	2.716921	-0.815469
C	-2.514920	0.242475	1.609909
C	-2.545951	0.769711	2.842829
H	-3.447770	-0.145194	1.169778
H	-3.488821	0.801889	3.408147
H	-1.667045	1.174935	3.356729

DBI-[Co^{III}(corrin)]-CH=CCl_2^+

Co	0.647966	0.244878	0.081755
N	0.193688	-1.293956	-0.876221
N	0.018528	-0.550089	1.721857
N	1.038333	1.976828	0.869511
N	1.327747	0.795860	-1.572841
C	0.194802	-1.164193	-2.357582
C	0.235017	-2.624045	-2.862667
C	-0.337048	-3.437237	-1.667941
C	-0.118293	-2.509698	-0.486194
C	-0.270625	-2.847654	0.892913
C	-0.213992	-1.911716	1.903772
C	-0.413751	-2.219425	3.376741
C	-0.586006	-0.821424	4.007421
C	-0.101079	0.103393	2.907464
C	0.201028	1.454433	3.109079
C	0.755594	2.314978	2.159222
C	1.123057	3.758429	2.452547
C	1.885921	4.192277	1.183087
C	1.658015	3.037460	0.221333

C	2.014393	3.056084	-1.113680
C	1.834179	1.940677	-1.985242
C	2.196885	1.878388	-3.461508
C	1.421117	0.620123	-3.936559
C	1.370826	-0.227987	-2.652669
N	-2.724131	2.575133	-1.178962
C	-1.419226	2.252264	-0.932773
N	-1.286031	1.038899	-0.395600
C	-3.094678	-0.691895	0.198509
C	-4.477458	-0.926869	0.181496
C	-5.386104	0.064987	-0.321764
C	-4.896736	1.287111	-0.803984
C	-3.511447	1.499275	-0.778056
C	-2.595134	0.532825	-0.285005
C	-5.016449	-2.243124	0.701057
C	-6.875073	-0.202867	-0.335514
H	0.163343	-4.409949	-1.521092
H	-0.017972	-0.682408	4.942225
H	0.039824	1.857073	4.113515
H	2.968980	4.304697	1.375676
H	0.397028	0.900038	-4.247467
H	2.310524	-0.802793	-2.529131
H	-0.596710	2.929449	-1.158241
H	-2.419024	-1.458999	0.585121
H	-5.584260	2.048271	-1.188864
H	-4.201262	-2.897489	1.052380
H	-5.577079	-2.793379	-0.077874
H	-5.716382	-2.094933	1.544906
H	-7.124135	-1.091043	-0.946192
H	-7.433195	0.654032	-0.747265
H	-7.263995	-0.400340	0.681089
H	-3.052988	3.450658	-1.582481
H	1.277720	-2.925320	-3.061900
H	-1.418898	-3.643999	-1.784460
H	-0.465183	-3.890623	1.157085
H	-1.267816	-2.894824	3.548521
H	0.487177	-2.726448	3.771120
H	-1.646899	-0.602655	4.236256
H	1.721912	3.844667	3.375146
H	0.204779	4.354588	2.612721
H	1.535989	5.150836	0.764015
H	2.476364	3.962035	-1.515935
H	1.928053	2.801374	-4.003241
H	3.291866	1.745420	-3.569602
H	1.909009	0.101815	-4.777121
H	-0.343190	-2.764359	-3.789397
H	-0.748992	-0.659255	-2.651002
C	2.401809	-0.320542	0.650473
C	3.298475	-1.290714	0.408841
H	2.750693	0.372897	1.428486
Cl	3.186735	-2.620429	-0.739002
Cl	4.829416	-1.348357	1.300443

DBI-[Co^{III}(corrin)]-CHF_2^+

Co	-0.944020	0.056025	0.331223

N	-0.103907	1.714309	0.573996
N	0.015942	-0.682520	1.835450
N	-1.811113	-1.604005	-0.138738
N	-1.858414	0.979079	-1.009529
C	-0.295314	2.718917	-0.507045
C	0.020959	4.066551	0.177599
C	0.962683	3.660330	1.341722
C	0.588422	2.207557	1.577567
C	0.956299	1.417505	2.707477
C	0.692375	0.066603	2.795744
C	1.109529	-0.813733	3.961482
C	0.854399	-2.240402	3.433082
C	0.004204	-1.994929	2.201012
C	-0.708142	-2.998845	1.540945
C	-1.567100	-2.804691	0.456271
C	-2.336837	-3.931150	-0.207441
C	-3.263995	-3.188540	-1.191202
C	-2.741694	-1.762621	-1.160689
C	-3.144524	-0.773232	-2.035659
C	-2.708862	0.580733	-1.934571
C	-3.166370	1.745039	-2.799222
C	-2.127695	2.845488	-2.451331
C	-1.712614	2.458548	-1.019695
N	1.489444	-1.232952	-3.014397
C	0.367008	-0.980073	-2.273782
N	0.648183	-0.494458	-1.065180
C	2.932381	0.004469	0.000005
C	4.315997	-0.035510	-0.226730
C	4.841917	-0.506071	-1.477391
C	3.972360	-0.936202	-2.489930
C	2.593839	-0.888176	-2.240099
C	2.052179	-0.423573	-1.012312
C	5.264249	0.421245	0.862416
C	6.336585	-0.540744	-1.709772
C	-2.397947	0.452657	1.556826
H	0.832525	4.274939	2.249000
H	0.350026	-2.900253	4.158509
H	-0.615380	-4.017481	1.929391
H	-4.314975	-3.200503	-0.847095
H	-1.257123	2.774610	-3.129828
H	-2.429430	2.865294	-0.277640
H	-0.637241	-1.162464	-2.654189
H	2.548509	0.365039	0.957951
H	4.368441	-1.297895	-3.445253
H	4.712026	0.760947	1.754555
H	5.906032	1.257152	0.525610
H	5.947340	-0.389886	1.177933
H	6.787159	0.465519	-1.618577
H	6.577648	-0.925900	-2.714251
H	6.850077	-1.184128	-0.970802
H	-2.321862	-0.163202	2.473152
H	1.504966	-1.605827	-3.962065
H	-0.908411	4.506900	0.581786
H	2.030504	3.728747	1.054275
H	1.492212	1.899154	3.529996
H	2.153962	-0.631242	4.263432
H	0.475182	-0.591442	4.840453

H	1.796382	-2.742484	3.139542
H	-2.880846	-4.542550	0.532605
H	-1.634129	-4.610498	-0.726497
H	-3.256733	-3.610540	-2.210286
H	-3.870541	-1.031145	-2.811887
H	-3.203079	1.488587	-3.872005
H	-4.191489	2.044108	-2.502682
H	-2.538210	3.865166	-2.520880
H	0.475284	4.797821	-0.509307
H	0.430539	2.489838	-1.314846
F	-2.431351	1.777089	1.951376
F	-3.626150	0.199787	0.987957

DBI-[Co^{III}(corrin)]-CF_3^+

Co	-0.882238	0.008553	0.232880
N	-0.097250	1.594187	0.858976
N	0.063510	-1.016562	1.566326
N	-1.690923	-1.525724	-0.614838
N	-1.780955	1.186140	-0.914120
C	-0.267065	2.799893	0.004692
C	-0.009646	3.975652	0.971863
C	0.895687	3.345723	2.063868
C	0.547748	1.869997	1.971686
C	0.896816	0.861578	2.918113
C	0.674015	-0.481688	2.695960
C	1.072458	-1.587243	3.656136
C	0.901866	-2.865092	2.808850
C	0.091469	-2.374391	1.625508
C	-0.559843	-3.226874	0.730328
C	-1.415631	-2.821229	-0.294441
C	-2.150300	-3.791572	-1.200474
C	-3.081831	-2.872638	-2.017101
C	-2.596457	-1.476873	-1.667994
C	-2.999187	-0.330404	-2.326566
C	-2.592167	0.977508	-1.931911
C	-3.036604	2.292552	-2.553833
C	-2.020757	3.302999	-1.954835
C	-1.657052	2.637351	-0.614825
N	1.652461	-0.482577	-3.198524
C	0.501286	-0.381525	-2.468373
N	0.735342	-0.186970	-1.170166
C	2.977399	0.029662	0.070494
C	4.368784	0.016926	-0.106216
C	4.942889	-0.179955	-1.407704
C	4.112466	-0.359609	-2.523061
C	2.725246	-0.342035	-2.322404
C	2.136526	-0.153427	-1.043986
C	5.273872	0.212660	1.092157
C	6.445547	-0.193423	-1.583268
C	-2.406963	0.118086	1.435469
H	0.715779	3.751969	3.073943
H	0.394103	-3.686360	3.341234
H	-0.437649	-4.303147	0.883998
H	-4.136778	-2.981206	-1.703452
H	-1.124217	3.370021	-2.599120

H	-2.412250	2.883817	0.159716
H	-0.486880	-0.460052	-2.919720
H	2.558171	0.182336	1.068148
H	4.544017	-0.508106	-3.519010
H	4.687622	0.368128	2.013199
H	5.939516	1.087143	0.965898
H	5.932521	-0.661121	1.256042
H	6.903284	0.759363	-1.256938
H	6.725182	-0.355617	-2.637246
H	6.919501	-0.992434	-0.982742
H	1.706025	-0.634960	-4.204183
H	-0.964350	4.305122	1.420180
H	1.971964	3.489062	1.843684
H	1.385292	1.163392	3.848538
H	2.091343	-1.445960	4.052527
H	0.382573	-1.587176	4.521117
H	1.875509	-3.257628	2.457507
H	-2.689885	-4.556842	-0.617056
H	-1.426444	-4.329754	-1.841284
H	-3.049437	-3.061788	-3.103242
H	-3.698889	-0.429633	-3.161105
H	-3.040138	2.261684	-3.656914
H	-4.072675	2.519633	-2.232477
H	-2.437031	4.315685	-1.835283
H	0.452512	4.843474	0.475531
H	0.497033	2.756528	-0.799361
F	-2.475615	1.295241	2.141141
F	-3.600902	0.024712	0.767649
F	-2.443887	-0.879021	2.373181

DBI-[Co^{III}(corrin)]-CH_2F^+

Co	-1.020402	0.050547	0.391260
N	-0.142253	1.672772	0.710402
N	-0.051800	-0.791751	1.828305
N	-1.953398	-1.555878	-0.137448
N	-1.949382	1.065423	-0.868918
C	-0.330696	2.740110	-0.308748
C	0.022293	4.042373	0.442505
C	0.960472	3.556683	1.579417
C	0.567712	2.097887	1.732454
C	0.941870	1.235548	2.806550
C	0.659081	-0.113764	2.817382
C	1.084674	-1.069583	3.918616
C	0.795755	-2.457051	3.309176
C	-0.077868	-2.121973	2.115526
C	-0.825866	-3.073327	1.415072
C	-1.716353	-2.797680	0.376918
C	-2.534493	-3.865409	-0.326343
C	-3.483080	-3.045497	-1.224463
C	-2.927009	-1.634468	-1.128094
C	-3.341117	-0.584286	-1.925929
C	-2.850195	0.746964	-1.779164
C	-3.293021	1.969422	-2.569233
C	-2.201606	3.011574	-2.203508
C	-1.762923	2.540121	-0.805562

N	1.291512	-1.112361	-3.083818
C	0.194171	-0.890828	-2.295886
N	0.516523	-0.465496	-1.075327
C	2.832720	-0.028401	-0.058633
C	4.208296	-0.057785	-0.330654
C	4.693389	-0.466686	-1.619151
C	3.791895	-0.847010	-2.623899
C	2.421808	-0.809371	-2.329327
C	1.921118	-0.403492	-1.064014
C	5.191159	0.346009	0.748604
C	6.180019	-0.488465	-1.900117
C	-2.468734	0.420686	1.651896
H	0.837798	4.119175	2.520995
H	0.298210	-3.153703	4.004279
H	-0.740399	-4.115205	1.738151
H	-4.521010	-3.061536	-0.842545
H	-1.354538	2.939441	-2.911011
H	-2.451534	2.921401	-0.025008
H	-0.823002	-1.048374	-2.652860
H	2.478200	0.282022	0.928121
H	4.157524	-1.161970	-3.607483
H	4.667867	0.636890	1.674784
H	5.818970	1.201167	0.434268
H	5.886834	-0.476941	0.999365
H	6.633178	0.512997	-1.775174
H	6.389129	-0.824687	-2.929045
H	6.716854	-1.165523	-1.209352
H	-2.318087	-0.181329	2.565778
H	-3.425382	0.160456	1.163569
H	1.275231	-1.439687	-4.048139
H	-0.893894	4.483662	0.874465
H	2.029134	3.629561	1.296332
H	1.500890	1.658148	3.646074
H	2.137406	-0.921947	4.210665
H	0.470096	-0.892755	4.821647
H	1.723219	-2.952656	2.962805
H	-3.062116	-4.514359	0.393308
H	-1.866398	-4.522158	-0.915519
H	-3.522773	-3.402408	-2.267421
H	-4.104530	-0.778993	-2.684632
H	-3.374632	1.767876	-3.651265
H	-4.295489	2.293083	-2.224469
H	-2.572962	4.048494	-2.213029
H	0.490841	4.796958	-0.208759
H	0.376224	2.541698	-1.141036
F	-2.545473	1.761520	2.040822

DBI-[Co^{III}(corrin)]-$CF_2CF_3^+$

Co	-0.648342	-0.111926	-0.043313
N	0.105460	-0.910287	1.478593
N	0.203564	-1.428171	-1.165719
N	-1.335758	0.956326	-1.496712
N	-1.367841	1.067431	1.227700
C	0.127613	-0.084876	2.714864
C	0.329342	-1.124463	3.837238

C	1.096345	-2.265425	3.117128
C	0.684365	-2.077915	1.666366
C	0.942803	-2.980059	0.592685
C	0.725335	-2.641161	-0.726829
C	1.039459	-3.535234	-1.911214
C	0.981946	-2.560546	-3.106158
C	0.248647	-1.368109	-2.524352
C	-0.320153	-0.353958	-3.298381
C	-1.084664	0.708755	-2.812775
C	-1.716413	1.756523	-3.710758
C	-2.546293	2.608361	-2.727994
C	-2.095363	2.113343	-1.366310
C	-2.379842	2.746539	-0.171837
C	-1.997568	2.220212	1.097151
C	-2.254461	2.861737	2.451304
C	-1.266938	2.094662	3.369697
C	-1.164983	0.728387	2.666374
N	2.276013	3.084496	-0.366147
C	1.057010	2.467675	-0.320809
N	1.154846	1.147252	-0.164211
C	3.263498	-0.312989	0.058478
C	4.665481	-0.272028	0.085913
C	5.367574	0.973437	-0.045734
C	4.653026	2.169214	-0.203898
C	3.253205	2.103402	-0.228737
C	2.537183	0.883153	-0.101093
C	5.445834	-1.558813	0.255996
C	6.879959	1.004458	-0.015314
C	-2.236284	-1.270158	-0.100415
H	0.847839	-3.272639	3.493367
H	0.468324	-2.969916	-3.991501
H	-0.199011	-0.425793	-4.383404
H	-3.629909	2.418900	-2.841761
H	-0.280352	2.594930	3.369223
H	-2.000015	0.072215	2.975524
H	0.122473	3.019780	-0.408056
H	2.747735	-1.270938	0.159828
H	5.182236	3.123137	-0.305477
H	4.770534	-2.426318	0.342585
H	6.082609	-1.536291	1.160429
H	6.123462	-1.743623	-0.598776
H	7.278276	0.600011	0.934126
H	7.261776	2.032553	-0.127788
H	7.317599	0.393091	-0.826742
H	2.431993	4.083749	-0.487546
H	-0.653114	-1.492050	4.185398
H	2.194015	-2.145943	3.209079
H	1.361095	-3.964214	0.820174
H	2.005243	-4.054477	-1.800277
H	0.256211	-4.312450	-1.997668
H	1.995515	-2.252917	-3.428910
H	-2.323509	1.290049	-4.505451
H	-0.929294	2.347008	-4.216484
H	-2.396883	3.694766	-2.845811
H	-2.955483	3.675867	-0.198733
H	-2.101550	3.954372	2.440473
H	-3.306898	2.682029	2.748406

H	-1.614954	2.016994	4.411886
H	0.872803	-0.720071	4.705705
H	0.996190	0.602693	2.642563
C	-3.655458	-0.825502	0.373333
F	-3.697113	-0.550848	1.705067
F	-4.538122	-1.821699	0.141982
F	-4.086642	0.272346	-0.295297
F	-2.461256	-1.636853	-1.419321
F	-2.011858	-2.447786	0.585018

DBI-[Co^{III}(corrin)]-CH_3^+

Co	-1.056554	-0.000893	0.511689
N	-0.134934	1.450095	1.243233
N	-0.045372	-1.230678	1.599127
N	-2.069811	-1.371059	-0.398035
N	-2.021290	1.341650	-0.350780
C	-0.340427	2.767875	0.583583
C	0.083921	3.795201	1.654238
C	1.076292	2.995087	2.538727
C	0.646052	1.557330	2.299877
C	1.059629	0.419175	3.052305
C	0.737071	-0.874266	2.693188
C	1.193218	-2.106742	3.454672
C	0.778606	-3.268686	2.528603
C	-0.125818	-2.588137	1.519347
C	-0.951066	-3.285998	0.634269
C	-1.874774	-2.711014	-0.240015
C	-2.782428	-3.528812	-1.140716
C	-3.705314	-2.465089	-1.769062
C	-3.093482	-1.150953	-1.312548
C	-3.508735	0.088325	-1.761678
C	-2.973987	1.311961	-1.263601
C	-3.425208	2.714446	-1.642542
C	-2.299010	3.598170	-1.043002
C	-1.798106	2.731348	0.127295
N	1.037376	-0.205797	-3.273692
C	-0.011696	-0.169278	-2.395037
N	0.383945	-0.095698	-1.125279
C	2.762640	-0.016925	-0.160891
C	4.121911	-0.020121	-0.507340
C	4.528222	-0.089993	-1.882610
C	3.565151	-0.156810	-2.899941
C	2.213028	-0.150891	-2.530095
C	1.789318	-0.081366	-1.176342
C	5.169551	0.052622	0.583892
C	5.997717	-0.091639	-2.243971
C	-2.392059	0.002979	1.958792
H	1.039357	3.272169	3.606189
H	0.261689	-4.089054	3.054406
H	-0.906858	-4.379278	0.666193
H	-4.741658	-2.544837	-1.392328
H	-1.488952	3.738633	-1.782557
H	-2.439836	2.882647	1.022715
H	-1.050340	-0.193239	-2.724471
H	2.468571	0.030997	0.891569

H	3.871393	-0.212519	-3.950773
H	4.702200	0.084155	1.582587
H	5.806186	0.952194	0.482688
H	5.851888	-0.817867	0.559080
H	6.505357	0.827549	-1.895075
H	6.141742	-0.160374	-3.334983
H	6.532194	-0.942103	-1.780282
H	-2.004612	0.563445	2.826638
H	-2.593335	-1.040400	2.255049
H	-3.332173	0.464756	1.612017
H	0.962571	-0.263116	-4.287770
H	-0.795496	4.096580	2.252889
H	2.124783	3.129281	2.206393
H	1.677835	0.575226	3.940840
H	2.274050	-2.077270	3.671955
H	0.670600	-2.158635	4.428210
H	1.649338	-3.715384	2.011730
H	-3.329563	-4.298419	-0.569381
H	-2.181386	-4.065176	-1.898988
H	-3.762791	-2.528400	-2.869199
H	-4.312998	0.131316	-2.501677
H	-3.554588	2.836082	-2.731941
H	-4.406736	2.931575	-1.176096
H	-2.651024	4.592159	-0.724594
H	0.527848	4.705735	1.221827
H	0.320979	2.809312	-0.306862

DBI-[Co^{III}(corrin)]-$CH_2CHF_2^+$

Co	-0.910520	0.002432	0.102679
N	-0.295645	1.247267	-1.151381
N	-0.117431	1.017872	1.534656
N	-1.518156	-1.445862	1.230376
N	-1.679753	-0.785609	-1.408898
C	-0.364668	0.831424	-2.580702
C	-0.249714	2.160785	-3.352755
C	0.577303	3.047362	-2.383980
C	0.269377	2.433009	-1.028623
C	0.585024	2.992263	0.242165
C	0.383872	2.313703	1.425055
C	0.687541	2.885762	2.796741
C	0.599196	1.653785	3.719080
C	-0.079142	0.623857	2.836591
C	-0.595176	-0.582024	3.322915
C	-1.279188	-1.536445	2.570637
C	-1.846506	-2.814392	3.160359
C	-2.642911	-3.421383	1.986850
C	-2.276114	-2.530929	0.811115
C	-2.651801	-2.786447	-0.495767
C	-2.344271	-1.914162	-1.580069
C	-2.732637	-2.110669	-3.038255
C	-1.827678	-1.076842	-3.760915
C	-1.640297	-0.002798	-2.674005
N	2.095240	-3.035102	-0.617435
C	0.862788	-2.462966	-0.459366
N	0.931023	-1.156442	-0.205266

C	3.000504	0.355160	0.004172
C	4.402105	0.362905	-0.052651
C	5.133965	-0.844273	-0.315371
C	4.450106	-2.051168	-0.519687
C	3.049731	-2.034347	-0.458805
C	2.305549	-0.852473	-0.199991
C	5.150056	1.661510	0.166608
C	6.645663	-0.821285	-0.372874
C	-2.661418	0.849956	0.502741
H	0.311512	4.117517	-2.426705
H	0.034697	1.834079	4.649226
H	-0.482608	-0.776845	4.393779
H	-3.733548	-3.375599	2.162551
H	-0.852086	-1.533507	-4.011546
H	-2.511692	0.687796	-2.673634
H	-0.060211	-3.035823	-0.536444
H	2.460353	1.284300	0.204803
H	5.002628	-2.975633	-0.720715
H	4.453649	2.495484	0.355211
H	5.769234	1.932227	-0.709378
H	5.839847	1.597370	1.029265
H	7.014041	-0.128585	-1.152676
H	7.054427	-1.821370	-0.592532
H	7.085378	-0.481413	0.583746
H	-2.720331	0.960450	1.600377
H	-3.419941	0.112802	0.188201
H	2.273647	-4.018440	-0.813945
H	-1.254361	2.598075	-3.502199
H	1.664010	2.974331	-2.587779
H	0.986326	4.008502	0.283525
H	1.663824	3.396924	2.827174
H	-0.082267	3.637270	3.055092
H	1.601437	1.287956	4.014524
H	-2.468036	-2.606366	4.048202
H	-1.024616	-3.474383	3.496153
H	-2.397320	-4.478871	1.789710
H	-3.232453	-3.690164	-0.701369
H	-2.584565	-3.149586	-3.379551
H	-3.807207	-1.875949	-3.175197
H	-2.273215	-0.681827	-4.687612
H	0.221405	2.043989	-4.341479
H	0.508651	0.175847	-2.780994
C	-3.054303	2.177710	-0.100513
H	-2.940868	2.254643	-1.198144
F	-4.389562	2.411467	0.189341
F	-2.339813	3.222393	0.459487

DBI-[Co^{III}(corrin)]-$CH_2CF_3^+$

Co	0.819341	0.125437	0.123343
N	0.264858	-1.244784	-1.021462
N	0.093911	-0.816953	1.642193
N	1.354108	1.692786	1.130002
N	1.528144	0.840882	-1.453122
C	0.317620	-0.947986	-2.480834
C	0.296769	-2.343894	-3.135982

C	-0.470702	-3.200015	-2.093998
C	-0.212335	-2.451774	-0.797808
C	-0.490629	-2.925725	0.517631
C	-0.337777	-2.142434	1.640698
C	-0.617286	-2.613030	3.056022
C	-0.593304	-1.305450	3.872546
C	0.032788	-0.318297	2.906291
C	0.484465	0.948947	3.290657
C	1.113937	1.876104	2.459994
C	1.610692	3.226788	2.942262
C	2.373922	3.778589	1.720259
C	2.047444	2.782919	0.619146
C	2.392957	2.958200	-0.708278
C	2.123711	1.987917	-1.718814
C	2.491116	2.089555	-3.192453
C	1.650185	0.945357	-3.820780
C	1.537903	-0.046107	-2.649659
N	-2.337839	2.905064	-0.817221
C	-1.075330	2.428762	-0.596986
N	-1.065865	1.141650	-0.248729
C	-3.040460	-0.481122	0.043097
C	-4.437226	-0.583445	-0.036787
C	-5.237583	0.550401	-0.404544
C	-4.626612	1.780221	-0.687438
C	-3.229661	1.858377	-0.601481
C	-2.418160	0.749354	-0.242671
C	-5.106266	-1.906838	0.270567
C	-6.743106	0.425764	-0.488684
C	2.628142	-0.576139	0.568319
H	-0.126004	-4.247111	-2.043287
H	-0.022611	-1.378555	4.813479
H	0.361553	1.223917	4.342621
H	3.465953	3.797657	1.892577
H	0.647522	1.318308	-4.101832
H	2.446518	-0.675217	-2.585195
H	-0.189630	3.053287	-0.704258
H	-2.448118	-1.354808	0.326967
H	-5.231511	2.649720	-0.967396
H	-4.362994	-2.676949	0.536354
H	-5.687149	-2.283836	-0.592281
H	-5.817882	-1.820899	1.113335
H	-7.049036	-0.336344	-1.229946
H	-7.209124	1.381667	-0.779340
H	-7.182241	0.118224	0.478954
H	2.723852	-0.478075	1.663138
H	3.342579	0.122074	0.101303
H	-2.574140	3.857659	-1.089561
H	1.328969	-2.720844	-3.241667
H	-1.559202	-3.225826	-2.300116
H	-0.830826	-3.957411	0.641879
H	-1.567575	-3.166938	3.129501
H	0.186799	-3.301895	3.376997
H	-1.613369	-0.967369	4.138544
H	2.240702	3.126580	3.842655
H	0.752932	3.865862	3.224760
H	2.078343	4.805087	1.444234
H	2.919575	3.874055	-0.991165

H	2.277522	3.086853	-3.613884
H	3.577586	1.910659	-3.319223
H	2.118949	0.504986	-4.714995
H	-0.178057	-2.344373	-4.129754
H	-0.595953	-0.370103	-2.735289
C	3.114701	-1.964956	0.231067
F	3.015786	-2.286249	-1.104007
F	2.467190	-2.951534	0.917306
F	4.440708	-2.083063	0.545799

DBI-[Co^{III}(corrin)]-$CH_2CH_2F^+$

Co	-0.975704	0.126872	0.120300
N	-0.284412	1.457063	-0.996348
N	-0.121671	0.935478	1.648683
N	-1.679102	-1.383372	1.093955
N	-1.797305	-0.444072	-1.455966
C	-0.384913	1.204442	-2.460835
C	-0.191743	2.599724	-3.088953
C	0.679744	3.333357	-2.034979
C	0.335813	2.595474	-0.751877
C	0.663542	3.006293	0.573373
C	0.446531	2.205860	1.678125
C	0.808105	2.599346	3.099528
C	0.661152	1.275824	3.876910
C	-0.091987	0.394604	2.899179
C	-0.681861	-0.820352	3.255176
C	-1.439770	-1.635621	2.411968
C	-2.092500	-2.926683	2.870066
C	-2.940260	-3.343787	1.650704
C	-2.509120	-2.367352	0.569047
C	-2.894980	-2.463452	-0.755066
C	-2.531056	-1.503224	-1.743784
C	-2.933360	-1.516750	-3.211106
C	-1.972729	-0.462588	-3.825177
C	-1.713050	0.469182	-2.628069
N	1.845529	-3.010076	-0.919327
C	0.649970	-2.383182	-0.695352
N	0.797285	-1.114304	-0.316280
C	2.952997	0.243800	0.021872
C	4.352526	0.173829	-0.043428
C	5.010316	-1.043353	-0.428300
C	4.255420	-2.181846	-0.744818
C	2.858725	-2.088076	-0.672656
C	2.187061	-0.895056	-0.294065
C	5.177886	1.397156	0.297706
C	6.520611	-1.104518	-0.496263
C	-2.655961	1.066494	0.626280
H	0.472074	4.414979	-1.964641
H	0.125351	1.380057	4.835121
H	-0.573386	-1.142257	4.295362
H	-4.022546	-3.227828	1.845120
H	-1.028600	-0.945033	-4.139951
H	-2.536797	1.209520	-2.537199
H	-0.305828	-2.890360	-0.820357
H	2.468782	1.178842	0.316711

H	4.751831	-3.113164	-1.039101
H	4.533288	2.251843	0.562819
H	5.819237	1.709254	-0.547931
H	5.855495	1.209759	1.152002
H	6.926476	-0.375072	-1.222328
H	6.868315	-2.106198	-0.798163
H	6.983361	-0.867779	0.480131
H	-2.705960	0.999454	1.727594
H	-3.482467	0.464921	0.208431
H	1.964059	-3.978336	-1.212260
H	-1.169333	3.106497	-3.188956
H	1.761656	3.224991	-2.248313
H	1.124101	3.987062	0.721018
H	1.815078	3.044083	3.161651
H	0.094722	3.361734	3.465985
H	1.645251	0.822439	4.103781
H	-2.689638	-2.773180	3.785327
H	-1.317431	-3.675957	3.118875
H	-2.783016	-4.391554	1.342944
H	-3.533281	-3.300982	-1.050519
H	-2.844718	-2.518857	-3.664838
H	-3.993519	-1.209730	-3.312749
H	-2.400715	0.060110	-4.695204
H	0.275934	2.560870	-4.085383
H	0.442799	0.519642	-2.739949
C	-2.844392	2.515752	0.221985
H	-2.884998	2.648747	-0.876242
H	-2.054393	3.173888	0.626847
F	-4.075084	2.956139	0.744456

DBI-[Co^{III}(corrin)]-Ado^{+}

Co	1.056588	0.448075	0.080978
C	2.910185	2.624389	-0.122171
C	3.542352	3.653278	0.840364
C	3.910033	2.795423	2.080226
H	3.811694	3.337273	3.036625
C	2.938987	1.631204	1.975161
C	2.672548	0.661649	2.985270
C	1.897577	-0.459885	2.760219
C	1.642873	-1.541474	3.796426
C	1.002351	-2.674260	2.968201
H	0.125332	-3.137516	3.450142
C	0.636370	-1.974319	1.673069
C	-0.227447	-2.511669	0.720011
H	-0.644289	-3.502986	0.922298
C	-0.655684	-1.865591	-0.443144
C	-1.645896	-2.480256	-1.411480
C	-0.876815	-0.296499	-2.037059
C	-0.605925	0.833496	-2.789667
C	0.311133	1.843006	-2.377414
C	0.629421	3.133506	-3.118733
C	1.891968	3.640122	-2.372172
H	2.803442	3.224313	-2.840716
C	1.704471	3.035811	-0.968107
H	1.047880	3.688166	-0.351906

N	2.387007	1.563894	0.779384
N	1.244184	-0.757638	1.570608
N	-0.239951	-0.634131	-0.847371
N	0.964974	1.773099	-1.231487
C	-1.898336	-1.347180	-2.424732
N	3.523445	-1.535166	-2.907619
C	2.453657	-0.874527	-2.365144
H	1.582261	-0.590429	-2.954107
N	2.606334	-0.629416	-1.065027
C	4.571113	-1.211373	0.483132
H	4.145459	-0.779504	1.393248
C	5.832659	-1.823558	0.524361
C	6.407944	-2.400785	-0.657795
C	5.710638	-2.357738	-1.873887
H	6.145196	-2.796812	-2.778838
C	4.451913	-1.740971	-1.891151
C	3.863932	-1.164519	-0.733796
C	6.594439	-1.875877	1.832591
H	7.575083	-1.368884	1.758036
H	6.803152	-2.916522	2.145213
H	6.026878	-1.389651	2.643655
C	7.769332	-3.058811	-0.598359
H	8.553399	-2.347926	-0.275524
H	8.064646	-3.459069	-1.582320
H	7.786826	-3.896184	0.124278
N	-6.967556	-2.723074	-1.238715
C	-6.114186	-1.961854	-1.951333
H	-6.057723	-2.198768	-3.021440
N	-5.320798	-0.948226	-1.533269
C	-5.473888	-0.739888	-0.210387
C	-6.304220	-1.449761	0.676241
C	-7.080901	-2.488323	0.094802
N	-6.187493	-0.971899	1.977681
C	-5.307397	0.008698	1.877074
H	-4.949725	0.612571	2.712546
N	-4.845845	0.222955	0.576928
N	-7.915085	-3.273073	0.823712
H	-8.530139	-3.915986	0.328609
H	-8.117239	-3.032584	1.791265
C	-3.844951	1.151581	0.099435
H	-3.986790	1.222336	-0.996790
C	-3.911866	2.594174	0.697887
H	-4.720691	2.707968	1.440141
C	-2.493358	2.790351	1.311384
H	-2.493476	2.470987	2.371073
C	-1.652304	1.768943	0.486593
H	-1.513824	2.207635	-0.524371
C	-0.339372	1.404504	1.135575
H	-0.548173	0.786947	2.027201
H	0.137528	2.343652	1.467597
O	-2.541578	0.631150	0.407693
O	-4.041596	3.573194	-0.347407
H	-4.966609	3.888189	-0.371670
O	-2.040970	4.122652	1.241638
H	-2.557465	4.507513	0.490438
H	-2.924405	-0.942560	-2.316576
H	-1.782239	-1.660859	-3.476591

H	-1.147487	0.970850	-3.729935
H	-0.216390	3.842604	-3.016339
H	0.784442	2.973151	-4.199666
H	1.979500	4.738242	-2.362233
H	2.790186	4.414359	1.118029
H	4.408950	4.173490	0.402528
H	4.950889	2.419327	2.026879
H	3.673271	2.160801	-0.781884
H	0.943292	-1.161886	4.565320
H	2.567022	-1.838755	4.319167
H	3.129575	0.791373	3.970297
H	1.725491	-3.486541	2.761239
H	-2.564964	-2.799109	-0.890584
H	-1.211422	-3.383953	-1.879472
H	3.612316	-1.826634	-3.879365

DBI-[Co^{III}(corrin)]-$CH_2OCH_3^+$

Co	-0.951478	0.015806	0.365986
N	-0.131713	1.652177	0.719887
N	0.013408	-0.813004	1.815223
N	-1.792587	-1.620006	-0.219882
N	-1.788965	0.982027	-0.988483
C	-0.253071	2.701098	-0.328611
C	0.014718	4.016099	0.432731
C	0.916244	3.559502	1.610455
C	0.537758	2.096103	1.765733
C	0.904983	1.237322	2.844301
C	0.680144	-0.125089	2.826175
C	1.112146	-1.078916	3.926795
C	0.911525	-2.465015	3.280989
C	0.025161	-2.148479	2.092042
C	-0.697437	-3.110317	1.384725
C	-1.557881	-2.853452	0.314947
C	-2.311658	-3.948232	-0.419038
C	-3.189113	-3.163710	-1.415058
C	-2.669861	-1.740472	-1.295235
C	-3.012509	-0.720380	-2.161977
C	-2.558091	0.621998	-1.999259
C	-2.920080	1.809406	-2.878730
C	-1.908313	2.888188	-2.409352
C	-1.624709	2.462339	-0.956912
N	1.669895	-1.172604	-3.005978
C	0.522905	-0.975956	-2.281593
N	0.756880	-0.490158	-1.065138
C	2.991889	0.095027	0.050295
C	4.380696	0.119631	-0.145380
C	4.954044	-0.315610	-1.387791
C	4.127337	-0.773241	-2.424465
C	2.742680	-0.789141	-2.205856
C	2.154303	-0.361453	-0.985751
C	5.283330	0.609662	0.967800
C	6.453866	-0.283166	-1.587214
C	-2.377462	0.392204	1.714969
H	0.755130	4.134069	2.538957
H	0.457203	-3.211214	3.953599

H	-0.597780	-4.151158	1.707570
H	-4.258035	-3.196125	-1.132824
H	-0.981415	2.825479	-3.009397
H	-2.397017	2.854289	-0.264821
H	-0.465159	-1.196516	-2.684648
H	2.569200	0.425617	1.003455
H	4.561560	-1.107745	-3.373195
H	4.696538	0.916488	1.849870
H	5.893887	1.476503	0.651785
H	5.995207	-0.172418	1.293199
H	6.858744	0.740879	-1.480471
H	6.732932	-0.650803	-2.588474
H	6.978995	-0.908992	-0.841238
H	-1.803194	0.716418	2.597668
H	-2.889841	-0.572564	1.901952
H	1.720958	-1.537825	-3.955350
H	-0.937292	4.420645	0.822183
H	1.993021	3.642614	1.362016
H	1.424326	1.668848	3.704647
H	2.144098	-0.886855	4.263468
H	0.453436	-0.951175	4.807211
H	1.870426	-2.888919	2.924484
H	-2.893228	-4.576996	0.276887
H	-1.596818	-4.619466	-0.931492
H	-3.123630	-3.539489	-2.450231
H	-3.682621	-0.949181	-2.995849
H	-2.852822	1.573825	-3.955017
H	-3.966354	2.118003	-2.682377
H	-2.301816	3.913976	-2.489233
H	0.484054	4.788321	-0.197111
H	0.533106	2.505755	-1.087855
O	-3.305820	1.405055	1.457932
C	-4.567195	0.968631	0.947202
H	-5.237454	1.842239	0.977903
H	-4.494459	0.603278	-0.095307
H	-4.993967	0.166501	1.581932

DBI-[Co^{III}(corrin)]-$CH_2CH_3^+$

Co	-1.057093	0.137061	0.351256
N	-0.247658	1.818017	0.328385
N	-0.078054	-0.341283	1.939045
N	-1.904324	-1.586352	0.146319
N	-1.984519	0.819539	-1.116687
C	-0.423410	2.618950	-0.914399
C	-0.094241	4.060524	-0.476260
C	0.882070	3.845708	0.710290
C	0.499320	2.460478	1.204377
C	0.913302	1.857968	2.428205
C	0.639287	0.541594	2.741875
C	1.090827	-0.140411	4.021756
C	0.801824	-1.629588	3.746101
C	-0.079246	-1.577486	2.512407
C	-0.802273	-2.674866	2.038382
C	-1.668375	-2.667295	0.943425
C	-2.457604	-3.885635	0.500221

C	-3.348688	-3.336088	-0.632680
C	-2.845775	-1.914165	-0.822522
C	-3.274393	-1.076178	-1.835235
C	-2.837038	0.274005	-1.965250
C	-3.284226	1.272177	-3.023216
C	-2.233208	2.404132	-2.871903
C	-1.832475	2.273875	-1.391117
N	1.374802	-1.709319	-2.773888
C	0.264069	-1.306937	-2.080853
N	0.564625	-0.621254	-0.979515
C	2.864493	0.026689	-0.041663
C	4.245382	-0.074578	-0.266674
C	4.752856	-0.777079	-1.411523
C	3.867953	-1.369979	-2.324031
C	2.492400	-1.253521	-2.080171
C	1.969258	-0.566621	-0.952347
C	5.208669	0.567081	0.710494
C	6.244693	-0.882714	-1.641725
C	-2.608851	0.623092	1.520470
H	0.792887	4.611277	1.500255
H	0.307891	-2.148898	4.584400
H	-0.707034	-3.612933	2.593975
H	-4.416644	-3.320885	-0.347515
H	-1.359363	2.202366	-3.519150
H	-2.560886	2.815656	-0.750364
H	-0.747156	-1.536719	-2.415084
H	2.492943	0.563692	0.835872
H	4.250851	-1.905989	-3.199547
H	4.668083	1.059508	1.536064
H	5.842101	1.331162	0.221429
H	5.899186	-0.174038	1.155459
H	6.714925	0.113668	-1.741159
H	6.469338	-1.451974	-2.558808
H	6.753347	-1.388737	-0.799702
H	-2.627878	-0.185340	2.273469
H	-3.494177	0.499286	0.871114
H	1.374864	-2.248377	-3.638001
H	-1.012872	4.564404	-0.123201
H	1.939243	3.845592	0.378285
H	1.490251	2.455503	3.139720
H	2.148112	0.072442	4.251308
H	0.493407	0.234623	4.874235
H	1.728010	-2.191367	3.518267
H	-3.034499	-4.314667	1.337827
H	-1.770741	-4.678767	0.150006
H	-3.278354	-3.919968	-1.566451
H	-4.004759	-1.460346	-2.553219
H	-3.321643	0.830133	-4.033775
H	-4.306282	1.632836	-2.790991
H	-2.628003	3.400462	-3.126753
H	0.337475	4.667751	-1.287587
H	0.309851	2.247787	-1.660693
C	-2.650566	1.978230	2.214658
H	-2.688139	2.826606	1.508450
H	-1.794436	2.140724	2.891369
H	-3.568695	2.039249	2.834402

DBI-[Co^{III}(corrin)]-$CH_2CH_2CH(CH_3)_2^+$

Co	-0.666735	0.180628	0.169324
N	0.144242	-0.268148	1.789518
N	-0.302717	-1.570394	-0.535883
N	-1.414689	0.862260	-1.472126
N	-1.005365	1.788815	1.048364
C	0.432905	0.852688	2.723418
C	0.591369	0.162792	4.095727
C	1.030654	-1.277258	3.719413
C	0.487409	-1.430769	2.308361
C	0.404319	-2.643703	1.561856
C	0.059005	-2.677845	0.224755
C	0.035021	-3.937902	-0.622543
C	-0.054376	-3.386508	-2.060928
C	-0.457976	-1.941310	-1.838117
C	-0.940668	-1.105215	-2.847550
C	-1.410317	0.197115	-2.662748
C	-1.973596	1.045060	-3.788783
C	-2.522268	2.283495	-3.051465
C	-1.972962	2.124163	-1.643848
C	-2.016111	3.115384	-0.681224
C	-1.525053	2.933649	0.644383
C	-1.543443	3.961805	1.765759
C	-0.578302	3.331207	2.805279
C	-0.725078	1.827571	2.509168
N	2.688704	2.478669	-1.445360
C	1.399691	2.165097	-1.103701
N	1.292947	0.958815	-0.550511
C	3.119461	-0.778068	-0.063618
C	4.495942	-1.027980	-0.165504
C	5.379117	-0.050107	-0.736612
C	4.871906	1.171691	-1.202533
C	3.493145	1.399296	-1.090516
C	2.602358	0.447052	-0.527285
C	5.054434	-2.344966	0.332077
C	6.862386	-0.331910	-0.839496
C	-2.410925	-0.534601	0.850969
H	0.639835	-2.050020	4.403668
H	-0.773839	-3.924377	-2.700481
H	-1.000454	-1.520862	-3.858082
H	-3.627940	2.280414	-3.019444
H	0.460318	3.654193	2.605097
H	-1.616601	1.419390	3.033772
H	0.568261	2.847990	-1.275470
H	2.458697	-1.533562	0.370571
H	5.542243	1.920060	-1.639591
H	4.257045	-2.984895	0.745816
H	5.811808	-2.197389	1.124938
H	5.553904	-2.911171	-0.476658
H	7.311243	-0.525802	0.152869
H	7.401536	0.517238	-1.290883
H	7.066728	-1.226323	-1.457776
H	-2.114430	-1.423273	1.434377
H	-2.803094	0.220638	1.556477
H	2.995063	3.346021	-1.882520

H	-0.384211	0.135823	4.615125
H	2.133466	-1.383186	3.709337
H	0.665159	-3.582880	2.057785
H	0.916021	-4.575510	-0.442362
H	-0.859060	-4.539045	-0.369297
H	0.926671	-3.424945	-2.572842
H	-2.742027	0.499736	-4.362955
H	-1.169521	1.307464	-4.502526
H	-2.219120	3.241126	-3.507130
H	-2.460138	4.079117	-0.946732
H	-1.237167	4.966009	1.425365
H	-2.570749	4.058335	2.170571
H	-0.827651	3.594734	3.845420
H	1.311800	0.675932	4.752115
H	1.378960	1.331893	2.396134
C	-3.492477	-0.883800	-0.165505
H	-3.111751	-1.587593	-0.931972
H	-3.808032	0.028944	-0.706214
C	-4.765267	-1.511017	0.478548
H	-5.087480	-0.841984	1.304086
C	-4.503787	-2.908651	1.070080
H	-3.727135	-2.893950	1.855012
H	-5.422904	-3.323178	1.521538
H	-4.176528	-3.613024	0.280679
C	-5.905696	-1.568005	-0.556349
H	-5.632436	-2.215002	-1.411891
H	-6.828359	-1.980269	-0.109690
H	-6.143062	-0.564575	-0.954799

DBI-[Co^{III}(corrin)]-$CH_2NH_2^+$

Co	-1.102433	0.180615	0.339495
N	-0.258549	1.838700	0.226847
N	-0.156415	-0.220943	1.965806
N	-1.956603	-1.540826	0.210293
N	-1.978640	0.783236	-1.187687
C	-0.378725	2.556453	-1.071502
C	-0.024682	4.017044	-0.724602
C	0.913974	3.862355	0.501180
C	0.478511	2.525904	1.079623
C	0.841528	1.996731	2.352736
C	0.557649	0.696808	2.730608
C	0.996731	0.078952	4.048388
C	0.693431	-1.420157	3.850229
C	-0.175320	-1.426257	2.606925
C	-0.905106	-2.537339	2.181775
C	-1.746114	-2.581892	1.067241
C	-2.525432	-3.820808	0.665986
C	-3.388841	-3.327408	-0.513030
C	-2.870451	-1.921499	-0.768271
C	-3.262676	-1.140087	-1.838539
C	-2.807385	0.195110	-2.034728
C	-3.201745	1.125923	-3.171587
C	-2.137556	2.248956	-3.058761
C	-1.783427	2.211315	-1.561048
N	1.461572	-1.917859	-2.660194

C	0.336713	-1.469555	-2.014802
N	0.614369	-0.706429	-0.961576
C	2.889089	0.006530	-0.023028
C	4.274929	-0.105092	-0.209010
C	4.808639	-0.879029	-1.294624
C	3.946123	-1.535776	-2.185102
C	2.564971	-1.410025	-1.979602
C	2.016433	-0.649001	-0.912772
C	5.215809	0.597586	0.747857
C	6.305715	-0.991755	-1.485592
C	-2.677069	0.771839	1.492206
H	0.830347	4.686847	1.230451
H	0.187534	-1.888215	4.711398
H	-0.829361	-3.446239	2.786861
H	-4.462079	-3.289409	-0.250044
H	-1.246536	1.989844	-3.660316
H	-2.514621	2.818644	-0.981646
H	-0.668289	-1.726830	-2.349551
H	2.493981	0.596256	0.810274
H	4.351096	-2.127344	-3.013737
H	4.656151	1.154065	1.518311
H	5.873493	1.317621	0.225224
H	5.883357	-0.115889	1.267137
H	6.773374	-0.002112	-1.646590
H	6.552143	-1.623404	-2.355062
H	6.799425	-1.433195	-0.599413
H	-2.763605	-0.066097	2.202821
H	-3.532834	0.772375	0.797994
H	1.479370	-2.516152	-3.484245
H	-0.939946	4.566411	-0.433940
H	1.978133	3.808910	0.197051
H	1.416381	2.625124	3.039327
H	2.056391	0.291307	4.267574
H	0.405398	0.503375	4.881900
H	1.616364	-2.001797	3.662646
H	-3.121845	-4.210863	1.509017
H	-1.830443	-4.628950	0.369800
H	-3.305224	-3.961716	-1.412118
H	-3.973009	-1.561104	-2.556108
H	-3.209338	0.617905	-4.151339
H	-4.225660	1.516025	-3.003934
H	-2.504437	3.232635	-3.392474
H	0.442410	4.557762	-1.562862
H	0.362552	2.115728	-1.769853
N	-2.646537	1.992211	2.206532
H	-1.886204	2.069283	2.888733
H	-2.667451	2.831021	1.621294

DBI-[Co^{III}(corrin)]-$CCl_2NO_2^+$

Co	-0.658241	0.058940	-0.033153
N	0.023482	-1.162675	1.222749
N	0.157240	-0.948095	-1.464619
N	-1.270329	1.508358	-1.157043
N	-1.320934	0.907380	1.503733
C	0.009549	-0.723673	2.647194

C	0.118477	-2.049420	3.427878
C	0.896033	-2.964458	2.444049
C	0.559867	-2.359653	1.092075
C	0.825925	-2.938406	-0.184549
C	0.636419	-2.251209	-1.365720
C	0.937473	-2.802220	-2.744051
C	0.952703	-1.536781	-3.626799
C	0.260613	-0.512316	-2.749149
C	-0.226564	0.709588	-3.222362
C	-0.974987	1.626857	-2.482553
C	-1.543008	2.906065	-3.068456
C	-2.389527	3.478368	-1.912130
C	-1.990939	2.618241	-0.727201
C	-2.267450	2.924603	0.591366
C	-1.921171	2.066960	1.679076
C	-2.233898	2.301564	3.148018
C	-1.344192	1.241475	3.851861
C	-1.243136	0.142419	2.778317
N	2.355040	3.040332	0.507029
C	1.112506	2.488977	0.397269
N	1.155173	1.171848	0.180687
C	3.209564	-0.377650	-0.027742
C	4.612184	-0.396465	-0.001574
C	5.361729	0.810292	0.205023
C	4.691268	2.027609	0.385575
C	3.290090	2.020941	0.356999
C	2.526717	0.840558	0.152220
C	5.342043	-1.709381	-0.193629
C	6.873775	0.775933	0.229131
C	-2.433622	-0.912526	-0.318584
H	0.603561	-4.026614	2.503574
H	0.439014	-1.661837	-4.594221
H	-0.064262	0.935856	-4.280362
H	-3.471743	3.353466	-2.103433
H	-0.343129	1.662527	4.062888
H	-2.127668	-0.524480	2.808297
H	0.202633	3.080078	0.480540
H	2.662984	-1.309439	-0.187198
H	5.253089	2.954496	0.544941
H	4.634382	-2.542461	-0.338460
H	5.977948	-1.955920	0.677383
H	6.013276	-1.680277	-1.072473
H	7.253756	0.103101	1.020483
H	7.295304	1.778344	0.410171
H	7.288645	0.404588	-0.726781
H	2.552441	4.026081	0.671662
H	-0.890742	-2.461677	3.600629
H	1.990799	-2.916357	2.608996
H	1.199349	-3.964599	-0.227409
H	1.874443	-3.381655	-2.770486
H	0.117666	-3.483656	-3.041462
H	1.985637	-1.203263	-3.845387
H	-2.128051	2.703275	-3.981618
H	-0.720051	3.585488	-3.360913
H	-2.217704	4.551086	-1.723380
H	-2.810556	3.848527	0.808251
H	-2.036176	3.339420	3.466629

H	-3.310791	2.105952	3.323111
H	-1.773704	0.878585	4.798809
H	0.623458	-1.933830	4.399791
H	0.907200	-0.089394	2.807081
Cl	-2.809646	-1.205536	-2.056106
Cl	-3.883505	-0.087866	0.376422
N	-2.418500	-2.351661	0.369703
O	-2.708304	-2.399945	1.571317
O	-2.052170	-3.301945	-0.320677

DBI-[Co^{III}(corrin)]-CBr_3^+

Co	-0.196671	0.236075	0.010443
N	0.439925	-0.817026	1.427272
N	0.465017	-1.051911	-1.258786
N	-0.722467	1.538627	-1.319007
N	-0.726020	1.373981	1.403272
C	0.502245	-0.166530	2.763556
C	0.518797	-1.358035	3.744921
C	1.139103	-2.502268	2.898510
C	0.820684	-2.075257	1.476748
C	0.937532	-2.884266	0.306930
C	0.783078	-2.374390	-0.965013
C	0.960573	-3.161770	-2.247072
C	1.118551	-2.054591	-3.310620
C	0.569549	-0.835312	-2.596914
C	0.185976	0.339684	-3.249845
C	-0.458316	1.423825	-2.651906
C	-0.922616	2.646711	-3.420985
C	-1.665766	3.473187	-2.350705
C	-1.296852	2.777971	-1.054545
C	-1.473330	3.321996	0.203362
C	-1.190624	2.607188	1.405987
C	-1.442604	3.091963	2.823672
C	-0.656555	2.059563	3.675513
C	-0.677745	0.807975	2.776832
N	3.106491	2.940196	-0.019570
C	1.810756	2.514640	-0.011806
N	1.710611	1.182718	-0.009452
C	3.587258	-0.590644	-0.008082
C	4.980636	-0.754386	-0.013041
C	5.856515	0.382824	-0.022414
C	5.320645	1.677816	-0.025897
C	3.926101	1.816028	-0.020501
C	3.039159	0.706580	-0.012636
C	5.565079	-2.151519	-0.008668
C	7.356826	0.191140	-0.028876
C	-2.064885	-0.614551	-0.037945
H	0.720861	-3.497084	3.129962
H	0.579954	-2.258824	-4.250496
H	0.335520	0.382377	-4.332725
H	-2.762187	3.416268	-2.487046
H	0.384921	2.401822	3.823604
H	-1.612186	0.227679	2.926735
H	0.970180	3.205857	-0.005807
H	2.943365	-1.472384	-0.001744

H	5.979480	2.553117	-0.032636
H	4.771103	-2.916696	-0.000115
H	6.208181	-2.324166	0.874815
H	6.198725	-2.333410	-0.897111
H	7.699629	-0.375100	0.857368
H	7.885084	1.158717	-0.033599
H	7.691189	-0.378862	-0.915970
H	3.409405	3.912771	-0.024368
H	-0.516253	-1.620656	4.026573
H	2.236725	-2.571428	3.031973
H	1.188978	-3.941723	0.422851
H	1.805257	-3.867598	-2.198560
H	0.041648	-3.750565	-2.431720
H	2.182021	-1.887334	-3.570059
H	-1.558592	2.363855	-4.276919
H	-0.049655	3.186569	-3.834253
H	-1.395050	4.541990	-2.344046
H	-1.902642	4.324631	0.281072
H	-1.127618	4.137727	2.981187
H	-2.530736	3.043000	3.029073
H	-1.106414	1.884970	4.665482
H	1.085430	-1.145640	4.665164
H	1.447728	0.413555	2.815282
Br	-2.554386	-1.396932	-1.818661
Br	-3.571347	0.664085	0.318070
Br	-2.405337	-2.102781	1.272780

DBI-[Co^{III}(corrin)]-CCl_3^+

Co	-0.683089	-0.018748	-0.005242
N	0.087212	-0.997097	1.400970
N	0.126999	-1.204660	-1.288132
N	-1.385236	1.210351	-1.319353
N	-1.366758	1.015393	1.400347
C	0.062598	-0.358222	2.743986
C	0.244334	-1.545082	3.713898
C	1.010538	-2.587422	2.855345
C	0.634856	-2.192654	1.438273
C	0.858856	-2.966244	0.260529
C	0.631060	-2.470939	-1.006247
C	0.917314	-3.215625	-2.295000
C	0.907317	-2.090292	-3.351056
C	0.197380	-0.964758	-2.624923
C	-0.344085	0.152817	-3.266069
C	-1.118054	1.140882	-2.654669
C	-1.743913	2.297845	-3.411299
C	-2.581716	3.012792	-2.330596
C	-2.124927	2.356054	-1.041685
C	-2.379238	2.853146	0.222417
C	-1.997761	2.172149	1.417543
C	-2.306930	2.606004	2.840851
C	-1.388052	1.678704	3.681458
C	-1.239004	0.446761	2.767770
N	2.222405	3.105991	0.003575
C	0.996670	2.507209	-0.006152
N	1.079633	1.174205	-0.018298

C	3.179396	-0.326550	-0.021490
C	4.582179	-0.299697	-0.013652
C	5.294941	0.946036	0.000330
C	4.588279	2.156342	0.005760
C	3.187843	2.104184	-0.001680
C	2.460422	0.884257	-0.015319
C	5.350790	-1.604515	-0.019961
C	6.807771	0.961995	0.009550
C	-2.428150	-1.105130	-0.073644
H	0.731227	-3.631713	3.077705
H	0.397817	-2.362392	-4.289838
H	-0.207179	0.224226	-4.349095
H	-3.663022	2.823914	-2.467224
H	-0.402758	2.156386	3.837742
H	-2.086393	-0.255146	2.913909
H	0.069000	3.076688	-0.000054
H	2.660806	-1.287361	-0.032779
H	5.122765	3.112631	0.016263
H	4.667459	-2.469970	-0.030104
H	6.002442	-1.701175	0.868734
H	6.011488	-1.686975	-0.903355
H	7.215896	0.437098	0.893587
H	7.197476	1.993035	0.021811
H	7.226499	0.454281	-0.879547
H	2.389799	4.110775	0.012346
H	-0.743913	-1.947544	3.999365
H	2.107836	-2.509986	2.987221
H	1.254746	-3.979855	0.364682
H	1.858519	-3.787047	-2.252245
H	0.099002	-3.936905	-2.483119
H	1.934846	-1.772300	-3.614664
H	-2.342948	1.940249	-4.265926
H	-0.951992	2.949935	-3.826030
H	-2.445129	4.106818	-2.312034
H	-2.943386	3.785578	0.311446
H	-2.127853	3.682425	3.005551
H	-3.378487	2.418431	3.052378
H	-1.811033	1.432113	4.667959
H	0.781529	-1.265977	4.633979
H	0.919433	0.345957	2.800387
Cl	-2.757872	-1.800176	-1.734032
Cl	-3.919792	-0.110489	0.308128
Cl	-2.499698	-2.523427	1.083734

DBI-[Co^{III}(corrin)]-$CH(CH_3)_2^+$

Co	1.044585	0.180738	0.230740
N	0.195596	-0.371080	1.793193
N	0.165237	1.882922	0.323482
N	1.832217	0.503592	-1.496246
N	1.843134	-1.502632	0.342069
C	0.225266	-1.833030	2.078827
C	-0.110074	-1.919887	3.582330
C	-0.965172	-0.646314	3.819360
C	-0.493462	0.278778	2.709570
C	-0.776566	1.671372	2.587470

C	-0.477062	2.394001	1.449152
C	-0.841537	3.852135	1.236550
C	-0.674775	4.030930	-0.287098
C	0.118811	2.799748	-0.682725
C	0.724845	2.639292	-1.932574
C	1.544363	1.570396	-2.298594
C	2.226949	1.457378	-3.649950
C	3.212116	0.289196	-3.439613
C	2.724139	-0.342258	-2.147330
C	3.098729	-1.597942	-1.706069
C	2.625768	-2.168991	-0.488494
C	2.925538	-3.566886	0.032960
C	1.827001	-3.751052	1.114184
C	1.590710	-2.300842	1.573809
N	-1.633350	-2.002020	-2.509179
C	-0.476054	-1.545813	-1.934374
N	-0.697727	-0.709968	-0.922352
C	-2.924559	0.109892	0.054710
C	-4.318044	0.014997	-0.075082
C	-4.905843	-0.810276	-1.092921
C	-4.088623	-1.534915	-1.972722
C	-2.699007	-1.425447	-1.823450
C	-2.096574	-0.615000	-0.824219
C	-5.210883	0.791982	0.869943
C	-6.410644	-0.904602	-1.221045
C	2.725236	0.954601	1.129319
H	-0.829014	-0.202820	4.820830
H	-0.158162	4.963092	-0.571186
H	0.584848	3.440042	-2.665121
H	4.246650	0.657229	-3.301191
H	0.905794	-4.157940	0.656767
H	2.359895	-2.021164	2.323594
H	0.509213	-1.850141	-2.286566
H	-2.490655	0.745458	0.832075
H	-4.533293	-2.165991	-2.750193
H	-4.615048	1.374363	1.592582
H	-5.878897	0.124053	1.445916
H	-5.867228	1.499336	0.328511
H	-6.875839	-1.291225	-0.294633
H	-6.701801	-1.574593	-2.046827
H	-6.867675	0.084118	-1.414002
H	3.486481	0.275650	0.702481
H	-1.694903	-2.646220	-3.295666
H	0.819385	-1.867738	4.178796
H	-2.047705	-0.851034	3.700776
H	-1.298043	2.176360	3.405563
H	-1.853430	4.085648	1.606204
H	-0.135460	4.498070	1.792849
H	-1.651790	4.030295	-0.807687
H	2.714881	2.401194	-3.945930
H	1.476809	1.225961	-4.430736
H	3.236568	-0.431041	-4.274130
H	3.783685	-2.183655	-2.325833
H	2.901560	-4.330997	-0.762786
H	3.940292	-3.595527	0.478413
H	2.131780	-4.421051	1.933959
H	-0.635906	-2.849491	3.852021

H	-0.566956	-2.308878	1.463846
C	3.065008	2.383649	0.701188
H	2.404022	3.131631	1.173891
H	4.096406	2.617383	1.036784
H	3.038734	2.539160	-0.388174
C	2.759688	0.862234	2.654380
H	2.640450	-0.160007	3.046014
H	3.743138	1.231165	3.012496
H	1.989943	1.499721	3.124596

DBI-[Co^{III}(corrin)]-CCl_2CN^+

Co	-0.691526	-0.028020	-0.019683
N	0.063929	-1.197067	1.245953
N	0.137543	-1.009687	-1.454277
N	-1.429302	1.354503	-1.154311
N	-1.416906	0.776775	1.514412
C	0.002028	-0.773462	2.672349
C	0.158104	-2.097082	3.452490
C	0.930233	-3.007729	2.460005
C	0.598777	-2.392640	1.113811
C	0.850464	-2.977008	-0.164013
C	0.653551	-2.297730	-1.348436
C	0.976572	-2.846796	-2.724280
C	0.915826	-1.593498	-3.622856
C	0.190278	-0.591798	-2.747000
C	-0.388447	0.584793	-3.231461
C	-1.179312	1.464051	-2.490023
C	-1.844221	2.690979	-3.085711
C	-2.665246	3.255669	-1.907647
C	-2.194624	2.432752	-0.722758
C	-2.464999	2.740849	0.597296
C	-2.080887	1.902620	1.686399
C	-2.419369	2.117377	3.152610
C	-1.481494	1.105185	3.863249
C	-1.303939	0.016261	2.787872
N	2.141624	3.097774	0.449461
C	0.924680	2.490017	0.353492
N	1.027599	1.173003	0.155325
C	3.147989	-0.286657	-0.038945
C	4.550009	-0.241346	-0.019517
C	5.244724	1.001675	0.163719
C	4.520843	2.190104	0.329744
C	3.121282	2.119502	0.309697
C	2.412159	0.902697	0.126146
C	5.338576	-1.522389	-0.193705
C	6.756787	1.036205	0.179707
C	-2.398311	-1.160971	-0.224205
H	0.618386	-4.064955	2.507191
H	0.392800	-1.756698	-4.579513
H	-0.267672	0.799666	-4.297327
H	-3.749590	3.094717	-2.053653
H	-0.506934	1.579351	4.084423
H	-2.148835	-0.703010	2.822439
H	-0.011828	3.038673	0.433633
H	2.643521	-1.244652	-0.180845

H	5.041099	3.143676	0.471949
H	4.669497	-2.390659	-0.313170
H	5.994720	-1.720456	0.674618
H	5.998274	-1.480233	-1.080834
H	7.170800	0.405935	0.988948
H	7.133106	2.061714	0.327814
H	7.183424	0.654778	-0.766878
H	2.295118	4.093575	0.599575
H	-0.836823	-2.531731	3.651773
H	2.025028	-2.977919	2.627126
H	1.245449	-3.995529	-0.202951
H	1.946636	-3.369296	-2.747929
H	0.200244	-3.580232	-3.013604
H	1.927457	-1.213482	-3.863611
H	-2.461845	2.424455	-3.960419
H	-1.075656	3.402193	-3.442391
H	-2.520527	4.336742	-1.744118
H	-3.049610	3.639597	0.812197
H	-2.276663	3.163445	3.473765
H	-3.486750	1.868706	3.317774
H	-1.898625	0.715436	4.804959
H	0.681795	-1.965114	4.412310
H	0.855253	-0.087477	2.857846
C	-2.422146	-2.326692	0.648005
N	-2.419619	-3.242253	1.388935
Cl	-2.674345	-1.805313	-1.923720
Cl	-3.942917	-0.245607	0.196406

DBI-[Co^{III}(corrin)]-$CF(CF_3)_2^+$

Co	-0.507743	0.096377	-0.072032
N	0.084117	-1.109614	1.235211
N	0.293694	-1.004466	-1.451100
N	-0.903140	1.590296	-1.240298
N	-1.162634	1.034730	1.413715
C	0.045131	-0.614209	2.639908
C	0.124764	-1.905182	3.474596
C	0.972605	-2.829873	2.560816
C	0.673156	-2.287783	1.172339
C	1.015762	-2.903896	-0.064242
C	0.815540	-2.283765	-1.279288
C	1.141475	-2.911896	-2.620111
C	1.036370	-1.727292	-3.599992
C	0.372883	-0.651141	-2.762996
C	-0.068597	0.561189	-3.297121
C	-0.655552	1.603276	-2.580708
C	-1.065256	2.915284	-3.221435
C	-1.578765	3.750145	-2.030728
C	-1.397854	2.826132	-0.839913
C	-1.687712	3.185364	0.462641
C	-1.580285	2.279667	1.556977
C	-1.924895	2.581363	3.005179
C	-1.208559	1.434006	3.764077
C	-1.171479	0.305016	2.714606
N	2.817419	2.914113	0.594647
C	1.548206	2.426496	0.466300

N	1.517781	1.117053	0.211320
C	3.497334	-0.523272	-0.035000
C	4.897243	-0.614727	-0.010269
C	5.707134	0.545263	0.229072
C	5.098293	1.788872	0.445146
C	3.698755	1.853748	0.415937
C	2.873480	0.721402	0.177107
C	5.558974	-1.957836	-0.238360
C	7.215796	0.434558	0.250293
C	-2.350232	-0.748065	-0.463770
H	0.717740	-3.899691	2.652043
H	0.449226	-1.953142	-4.506241
H	0.067506	0.710322	-4.372567
H	-2.643548	4.024345	-2.135281
H	-0.179104	1.739296	4.029592
H	-2.091031	-0.305969	2.756396
H	0.673255	3.066423	0.558165
H	2.903339	-1.422205	-0.210765
H	5.705982	2.681307	0.631323
H	4.809391	-2.746997	-0.415838
H	6.171770	-2.266695	0.629497
H	6.239502	-1.937081	-1.110249
H	7.562252	-0.281672	1.018714
H	7.686441	1.408568	0.463040
H	7.612355	0.074709	-0.717807
H	3.064100	3.883482	0.787140
H	-0.885352	-2.329643	3.609871
H	2.056454	-2.733713	2.771038
H	1.435834	-3.913335	-0.052317
H	2.129061	-3.402104	-2.618422
H	0.391134	-3.692252	-2.847717
H	2.030720	-1.378952	-3.938142
H	-1.842462	2.742663	-3.987483
H	-0.208198	3.382197	-3.738981
H	-1.020182	4.692952	-1.894554
H	-2.062848	4.194456	0.654555
H	-1.608386	3.591216	3.317372
H	-3.024229	2.529710	3.133099
H	-1.727705	1.138799	4.689468
H	0.574479	-1.748322	4.467746
H	0.956500	0.003113	2.791068
C	-2.581506	-2.206689	0.053001
C	-3.635868	0.077968	-0.117816
F	-2.455389	-2.285166	1.408660
F	-3.811490	-2.686921	-0.248871
F	-1.702119	-3.067881	-0.510863
F	-3.858287	0.108404	1.228380
F	-4.736425	-0.449604	-0.701104
F	-3.576636	1.357218	-0.559358
F	-2.424506	-0.864216	-1.858051

DBI-[Co^{III}(corrin)]-$CCl(CN)_2^+$

Co	0.725738	0.058931	-0.011697
N	-0.070868	1.168834	1.279037
N	-0.107833	1.060562	-1.427002

N	1.508815	-1.275665	-1.178898
N	1.454962	-0.777144	1.507574
C	-0.025084	0.696295	2.690753
C	-0.226409	1.988763	3.512465
C	-0.995702	2.919137	2.535844
C	-0.625853	2.357854	1.176155
C	-0.864643	2.978524	-0.087383
C	-0.639994	2.339122	-1.289310
C	-0.945958	2.927057	-2.652987
C	-0.859813	1.701781	-3.587599
C	-0.130042	0.684235	-2.733627
C	0.478513	-0.465246	-3.245928
C	1.277692	-1.350900	-2.520707
C	1.976957	-2.545369	-3.142450
C	2.802408	-3.120764	-1.972507
C	2.293259	-2.350558	-0.769362
C	2.557759	-2.689259	0.543695
C	2.145073	-1.892161	1.652821
C	2.473819	-2.140773	3.114840
C	1.493147	-1.183643	3.844653
C	1.299920	-0.063208	2.804930
N	-2.039413	-3.137628	0.308460
C	-0.833757	-2.504424	0.247295
N	-0.961180	-1.181403	0.107784
C	-3.109138	0.245430	-0.034980
C	-4.510117	0.171958	-0.027393
C	-5.181219	-1.091252	0.094910
C	-4.434708	-2.271319	0.213035
C	-3.036735	-2.172747	0.205914
C	-2.350501	-0.935463	0.081354
C	-5.321909	1.444360	-0.150095
C	-6.692418	-1.156519	0.096948
C	2.435955	1.224599	-0.155225
H	-0.705616	3.979705	2.626685
H	-0.329892	1.899776	-4.533749
H	0.377702	-0.648448	-4.319715
H	3.882710	-2.918703	-2.096738
H	0.530205	-1.694116	4.033181
H	2.122166	0.678719	2.882085
H	0.112148	-3.039364	0.307806
H	-2.624460	1.219050	-0.131474
H	-4.936555	-3.240342	0.309287
H	-4.668539	2.328936	-0.231328
H	-5.983170	1.594153	0.723969
H	-5.978619	1.427349	-1.040152
H	-7.125147	-0.571389	0.929952
H	-7.048809	-2.194927	0.195704
H	-7.119284	-0.741466	-0.835211
H	-2.174666	-4.142112	0.411419
H	0.754911	2.435436	3.749505
H	-2.092868	2.863152	2.678400
H	-1.271913	3.992823	-0.101961
H	-1.919326	3.443243	-2.677038
H	-0.170053	3.673912	-2.907186
H	-1.864162	1.316202	-3.849335
H	2.594155	-2.241368	-4.005108
H	1.228527	-3.265449	-3.523684

H	2.691720	-4.210471	-1.844366
H	3.171442	-3.572630	0.738666
H	2.365399	-3.200488	3.402406
H	3.530527	-1.859177	3.294396
H	1.883519	-0.814631	4.805948
H	-0.767350	1.812893	4.455447
H	-0.863316	-0.017004	2.835669
C	2.403859	2.376724	0.737331
N	2.365619	3.285704	1.484480
Cl	2.759723	1.894255	-1.859545
C	3.617980	0.433416	0.164025
N	4.571951	-0.203350	0.427155

DBI-[Co^{III}(corrin)]-$C(CH_3)_3^+$

Co	1.026784	0.268295	-0.031364
N	0.207901	1.202927	1.361092
N	0.090302	1.357726	-1.312182
N	1.702580	-0.976458	-1.335694
N	1.784906	-0.701287	1.366176
C	0.250942	0.553998	2.699767
C	-0.049829	1.706479	3.677864
C	-0.937071	2.649042	2.822121
C	-0.496741	2.317127	1.405757
C	-0.824719	3.046377	0.226184
C	-0.557435	2.560430	-1.038072
C	-0.969960	3.249388	-2.325956
C	-0.851400	2.120738	-3.369840
C	-0.014621	1.084003	-2.643965
C	0.568345	-0.014836	-3.278506
C	1.375824	-0.971576	-2.662037
C	1.968665	-2.158710	-3.399605
C	2.890267	-2.799481	-2.342537
C	2.486095	-2.094720	-1.059437
C	2.827019	-2.532593	0.206028
C	2.446338	-1.845663	1.395403
C	2.757028	-2.278114	2.819078
C	1.783930	-1.400799	3.648740
C	1.595130	-0.168378	2.743345
N	-1.871283	-3.184010	0.127973
C	-0.687067	-2.493025	0.098495
N	-0.857235	-1.173981	0.049991
C	-3.036767	0.180275	0.011711
C	-4.435444	0.073271	0.022300
C	-5.072401	-1.212605	0.069767
C	-4.298089	-2.381537	0.107915
C	-2.902435	-2.249629	0.097487
C	-2.250736	-0.987830	0.048660
C	-5.280010	1.330128	-0.017773
C	-6.582288	-1.314652	0.077996
C	2.760752	1.510333	-0.172843
H	-0.805488	3.718809	3.060391
H	-0.386013	2.436794	-4.318388
H	0.388342	-0.127470	-4.352094
H	3.956162	-2.593965	-2.557345
H	0.817591	-1.922723	3.778928

H	2.397507	0.576367	2.933072
H	0.279251	-2.996189	0.113350
H	-2.566479	1.167155	-0.024536
H	-4.780075	-3.364813	0.145356
H	-4.647429	2.233042	-0.051630
H	-5.936778	1.413651	0.868636
H	-5.944185	1.351637	-0.902403
H	-7.023246	-0.790048	0.946471
H	-6.912973	-2.365643	0.118097
H	-7.027435	-0.856815	-0.825415
H	-1.970705	-4.196988	0.164513
H	0.888610	2.219379	3.958491
H	-2.014348	2.419979	2.943487
H	-1.353984	3.998514	0.322556
H	-1.975979	3.694413	-2.257980
H	-0.264059	4.072790	-2.549218
H	-1.841445	1.692792	-3.619719
H	2.499047	-1.845136	-4.314954
H	1.161998	-2.846099	-3.718376
H	2.785334	-3.894544	-2.265891
H	3.419468	-3.447459	0.298585
H	2.621234	-3.362321	2.973856
H	3.815561	-2.049064	3.056537
H	2.172923	-1.145634	4.647281
H	-0.544501	1.368289	4.602162
H	-0.557460	-0.206784	2.724434
C	2.621359	2.751268	0.715878
H	2.548251	2.508170	1.789686
H	3.533927	3.372387	0.591180
H	1.762902	3.384531	0.439688
C	2.942496	1.960109	-1.628858
H	2.159449	2.660007	-1.960745
H	3.907514	2.502920	-1.708687
H	2.989327	1.122396	-2.342136
C	4.012365	0.731112	0.254537
H	4.900291	1.367673	0.058491
H	4.029031	0.495902	1.331520
H	4.158260	-0.203835	-0.309555

DBI-[Co^{III}(corrin)]-$C(CN)_3^+$

Co	0.734446	0.076229	-0.022140
N	-0.045813	1.121568	1.327869
N	-0.127509	1.127299	-1.384812
N	1.539155	-1.182429	-1.260949
N	1.537811	-0.788934	1.445435
C	0.028745	0.586486	2.715049
C	-0.185819	1.836446	3.598783
C	-0.964511	2.808680	2.670571
C	-0.608093	2.310775	1.282828
C	-0.863830	2.984952	0.049808
C	-0.656696	2.400456	-1.183613
C	-0.963331	3.052584	-2.516204
C	-0.876950	1.876188	-3.511097
C	-0.147082	0.818852	-2.710205
C	0.471556	-0.298281	-3.279296

C	1.290156	-1.203864	-2.602446
C	2.001318	-2.358601	-3.282737
C	2.871940	-2.949995	-2.154672
C	2.357743	-2.253147	-0.910773
C	2.656385	-2.639452	0.381591
C	2.251044	-1.896099	1.529922
C	2.596578	-2.210507	2.976342
C	1.599470	-1.314308	3.760023
C	1.372679	-0.147717	2.780087
N	-1.919349	-3.162969	0.231051
C	-0.725907	-2.508798	0.180692
N	-0.880961	-1.184059	0.077581
C	-3.057207	0.207171	-0.014975
C	-4.456271	0.105050	-0.002534
C	-5.101585	-1.174235	0.090284
C	-4.330787	-2.341426	0.172704
C	-2.935136	-2.214673	0.159880
C	-2.274895	-0.960953	0.064902
C	-5.293289	1.363826	-0.088797
C	-6.610976	-1.269666	0.098780
C	2.464902	1.360801	-0.177661
H	-0.675309	3.864569	2.807687
H	-0.339684	2.123557	-4.440873
H	0.370367	-0.428060	-4.360575
H	3.939503	-2.691649	-2.286924
H	0.650679	-1.856437	3.931309
H	2.175036	0.609029	2.892685
H	0.230022	-3.027459	0.220456
H	-2.593698	1.192628	-0.088072
H	-4.811674	-3.322923	0.245853
H	-4.657894	2.262322	-0.157925
H	-5.947365	1.481867	0.795435
H	-5.959204	1.352848	-0.971945
H	-7.050343	-0.710558	0.945953
H	-6.946595	-2.316679	0.177064
H	-7.050597	-0.843515	-0.822345
H	-2.035349	-4.172378	0.306318
H	0.791106	2.279807	3.857431
H	-2.060484	2.745948	2.818852
H	-1.271743	3.998533	0.084156
H	-1.933210	3.575816	-2.515696
H	-0.175983	3.799090	-2.733087
H	-1.880011	1.503054	-3.795401
H	2.584761	-2.012888	-4.152883
H	1.258493	-3.084606	-3.664296
H	2.812511	-4.047973	-2.073037
H	3.295085	-3.514433	0.527623
H	2.512320	-3.285971	3.208052
H	3.647833	-1.917556	3.168611
H	1.990093	-0.984550	4.735384
H	-0.725763	1.608456	4.531037
H	-0.792352	-0.150452	2.837237
C	2.476529	2.337904	0.911860
N	2.482165	3.107105	1.801985
C	3.663235	0.525620	-0.088041
N	4.631650	-0.138507	-0.027201
C	2.464996	2.056296	-1.465685

N	2.458556	2.610958	-2.502752

DBI-[Co^{III}(corrin)]-$C(CF_3)_3^+$

Co	-0.258691	0.217354	-0.006677
N	0.375728	-0.784841	1.446539
N	0.401766	-1.130117	-1.218850
N	-0.696473	1.504820	-1.391209
N	-0.717185	1.450116	1.337443
C	0.556560	-0.036027	2.721345
C	0.624983	-1.152377	3.782422
C	1.222349	-2.341268	2.981883
C	0.820608	-2.019524	1.552227
C	0.967674	-2.873939	0.420219
C	0.775060	-2.425944	-0.868743
C	0.992326	-3.263471	-2.112476
C	1.087639	-2.203858	-3.229192
C	0.522273	-0.964941	-2.563209
C	0.168916	0.189524	-3.265233
C	-0.418425	1.328088	-2.713743
C	-0.798625	2.544137	-3.537043
C	-1.484524	3.465394	-2.507978
C	-1.189675	2.788948	-1.183496
C	-1.347182	3.390218	0.049803
C	-1.091423	2.714366	1.279242
C	-1.204532	3.317049	2.669450
C	-0.383398	2.319226	3.527159
C	-0.564814	1.000464	2.752120
N	3.125691	2.834519	-0.153220
C	1.824441	2.432884	-0.122553
N	1.698991	1.103342	-0.068111
C	3.559807	-0.697401	-0.001974
C	4.951390	-0.878175	-0.004924
C	5.841579	0.245310	-0.063904
C	5.319106	1.544198	-0.118408
C	3.926423	1.698580	-0.113540
C	3.022595	0.603349	-0.057390
C	5.517068	-2.281818	0.055035
C	7.339407	0.035925	-0.068263
C	-2.393487	-0.677191	0.008587
H	0.842648	-3.326357	3.303670
H	0.527193	-2.466661	-4.141596
H	0.331206	0.185413	-4.347192
H	-2.579481	3.499937	-2.660133
H	0.683166	2.613529	3.538168
H	-1.505468	0.506419	3.048992
H	0.999589	3.141813	-0.140979
H	2.909788	-1.572253	0.042940
H	5.986372	2.412007	-0.162946
H	4.713061	-3.035353	0.095943
H	6.159608	-2.427422	0.943803
H	6.146324	-2.507913	-0.826239
H	7.678066	-0.505183	0.835024
H	7.878975	0.996446	-0.106247
H	7.664097	-0.566797	-0.937154
H	3.444123	3.801209	-0.197837

H	-0.391401	-1.404425	4.129636
H	2.327190	-2.377954	3.058190
H	1.264368	-3.914102	0.578501
H	1.880257	-3.911071	-2.031117
H	0.116080	-3.921118	-2.264014
H	2.136498	-2.019312	-3.531249
H	-1.453596	2.264237	-4.379800
H	0.107016	3.003989	-3.975493
H	-1.123424	4.507082	-2.532222
H	-1.709401	4.421199	0.086109
H	-0.839533	4.357244	2.714422
H	-2.270123	3.329085	2.972947
H	-0.734032	2.254851	4.569424
H	1.233397	-0.873367	4.657083
H	1.529579	0.495209	2.650520
C	-2.543957	-1.860110	1.002168
C	-3.470517	0.379609	0.400288
C	-2.785584	-1.204353	-1.403820
F	-2.187866	-1.517002	2.277680
F	-3.817797	-2.324181	1.094320
F	-1.780796	-2.925505	0.645236
F	-3.335493	0.800097	1.693659
F	-4.744038	-0.082757	0.304309
F	-2.786295	-0.204662	-2.328040
F	-1.950259	-2.179802	-1.861164
F	-4.027273	-1.755743	-1.441461
F	-3.422569	1.481217	-0.392915