Ligand Conformation and Spin States in Sandwich-type Complexes of the Split (3+2) Five-electron Donor Hydrocarbon Ligand Bicyclo[3.2.1] octa-2,6-dien-4-yl (bcod)

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Supporting Information

Table S1 to Table S51: Atomic coordinates of the optimized structures for the $(bcod)_2M$ (M =Ti, V, Cr, Mn, Fe, Co, Ni, Cu) complexes.

Table S52 to Table S102: Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the $(bcod)_2M$ (M =Ti, V, Cr, Mn, Fe, Co, Ni, Cu) complexes.

Table S103 to Table S110: Total energies (E in hartree), total free energies (G, in hartree), relative energies (ΔE and ΔG in kcal mol^{-1}), and the staggered angles χ for the $(bcod)_2M$ (M=Ti, V, Cr, Mn, Fe, Co, Ni, Cu)structures optimized at the M06-L/DZP level.

Table S111. Energy gaps between the lowest unoccupied and the highest occupied molecular orbitals (in eV) and the spin values $\langle S^2 \rangle$for the $(BCOD)_2M$ structures optimized at the M06-L/DZP level.

Table S112 to Table S120: Atomic coordinates of the optimized structures for the (bcod)M (M =Ti, V, Cr, Mn, Fe, Co, Ni, Cu) structures and bcod structure predictedby the M06-L/DZP.

Table S121 to Table S128: The single point energies (kcal/mol),relative energies (ΔE in kcal mol^{-1}),and the spin values $\langle S^2 \rangle$ for $(bcod)_2M$ (M=Ti, V, Cr, Mn, Fe, Co, Ni, Cu)structures at the M06-L/cc-pVTZ level.

Table S129to Table S134: Atomic coordinates of the optimized structures for the (bcod)Fe(C_5H_6), (bcod)Fe(C_6H_7), (bcod)Cr(C_5H_6), (bcod)Cr(C_6H_7),C_3H_3(Quartet), and C_2H_2(Singlet) structures calculated at the M06-L/cc-pVTZ level.

Table S135. Energies (kcal/mol) and the spin values $\langle S^2 \rangle$ for the structures(bcod)Fe(C_5H_6), (bcod)Fe(C_6H_7), (bcod)Cr(C_5H_6), (bcod)Cr(C_6H_7),C_3H_3(Quartet), and C_2H_2(Singlet)optimized at the M06-L/cc-pVTZ level.

Complete Gaussian 09 reference.

Table S1. Optimized coordinates for the **(bcod)$_2$Ti** structure **Ti-1S.**

	M06-L				OPBE		
	x	y	z		x	y	z
C	0.101114	2.299781	-1.307069	C	0.246630	2.304483	-1.276487
C	-1.185034	2.434934	0.652933	C	-1.126099	2.461091	0.621139
C	-0.663216	3.339631	-0.472209	C	-0.524725	3.362888	-0.469458
H	-1.503231	3.743300	-1.047755	H	-1.330727	3.791930	-1.082528
H	-0.027762	4.159578	-0.118511	H	0.116679	4.166345	-0.078807
C	-0.883225	1.126272	-1.317538	C	-0.771883	1.160154	-1.354840
C	-1.676649	1.225746	-0.155645	C	-1.616433	1.276201	-0.219831
H	0.386377	2.645056	-2.305644	H	0.597478	2.651246	-2.258670
H	-1.967793	2.882008	1.272182	H	-1.925750	2.928292	1.212799
C	1.266605	1.928635	0.877908	C	1.295496	1.877290	0.967713
C	0.000000	1.968115	1.532706	C	0.000000	1.953060	1.546746
C	1.315694	1.860397	-0.505529	C	1.408557	1.813271	-0.422354
H	-1.133885	0.570773	-2.215069	H	-1.040946	0.676275	-2.291914
H	-2.636557	0.737785	-0.002751	H	-2.613522	0.844796	-0.125704
H	2.249127	1.633608	-1.015096	H	2.372645	1.605437	-0.888822
H	2.168598	1.718647	1.455842	H	2.165392	1.649213	1.594241
H	-0.044741	2.109133	2.610309	H	-0.114632	2.018169	2.631400
C	-0.101114	-2.299781	-1.307069	C	-0.246630	-2.304483	-1.276487
C	1.185034	-2.434934	0.652933	C	1.126099	-2.461091	0.621139
C	0.663216	-3.339631	-0.472209	C	0.524725	-3.362888	-0.469458
H	1.503231	-3.743300	-1.047755	H	1.330727	-3.791930	-1.082528
H	0.027762	-4.159578	-0.118511	H	-0.116679	-4.166345	-0.078807
C	0.883225	-1.126272	-1.317538	C	0.771883	-1.160154	-1.354840
C	1.676649	-1.225746	-0.155645	C	1.616433	-1.276201	-0.219831
H	-0.386377	-2.645056	-2.305644	H	-0.597478	-2.651246	-2.258670
H	1.967793	-2.882008	1.272182	H	1.925750	-2.928292	1.212799
C	-1.266605	-1.928635	0.877908	C	-1.295496	-1.877290	0.967713
C	0.000000	-1.968115	1.532706	C	0.000000	-1.953060	1.546746
C	-1.315694	-1.860397	-0.505529	C	-1.408557	-1.813271	-0.422354
H	1.133885	-0.570773	-2.215069	H	1.040946	-0.676275	-2.291914
H	2.636557	-0.737785	-0.002751	H	2.613522	-0.844796	-0.125704
H	-2.249127	-1.633608	-1.015096	H	-2.372645	-1.605437	-0.888822
H	-2.168598	-1.718647	1.455842	H	-2.165392	-1.649213	1.594241
H	0.044741	-2.109133	2.610309	H	0.114632	-2.018169	2.631400
Ti	0.000000	0.000000	0.503014	Ti	0.000000	0.000000	0.448386

Table S2. Optimized coordinates for the **(bcod)$_2$Ti** structure **Ti-2S.**

	M06-L				OPBE		
	x	y	z		x	y	z
C	2.542848	-0.737001	1.078489	C	2.588013	-0.826766	1.001235
C	2.804422	0.247833	-1.053181	C	2.826318	0.353739	-1.035293
C	3.629917	-0.118050	0.187735	C	3.664343	-0.125687	0.158659
H	4.384628	-0.871479	-0.065274	H	4.416325	-0.856957	-0.175223
H	4.117203	0.747214	0.647785	H	4.162204	0.695647	0.691876
C	1.749082	-1.534034	0.060746	C	1.760683	-1.514389	-0.065636
C	1.900336	-0.967533	-1.167641	C	1.889631	-0.819009	-1.245401
H	2.920518	-1.319163	1.922645	H	2.976048	-1.488100	1.786790
H	3.398283	0.466321	-1.944412	H	3.409621	0.653360	-1.915734
C	1.431955	1.449541	0.654175	C	1.424191	1.371387	0.772027
C	1.808241	1.352191	-0.714797	C	1.819513	1.401782	-0.593363
C	1.560858	0.343164	1.502959	C	1.584306	0.188085	1.524375
H	1.072020	-2.342298	0.316774	H	1.109691	-2.366512	0.121076
H	1.359438	-1.255034	-2.069618	H	1.351192	-1.021832	-2.176736
H	1.172775	0.365735	2.516682	H	1.220022	0.123517	2.549836
H	0.843633	2.305739	0.987529	H	0.844607	2.199354	1.189096
H	1.734782	2.230481	-1.352765	H	1.675662	2.309486	-1.183593
C	-2.454010	-0.476636	-1.117636	C	-2.395163	-0.437342	-1.168892
C	-2.493434	-0.382999	1.222241	C	-2.605411	-0.375503	1.165944
C	-3.460045	-0.530680	0.043974	C	-3.488149	-0.483477	-0.081914
H	-3.943777	-1.512681	0.073337	H	-3.992545	-1.460292	-0.102804
H	-4.222144	0.256347	-0.000895	H	-4.230963	0.322649	-0.171600
C	-1.359967	-1.470984	-0.630361	C	-1.368266	-1.470088	-0.611789
C	-1.329320	-1.290875	0.825323	C	-1.433676	-1.299293	0.840586
H	-2.837791	-0.771395	-2.097119	H	-2.711379	-0.718821	-2.181748
H	-2.941785	-0.603557	2.196982	H	-3.132871	-0.593734	2.106462
C	-1.853919	1.720211	-0.009894	C	-1.813420	1.730131	0.009191
C	-1.902640	1.022445	1.190070	C	-1.956250	1.002524	1.193689
C	-1.906197	0.982571	-1.230118	C	-1.822032	1.013523	-1.227093
H	-1.210617	-2.420464	-1.143942	H	-1.206598	-2.417683	-1.133120
H	-0.945867	-2.046963	1.507673	H	-1.089477	-2.056871	1.547036
H	-1.979769	1.492488	-2.186652	H	-1.815506	1.537053	-2.184652
H	-1.555896	2.769712	-0.024826	H	-1.505570	2.780449	0.030490
H	-1.637117	1.513543	2.124435	H	-1.738441	1.469126	2.157450
Ti	-0.169876	0.151839	-0.293675	Ti	-0.172264	0.119658	-0.216948

Table S3. Optimized coordinates for the **(bcod)$_2$Ti** structure **Ti-3S.**

	M06-L				OPBE		
	x	y	z		x	y	z
C	2.706845	-0.380573	-1.104973	C	2.663405	-0.454660	-1.114915
C	2.670586	0.720936	0.982812	C	2.753656	0.739197	0.923345
C	3.654471	0.025403	0.031870	C	3.673856	-0.021102	-0.041541
H	4.399475	0.743250	-0.329874	H	4.415870	0.668851	-0.471767
H	4.161068	-0.828690	0.492060	H	4.189078	-0.868382	0.431601
C	1.837459	0.865431	-1.214165	C	1.787982	0.785071	-1.230383
C	1.811960	1.496148	-0.001229	C	1.836729	1.475351	-0.031668
H	3.209736	-0.665348	-2.032724	H	3.116626	-0.784293	-2.059199
H	3.140209	1.331812	1.757859	H	3.271558	1.372759	1.655035
C	1.459053	-1.443581	0.778706	C	1.431808	-1.381911	0.853031
C	1.701134	-0.302173	1.544790	C	1.751472	-0.205303	1.552915
C	1.729428	-1.444726	-0.613625	C	1.684923	-1.471050	-0.542138
H	1.280001	1.163223	-2.101241	H	1.233406	1.082861	-2.123978
H	1.223312	2.370248	0.263885	H	1.314142	2.398601	0.218609
H	1.577378	-2.353185	-1.190318	H	1.479059	-2.400814	-1.074592
H	0.854755	-2.242097	1.204982	H	0.829759	-2.145401	1.348977
H	1.372812	-0.243169	2.579007	H	1.443542	-0.072848	2.591881
C	-2.444769	-0.019783	-1.210989	C	-2.365028	-0.051306	-1.242449
C	-2.681977	-0.334517	1.099538	C	-2.756685	-0.344058	1.051610
C	-3.543032	-0.050485	-0.134525	C	-3.538103	-0.088698	-0.240936
H	-4.223338	-0.888341	-0.320280	H	-4.190122	-0.946367	-0.461598
H	-4.114440	0.882905	-0.067401	H	-4.130594	0.837754	-0.227004
C	-1.636829	-1.308507	-0.856138	C	-1.562768	-1.320696	-0.804384
C	-1.708894	-1.399531	0.599993	C	-1.737082	-1.397355	0.635602
H	-2.788220	-0.053675	-2.247335	H	-2.634638	-0.117869	-2.304200
H	-3.257647	-0.609582	1.989936	H	-3.390078	-0.607259	1.911789
C	-1.498232	1.750237	0.323664	C	-1.538443	1.754366	0.326074
C	-1.799848	0.881785	1.364101	C	-1.874175	0.860756	1.348336
C	-1.598067	1.277741	-1.021708	C	-1.580565	1.280922	-1.025725
H	-1.612279	-2.155746	-1.537523	H	-1.439454	-2.170624	-1.478349
H	-1.552317	-2.332361	1.138450	H	-1.580300	-2.313445	1.208169
H	-1.512185	1.967459	-1.857675	H	-1.479489	1.968183	-1.867495
H	-1.006010	2.701671	0.529733	H	-1.088339	2.724389	0.558158
H	-1.525951	1.131670	2.386786	H	-1.633496	1.096485	2.387765
Ti	-0.162822	-0.087404	-0.184866	Ti	-0.159655	-0.030897	-0.124748

Table S4. Optimized coordinates for the **(bcod)$_2$Ti** structure **Ti-4T.**

	M06-L				OPBE		
	x	y	z		x	y	z
C	-0.245738	2.547770	-1.250954	C	0.000000	2.653023	-1.082851
C	-0.098812	2.842963	1.083880	C	0.867287	2.669987	1.110232
C	0.000000	3.654945	-0.214929	C	0.785188	3.571448	-0.131963
H	-0.802833	4.399734	-0.258602	H	0.193897	4.471717	0.094285
H	0.968711	4.149726	-0.337712	H	1.770333	3.861983	-0.522464
C	-1.385820	1.783368	-0.584420	C	-1.069315	2.098613	-0.145321
C	-1.303081	1.955662	0.777936	C	-0.539875	2.082870	1.142589
H	-0.481999	2.912897	-2.254353	H	-0.399154	3.156574	-1.974037
H	-0.203676	3.448816	1.988362	H	1.159813	3.193919	2.031001
C	1.685401	1.496664	-0.056501	C	1.879783	1.071311	-0.536604
C	1.078936	1.874007	1.165060	C	1.759230	1.468039	0.816865
C	0.937471	1.579330	-1.252384	C	0.864071	1.445024	-1.448305
H	-2.126571	1.197701	-1.122584	H	-2.096069	1.874406	-0.433061
H	-1.966484	1.528382	1.528290	H	-1.067008	1.785774	2.053897
H	1.373613	1.261642	-2.196195	H	0.911241	1.112880	-2.486208
H	2.633381	0.955575	-0.042261	H	2.655836	0.362379	-0.836651
H	1.627331	1.768074	2.098734	H	2.501480	1.143931	1.550680
C	0.245738	-2.547770	-1.250954	C	0.000000	-2.653023	-1.082851
C	0.098812	-2.842963	1.083880	C	-0.867287	-2.669987	1.110232
C	0.000000	-3.654945	-0.214929	C	-0.785188	-3.571448	-0.131963
H	0.802833	-4.399734	-0.258602	H	-0.193897	-4.471717	0.094285
H	-0.968711	-4.149726	-0.337712	H	-1.770333	-3.861983	-0.522464
C	1.385820	-1.783368	-0.584420	C	1.069315	-2.098613	-0.145321
C	1.303081	-1.955662	0.777936	C	0.539875	-2.082870	1.142589
H	0.481999	-2.912897	-2.254353	H	0.399154	-3.156574	-1.974037
H	0.203676	-3.448816	1.988362	H	-1.159813	-3.193919	2.031001
C	-1.685401	-1.496664	-0.056501	C	-1.879783	-1.071311	-0.536604
C	-1.078936	-1.874007	1.165060	C	-1.759230	-1.468039	0.816865
C	-0.937471	-1.579330	-1.252384	C	-0.864071	-1.445024	-1.448305
H	2.126571	-1.197701	-1.122584	H	2.096069	-1.874406	-0.433061
H	1.966484	-1.528382	1.528290	H	1.067008	-1.785774	2.053897
H	-1.373613	-1.261642	-2.196195	H	-0.911241	-1.112880	-2.486208
H	-2.633381	-0.955575	-0.042261	H	-2.655836	-0.362379	-0.836651
H	-1.627331	-1.768074	2.098734	H	-2.501480	-1.143931	1.550680
Ti	0.000000	0.000000	0.235472	Ti	0.000000	0.000000	0.197700

Table S5. Optimized coordinates for the **(bcod)$_2$Ti** structure **Ti-5T.**

	M06-L				OPBE		
	x	y	z		x	y	z
C	2.507079	0.002958	1.270028	C	2.713954	0.320853	1.128552
C	2.744359	-0.629505	-0.986970	C	2.688065	-0.871987	-0.909412
C	3.604944	-0.248143	0.224694	C	3.681331	-0.207329	0.056639
H	4.228384	-1.097282	0.526598	H	4.347858	-0.967918	0.490789
H	4.236283	0.628775	0.047585	H	4.279603	0.585274	-0.413553
C	1.566766	-1.170713	0.991407	C	1.747442	-0.854676	1.263772
C	1.716239	-1.547371	-0.332013	C	1.737065	-1.558717	0.063423
H	2.867560	0.046351	2.301708	H	3.197381	0.615389	2.070005
H	3.300950	-1.089762	-1.808420	H	3.150453	-1.544809	-1.644396
C	1.697040	1.596414	-0.481287	C	1.628871	1.402612	-0.857812
C	1.935803	0.584764	-1.443988	C	1.809433	0.188662	-1.562671
C	1.737493	1.262947	0.881135	C	1.857174	1.438407	0.541684
H	0.945399	-1.653408	1.740505	H	1.211092	-1.118221	2.178064
H	1.228100	-2.382786	-0.830194	H	1.214260	-2.493300	-0.145462
H	1.473810	1.995433	1.639891	H	1.706596	2.365244	1.098473
H	1.255041	2.544248	-0.794428	H	1.139126	2.248304	-1.351221
H	1.862332	0.818579	-2.503850	H	1.581513	0.132084	-2.628930
C	-2.833260	0.219774	-1.025397	C	-2.714003	0.320919	-1.128503
C	-2.443683	-0.817330	1.056159	C	-2.688026	-0.872043	0.909390
C	-3.601555	-0.253487	0.217795	C	-3.681334	-0.207332	-0.056582
H	-4.298600	-1.055353	-0.050841	H	-4.347875	-0.967898	-0.490752
H	-4.143144	0.554126	0.720843	H	-4.279591	0.585240	0.413682
C	-1.882074	-0.957564	-1.236353	C	-1.747490	-0.854596	-1.263831
C	-1.659627	-1.574305	-0.016729	C	-1.737062	-1.558709	-0.063524
H	-3.467179	0.438180	-1.889646	H	-3.197470	0.615510	-2.069917
H	-2.757909	-1.443001	1.896499	H	-3.150382	-1.544912	1.644350
C	-1.551356	1.496138	0.702456	C	-1.628844	1.402561	0.857883
C	-1.542298	0.335401	1.508401	C	-1.809376	0.188572	1.562681
C	-1.947016	1.406690	-0.646801	C	-1.857200	1.438438	-0.541601
H	-1.490519	-1.272282	-2.202537	H	-1.211165	-1.118075	-2.178156
H	-1.089842	-2.483852	0.158359	H	-1.214236	-2.493297	0.145284
H	-1.910069	2.285197	-1.286873	H	-1.706641	2.365308	-1.098343
H	-1.045644	2.396381	1.053505	H	-1.139088	2.248229	1.351324
H	-1.212470	0.390413	2.542546	H	-1.581425	0.131936	2.628930
Ti	-0.012528	0.097274	-0.243476	Ti	0.000000	0.093732	-0.000032

Table S6. Optimized coordinates for the **(bcod)$_2$Ti** structure **Ti-6T.**

	M06-L				OPBE		
	x	y	z		x	y	z
C	2.443680	-0.817341	1.056156	C	2.688015	-0.872081	0.909365
C	2.833276	0.219782	-1.025388	C	2.714022	0.320971	-1.128475
C	3.601559	-0.253491	0.217807	C	3.681337	-0.207326	-0.056563
H	4.298605	-1.055355	-0.050831	H	4.347885	-0.967872	-0.490756
H	4.143146	0.554117	0.720867	H	4.279586	0.585226	0.413745
C	1.659628	-1.574302	-0.016744	C	1.737064	-1.558703	-0.063593
C	1.882086	-0.957549	-1.236360	C	1.747512	-0.854538	-1.263869
H	2.757896	-1.443018	1.896495	H	3.150361	-1.544984	1.644301
H	3.467204	0.438189	-1.889629	H	3.197503	0.615606	-2.069869
C	1.551356	1.496132	0.702461	C	1.628826	1.402521	0.857942
C	1.947033	1.406696	-0.646790	C	1.857204	1.438460	-0.541538
C	1.542292	0.335388	1.508399	C	1.809355	0.188504	1.562691
H	1.089845	-2.483854	0.158328	H	1.214233	-2.493298	0.145169
H	1.490543	-1.272257	-2.202552	H	1.211188	-1.117969	-2.178210
H	1.212441	0.390389	2.542537	H	1.581391	0.131820	2.628934
H	1.045645	2.396374	1.053515	H	1.139061	2.248165	1.351411
H	1.910078	2.285206	-1.286858	H	1.706653	2.365355	-1.098240
C	-2.744364	-0.629491	-0.986979	C	-2.688077	-0.871959	-0.909426
C	-2.507089	0.002937	1.270030	C	-2.713937	0.320824	1.128573
C	-3.604952	-0.248150	0.224691	C	-3.681330	-0.207325	0.056657
H	-4.228390	-1.097296	0.526581	H	-4.347853	-0.967925	0.490795
H	-4.236294	0.628769	0.047594	H	-4.279605	0.585293	-0.413504
C	-1.716240	-1.547360	-0.332035	C	-1.737069	-1.558719	0.063379
C	-1.566770	-1.170723	0.991391	C	-1.747425	-0.854711	1.263748
H	-3.300954	-1.089742	-1.808433	H	-3.150476	-1.544759	-1.644421
H	-2.867570	0.046315	2.301711	H	-3.197351	0.615336	2.070040
C	-1.697048	1.596417	-0.481262	C	-1.628878	1.402636	-0.857776
C	-1.737497	1.262927	0.881155	C	-1.857162	1.438392	0.541723
C	-1.935818	0.584789	-1.443981	C	-1.809449	0.188706	-1.562667
H	-1.228091	-2.382760	-0.830231	H	-1.214277	-2.493302	-0.145536
H	-0.945401	-1.653424	1.740484	H	-1.211077	-1.118294	2.178029
H	-1.862349	0.818622	-2.503839	H	-1.581555	0.132162	-2.628934
H	-1.255047	2.544256	-0.794387	H	-1.139133	2.248340	-1.351165
H	-1.473827	1.995408	1.639922	H	-1.706556	2.365207	1.098540
Ti	0.012532	0.097277	-0.243481	Ti	-0.000001	0.093726	-0.000061

Table S7. Optimized coordinates for the **$(bcod)_2V$** structure **V-1Q.**

	M06-L				OPBE		
	x	y	z		x	y	z
C	0.000000	2.684343	1.179376	C	0.000000	2.709254	1.180977
C	0.000000	2.684343	-1.179376	C	0.000000	2.709254	-1.180977
C	-0.231751	3.639465	0.000000	C	-0.223527	3.665647	0.000000
H	0.524917	4.432381	0.000000	H	0.547276	4.451412	0.000000
H	-1.231548	4.085130	0.000000	H	-1.220818	4.126882	0.000000
C	1.217082	1.909574	0.685999	C	1.188505	1.893283	0.693521
C	1.217082	1.909574	-0.685999	C	1.188505	1.893283	-0.693521
H	0.144312	3.181326	2.142528	H	0.151486	3.205615	2.148901
H	0.144312	3.181326	-2.142528	H	0.151486	3.205615	-2.148901
C	-1.765097	1.366902	0.000000	C	-1.750099	1.360667	0.000000
C	-1.115181	1.644130	-1.220753	C	-1.102660	1.661191	-1.222362
C	-1.115181	1.644130	1.220753	C	-1.102660	1.661191	1.222362
H	1.936116	1.417053	1.336914	H	1.922769	1.426998	1.352520
H	1.936116	1.417053	-1.336914	H	1.922769	1.426998	-1.352520
H	-1.592119	1.397834	2.166508	H	-1.563168	1.391534	2.175173
H	-2.665767	0.748590	0.000000	H	-2.659540	0.750441	0.000000
H	-1.592119	1.397834	-2.166508	H	-1.563168	1.391534	-2.175173
C	0.000000	-2.684343	1.179376	C	0.000000	-2.709254	1.180977
C	0.000000	-2.684343	-1.179376	C	0.000000	-2.709254	-1.180977
C	0.231751	-3.639465	0.000000	C	0.223527	-3.665647	0.000000
H	-0.524917	-4.432381	0.000000	H	-0.547276	-4.451412	0.000000
H	1.231548	-4.085130	0.000000	H	1.220818	-4.126882	0.000000
C	-1.217082	-1.909574	0.685999	C	-1.188505	-1.893283	0.693521
C	-1.217082	-1.909574	-0.685999	C	-1.188505	-1.893283	-0.693521
H	-0.144312	-3.181326	2.142528	H	-0.151486	-3.205615	2.148901
H	-0.144312	-3.181326	-2.142528	H	-0.151486	-3.205615	-2.148901
C	1.765097	-1.366902	0.000000	C	1.750099	-1.360667	0.000000
C	1.115181	-1.644130	-1.220753	C	1.102660	-1.661191	-1.222362
C	1.115181	-1.644130	1.220753	C	1.102660	-1.661191	1.222362
H	-1.936116	-1.417053	1.336914	H	-1.922769	-1.426998	1.352520
H	-1.936116	-1.417053	-1.336914	H	-1.922769	-1.426998	-1.352520
H	1.592119	-1.397834	2.166508	H	1.563168	-1.391534	2.175173
H	2.665767	-0.748590	0.000000	H	2.659540	-0.750441	0.000000
H	1.592119	-1.397834	-2.166508	H	1.563168	-1.391534	-2.175173
V	0.000000	0.000000	0.000000	V	0.000000	0.000000	0.000000

Table S8. Optimized coordinates for the**(bcod)$_2$V** structure **V-2Q.**

	M06-L				OPBE		
	x	y	z		x	y	z
C	0.907280	2.656091	-0.788691	C	-1.125940	2.555609	-0.905595
C	-1.223638	2.644265	0.218719	C	-2.612556	1.265572	0.395021
C	-0.125883	3.629844	-0.205034	C	-2.470081	2.685172	-0.173796
H	-0.498437	4.300159	-0.988168	H	-3.274450	2.885452	-0.898046
H	0.264620	4.220317	0.629896	H	-2.468414	3.463376	0.601917
C	0.000000	1.706530	-1.561307	C	-1.259453	1.178143	-1.539699
C	-1.245400	1.702244	-0.982754	C	-2.133759	0.417328	-0.778949
H	1.682070	3.131206	-1.397107	H	-0.913777	3.366897	-1.615340
H	-2.187885	3.109632	0.441210	H	-3.620602	1.017392	0.754303
C	0.683947	1.610787	1.469701	C	-0.342050	1.772443	1.344363
C	-0.712375	1.785152	1.371131	C	-1.539255	1.020997	1.447802
C	1.488196	1.791578	0.326066	C	0.000000	2.344006	0.097567
H	0.315124	1.138073	-2.433803	H	-0.787185	0.889285	-2.479738
H	-2.107754	1.119816	-1.298124	H	-2.473472	-0.597447	-0.993476
H	2.560035	1.614409	0.374628	H	0.946258	2.876175	-0.023808
H	1.105042	1.128033	2.352863	H	0.387863	1.759036	2.159557
H	-1.350049	1.603346	2.233447	H	-1.804442	0.537009	2.390376
C	-0.907280	-2.656091	-0.788691	C	1.125940	-2.555609	-0.905595
C	1.223638	-2.644265	0.218719	C	2.612556	-1.265572	0.395021
C	0.125883	-3.629844	-0.205034	C	2.470081	-2.685172	-0.173796
H	0.498437	-4.300159	-0.988168	H	3.274450	-2.885452	-0.898046
H	-0.264620	-4.220317	0.629896	H	2.468414	-3.463376	0.601917
C	0.000000	-1.706530	-1.561307	C	1.259453	-1.178143	-1.539699
C	1.245400	-1.702244	-0.982754	C	2.133759	-0.417328	-0.778949
H	-1.682070	-3.131206	-1.397107	H	0.913777	-3.366897	-1.615340
H	2.187885	-3.109632	0.441210	H	3.620602	-1.017392	0.754303
C	-0.683947	-1.610787	1.469701	C	0.342050	-1.772443	1.344363
C	0.712375	-1.785152	1.371131	C	1.539255	-1.020997	1.447802
C	-1.488196	-1.791578	0.326066	C	0.000000	-2.344006	0.097567
H	-0.315124	-1.138073	-2.433803	H	0.787185	-0.889285	-2.479738
H	2.107754	-1.119816	-1.298124	H	2.473472	0.597447	-0.993476
H	-2.560035	-1.614409	0.374628	H	-0.946258	-2.876175	-0.023808
H	-1.105042	-1.128033	2.352863	H	-0.387863	-1.759036	2.159557
H	1.350049	-1.603346	2.233447	H	1.804442	-0.537009	2.390376
V	0.000000	0.000000	0.086798	V	0.000000	0.000000	0.068171

Table S9. Optimized coordinates for the**(bcod)$_2$V** structure **V-3D.**

	M06-L				OPBE		
	x	y	z		x	y	z
C	2.456880	-1.143657	-0.571809	C	2.417169	-1.146959	-0.589594
C	2.592877	1.145127	-0.035230	C	2.589728	1.132014	-0.017544
C	3.503797	-0.070604	-0.244150	C	3.483254	-0.092276	-0.256012
H	4.160531	0.094287	-1.105800	H	4.129220	0.081279	-1.130056
H	4.107157	-0.313278	0.636808	H	4.100833	-0.358318	0.613546
C	1.525682	-0.368725	-1.502354	C	1.471433	-0.354096	-1.491166
C	1.593036	0.965121	-1.168682	C	1.562467	0.989414	-1.130594
H	2.868162	-2.058888	-1.006673	H	2.812352	-2.066085	-1.044017
H	3.112681	2.107333	-0.034849	H	3.123561	2.092297	-0.002582
C	1.492299	-0.382944	1.613930	C	1.456555	-0.405273	1.615812
C	1.739699	0.938507	1.204674	C	1.725924	0.920575	1.214413
C	1.613465	-1.421017	0.668526	C	1.578584	-1.432722	0.652154
H	0.928605	-0.805491	-2.294616	H	0.934683	-0.758569	-2.347034
H	1.058143	1.778217	-1.651195	H	1.096785	1.829071	-1.646000
H	1.382542	-2.445528	0.946757	H	1.341646	-2.464212	0.916500
H	1.005996	-0.572346	2.572221	H	0.992489	-0.606344	2.587271
H	1.541355	1.770620	1.875507	H	1.535029	1.752941	1.894402
C	-2.628973	-0.169384	-1.162299	C	-2.651869	-0.182672	-1.138324
C	-2.230351	-0.334461	1.141925	C	-2.176279	-0.320497	1.157017
C	-3.404496	-0.191798	0.153092	C	-3.385670	-0.191934	0.201765
H	-4.046270	-1.077689	0.201295	H	-4.022521	-1.085166	0.279064
H	-4.002753	0.709457	0.326749	H	-3.984837	0.710883	0.386183
C	-1.607843	-1.279268	-0.964428	C	-1.618502	-1.282477	-0.958940
C	-1.418465	-1.485918	0.438223	C	-1.382067	-1.474151	0.437021
H	-3.265027	-0.252984	-2.050826	H	-3.315484	-0.272298	-2.011463
H	-2.485207	-0.631571	2.161607	H	-2.402334	-0.614023	2.190216
C	-1.462054	1.772262	-0.023494	C	-1.434440	1.771488	-0.055624
C	-1.495420	1.045272	1.208495	C	-1.458031	1.068008	1.191914
C	-1.749341	1.068966	-1.194937	C	-1.742887	1.030489	-1.210078
H	-1.349135	-2.001385	-1.734355	H	-1.355744	-2.000873	-1.736539
H	-1.206374	-2.419588	0.954646	H	-1.162672	-2.410425	0.953556
H	-1.468745	1.485164	-2.161424	H	-1.478577	1.421831	-2.195857
H	-0.993999	2.755847	-0.060594	H	-0.988007	2.767847	-0.118104
H	-1.396691	1.535606	2.173897	H	-1.354192	1.575591	2.152967
V	-0.133727	-0.007942	0.125302	V	-0.113672	0.010043	0.109766

Table S10. Optimized coordinates for the**(bcod)$_2$V** structure **V-4D.**

	M06-L				OPBE		
	x	y	z		x	y	z
C	2.544118	-0.907935	0.848396	C	2.531842	-1.234506	0.022919
C	2.605378	0.480978	-1.053830	C	2.515289	1.072095	-0.446282
C	3.546354	-0.110738	0.003037	C	3.501852	-0.053158	-0.103009
H	4.267689	-0.788797	-0.467183	H	4.190743	-0.221092	-0.944806
H	4.081294	0.653973	0.575592	H	4.077788	0.136558	0.814041
C	1.676189	-1.525720	-0.240693	C	1.578664	-0.995402	-1.140364
C	1.688872	-0.700028	-1.336630	C	1.576099	0.370692	-1.427672
H	3.000835	-1.632535	1.528073	H	3.009922	-2.223491	0.034754
H	3.108918	0.891124	-1.933344	H	2.983388	1.985274	-0.839326
C	1.405234	1.315934	0.978412	C	1.369717	0.291952	1.657584
C	1.669249	1.473296	-0.392718	C	1.609711	1.353000	0.747431
C	1.595850	0.047418	1.567621	C	1.603514	-1.020133	1.200725
H	1.148307	-2.465756	-0.141490	H	1.153710	-1.790952	-1.749480
H	1.141473	-0.843364	-2.264886	H	1.153164	0.842634	-2.312561
H	1.353107	-0.108977	2.615380	H	1.289449	-1.874748	1.802435
H	0.851978	2.085860	1.517080	H	0.839921	0.465009	2.598402
H	1.411097	2.399374	-0.900794	H	1.388498	2.381626	1.041415
C	-2.064939	-0.630208	-1.171790	C	-2.021173	-0.477899	-1.246118
C	-2.791677	-0.035453	0.977759	C	-2.714986	-0.235933	0.981221
C	-3.372003	-0.363477	-0.397422	C	-3.322322	-0.396873	-0.413340
H	-3.973557	-1.277059	-0.347584	H	-3.871044	-1.347448	-0.478003
H	-3.967397	0.448596	-0.829192	H	-3.977006	0.433227	-0.713880
C	-1.332661	-1.589972	-0.156226	C	-1.205294	-1.517788	-0.402182
C	-1.708426	-1.092551	1.134791	C	-1.572773	-1.236518	0.955434
H	-2.163350	-1.133536	-2.136297	H	-2.121223	-0.834597	-2.279296
H	-3.542999	0.003228	1.774709	H	-3.441807	-0.351437	1.799567
C	-1.534686	1.697494	-0.359712	C	-1.601444	1.753300	-0.123250
C	-1.985476	1.249899	0.878026	C	-1.951633	1.079997	1.059188
C	-1.359004	0.741122	-1.413102	C	-1.426976	0.973372	-1.307171
H	-1.101406	-2.613712	-0.446216	H	-0.921829	-2.482280	-0.827598
H	-1.508825	-1.603186	2.073670	H	-1.304104	-1.857288	1.811267
H	-1.156885	1.047322	-2.436422	H	-1.298255	1.429013	-2.289984
H	-1.092941	2.689324	-0.459924	H	-1.258027	2.792309	-0.101242
H	-1.881693	1.882758	1.757455	H	-1.861316	1.583961	2.024473
V	-0.150864	0.002827	0.057646	V	-0.124021	0.112023	0.022571

Table S11. Optimized coordinates for the**(bcod)$_2$V** structure **V-5D.**

	M06-L				OPBE		
	x	y	z		x	y	z
C	2.609236	-0.137832	-1.146441	C	2.560874	-0.172558	-1.158976
C	2.544147	0.492506	1.122349	C	2.557443	0.497854	1.101075
C	3.546096	0.023806	0.059506	C	3.531726	0.009415	0.020291
H	4.283608	0.811279	-0.133710	H	4.260621	0.801995	-0.208342
H	4.060543	-0.904394	0.329961	H	4.061709	-0.914749	0.292588
C	1.741593	1.119926	-1.008601	C	1.685352	1.082671	-1.027317
C	1.708947	1.481098	0.324935	C	1.681726	1.466766	0.324282
H	3.122767	-0.221008	-2.108898	H	3.049688	-0.275041	-2.138538
H	3.001859	0.907668	2.024839	H	3.040061	0.921393	1.992930
C	1.387978	-1.626940	0.459960	C	1.349527	-1.625177	0.501838
C	1.563652	-0.628311	1.428140	C	1.561271	-0.596877	1.441009
C	1.666748	-1.318249	-0.892759	C	1.627793	-1.351877	-0.862920
H	1.318357	1.689046	-1.834510	H	1.341115	1.700427	-1.860862
H	1.244537	2.364603	0.751609	H	1.342647	2.420730	0.726550
H	1.524128	-2.078524	-1.658281	H	1.463470	-2.128340	-1.614759
H	0.862973	-2.545183	0.713726	H	0.851479	-2.550503	0.797758
H	1.225161	-0.787027	2.448988	H	1.229108	-0.721792	2.473365
C	-2.618764	0.050713	-1.137662	C	-2.560894	0.172168	-1.158981
C	-2.480974	-0.423231	1.165548	C	-2.557205	-0.497622	1.101247
C	-3.524035	-0.068677	0.096857	C	-3.531644	-0.009637	0.020397
H	-4.224974	-0.901518	-0.029685	H	-4.260421	-0.802398	-0.207981
H	-4.080451	0.850131	0.317175	H	-4.061770	0.914512	0.292479
C	-1.687323	-1.158523	-0.961944	C	-1.685139	-1.082893	-1.027109
C	-1.604250	-1.427291	0.427495	C	-1.681323	-1.466611	0.324702
H	-3.155368	0.070567	-2.091553	H	-3.049789	0.274369	-2.138534
H	-2.906366	-0.792791	2.103837	H	-3.039712	-0.920986	1.993249
C	-1.419731	1.690743	0.344605	C	-1.349710	1.625476	0.501383
C	-1.554465	0.765168	1.387396	C	-1.561252	0.597426	1.440864
C	-1.717646	1.278176	-0.969803	C	-1.628013	1.351740	-0.863256
H	-1.441652	-1.869517	-1.749491	H	-1.341392	-1.701082	-1.860533
H	-1.274896	-2.361845	0.874106	H	-1.342634	-2.420676	0.727068
H	-1.563553	1.966914	-1.799357	H	-1.463683	2.127937	-1.615372
H	-0.896432	2.631594	0.513766	H	-0.851653	2.550912	0.796965
H	-1.214336	1.014060	2.389874	H	-1.229081	0.722703	2.473175
V	-0.037093	-0.022720	-0.228690	V	-0.000129	-0.000043	-0.217060

Table S12. Optimized coordinates for the**(bcod)$_2$V** structure **V-6Q.**

	M06-L				OPBE		
	x	y	z		x	y	z
C	-0.434764	2.492547	1.181251	C	-0.445643	2.481380	1.182899
C	-0.434764	2.492547	-1.181251	C	-0.445643	2.481380	-1.182899
C	-1.324373	2.072936	0.000000	C	-1.332871	2.060154	0.000000
H	-2.262118	2.638117	0.000000	H	-2.274755	2.628883	0.000000
H	-1.679411	1.014799	0.000000	H	-1.690408	0.999122	0.000000
C	0.019224	3.844666	0.674879	C	0.016617	3.832139	0.679080
C	0.019224	3.844666	-0.674879	C	0.016617	3.832139	-0.679080
H	-0.957940	2.501083	2.141463	H	-0.970207	2.489579	2.147805
H	-0.957940	2.501083	-2.141463	H	-0.970207	2.489579	-2.147805
C	1.499234	1.426624	0.000000	C	1.503695	1.426166	0.000000
C	0.803232	1.578000	-1.219816	C	0.800760	1.579340	-1.221062
C	0.803232	1.578000	1.219816	C	0.800760	1.579340	1.221062
H	0.452076	4.612254	1.311372	H	0.460859	4.598577	1.318661
H	0.452076	4.612254	-1.311372	H	0.460859	4.598577	-1.318661
H	1.342896	1.481604	2.159964	H	1.334770	1.476532	2.168740
H	2.503595	0.998197	0.000000	H	2.526272	1.034799	0.000000
H	1.342896	1.481604	-2.159964	H	1.334770	1.476532	-2.168740
C	0.196841	-2.793351	-1.179618	C	0.184539	-2.802263	-1.181356
C	0.196841	-2.793351	1.179618	C	0.184539	-2.802263	1.181356
C	0.068513	-3.768088	0.000000	C	0.051747	-3.775809	0.000000
H	0.905735	-4.475243	0.000000	H	0.893311	-4.485002	0.000000
H	-0.877683	-4.318462	0.000000	H	-0.897570	-4.329164	0.000000
C	1.326687	-1.894322	-0.688238	C	1.298175	-1.883090	-0.696685
C	1.326687	-1.894322	0.688238	C	1.298175	-1.883090	0.696685
H	0.392877	-3.271743	-2.142969	H	0.379728	-3.282669	-2.149560
H	0.392877	-3.271743	2.142969	H	0.379728	-3.282669	2.149560
C	-1.702714	-1.679658	0.000000	C	-1.691714	-1.635561	0.000000
C	-1.028707	-1.883422	1.222110	C	-1.020199	-1.869584	1.223850
C	-1.028707	-1.883422	-1.222110	C	-1.020199	-1.869584	-1.223850
H	2.007750	-1.350588	-1.338807	H	2.010866	-1.381082	-1.353236
H	2.007750	-1.350588	1.338807	H	2.010866	-1.381082	1.353236
H	-1.532188	-1.694295	-2.166584	H	-1.506453	-1.643710	-2.175198
H	-2.670976	-1.174024	0.000000	H	-2.663027	-1.126360	0.000000
H	-1.532188	-1.694295	2.166584	H	-1.506453	-1.643710	2.175198
V	-0.050617	-0.160013	0.000000	V	-0.022134	-0.162675	0.000000

Table S13. Optimized coordinates for the **(bcod)$_2$V** structure **V-7D.**

	M06-L				OPBE		
	x	y	z		x	y	z
C	-2.377610	1.077339	0.655860	C	-2.366207	1.030619	0.726140
C	-2.266797	-1.254318	0.343922	C	-2.234676	-1.278415	0.267300
C	-1.812559	-0.171148	1.338641	C	-1.799728	-0.257077	1.334705
H	-2.268551	-0.334065	2.320925	H	-2.269390	-0.485006	2.303360
H	-0.718937	-0.140242	1.575229	H	-0.702389	-0.240878	1.596915
C	-3.741928	0.560558	0.255450	C	-3.720955	0.536726	0.267881
C	-3.678727	-0.775930	0.081500	C	-3.645321	-0.792778	0.007059
H	-2.379974	1.966253	1.293070	H	-2.383183	1.880405	1.421963
H	-2.179622	-2.271618	0.736323	H	-2.148208	-2.323065	0.595530
C	-1.420903	0.215837	-1.506338	C	-1.372488	0.314476	-1.483831
C	-1.473445	-1.089771	-0.966916	C	-1.429059	-1.025693	-1.022559
C	-1.555172	1.306587	-0.623654	C	-1.531241	1.347196	-0.526332
H	-4.581104	1.197503	-0.012192	H	-4.561541	1.189793	0.021340
H	-4.457198	-1.399196	-0.351207	H	-4.413878	-1.393595	-0.485252
H	-1.467118	2.319995	-1.011415	H	-1.450786	2.389021	-0.845535
H	-1.088839	0.375406	-2.531880	H	-1.063861	0.541381	-2.508252
H	-1.393745	-1.950145	-1.626846	H	-1.337351	-1.848063	-1.734505
C	2.685640	-0.310051	1.218595	C	2.711991	-0.333803	1.185164
C	2.403071	-0.302914	-1.107940	C	2.322055	-0.317283	-1.129738
C	3.528515	-0.282157	-0.056310	C	3.497712	-0.319085	-0.127447
H	4.130620	-1.193070	-0.133113	H	4.078468	-1.246874	-0.230033
H	4.175397	0.598185	-0.138059	H	4.159893	0.550739	-0.240633
C	1.624802	-1.353147	0.890179	C	1.619627	-1.355030	0.902281
C	1.514607	-1.474963	-0.538684	C	1.437205	-1.474992	-0.518950
H	3.269802	-0.494227	2.127654	H	3.336809	-0.524089	2.071400
H	2.693848	-0.528916	-2.135851	H	2.560617	-0.553739	-2.174494
C	1.674731	1.759217	0.170425	C	1.674616	1.755981	0.182560
C	1.712623	1.098278	-1.103797	C	1.675349	1.103700	-1.100924
C	1.895588	0.991169	1.307861	C	1.916227	0.960212	1.307989
H	1.307437	-2.121091	1.592430	H	1.299125	-2.108870	1.624713
H	1.333624	-2.369801	-1.128671	H	1.230283	-2.375501	-1.099589
H	1.631217	1.384302	2.288039	H	1.677766	1.341136	2.305250
H	1.252622	2.760314	0.246261	H	1.282591	2.772019	0.279693
H	1.653415	1.652247	-2.037762	H	1.606974	1.663141	-2.036370
V	0.296196	0.025246	-0.140248	V	0.285540	0.061022	-0.108404

Table S14. Optimized coordinates for the **(bcod)$_2$Cr** structure **Cr-1T.**

	M06-L				OPBE		
	x	y	z		x	y	z
C	1.011432	2.583157	0.464076	C	0.994171	2.583099	0.487682
C	-0.809027	2.392202	-1.017569	C	-0.788615	2.376920	-1.039226
C	0.000000	3.466037	-0.276393	C	0.000000	3.459300	-0.285609
H	0.519872	4.109155	-0.995418	H	0.542785	4.095176	-1.001383
H	-0.610343	4.082460	0.393517	H	-0.628988	4.086813	0.362927
C	1.365863	1.555027	-0.605068	C	1.372412	1.533506	-0.552255
C	0.298020	1.453938	-1.510924	C	0.322433	1.423103	-1.492901
H	1.866676	3.125007	0.878681	H	1.842345	3.129728	0.922984
H	-1.455277	2.779989	-1.810410	H	-1.420307	2.757473	-1.853970
C	-1.077355	1.482200	1.309714	C	-1.106870	1.451556	1.285477
C	-1.594403	1.569551	0.003149	C	-1.591177	1.547945	-0.039021
C	0.292463	1.741882	1.509338	C	0.259345	1.733142	1.513737
H	2.363857	1.150926	-0.745455	H	2.389078	1.163888	-0.684770
H	0.342159	1.043250	-2.513697	H	0.414492	1.046518	-2.510288
H	0.745031	1.570951	2.483666	H	0.697558	1.560008	2.499177
H	-1.658387	0.993541	2.091573	H	-1.713429	0.975727	2.061379
H	-2.628424	1.297454	-0.193096	H	-2.622635	1.270639	-0.263519
C	-1.011432	-2.583157	0.464076	C	-0.994171	-2.583099	0.487682
C	0.809027	-2.392202	-1.017569	C	0.788615	-2.376920	-1.039226
C	0.000000	-3.466037	-0.276393	C	0.000000	-3.459300	-0.285609
H	-0.519872	-4.109155	-0.995418	H	-0.542785	-4.095176	-1.001383
H	0.610343	-4.082460	0.393517	H	0.628988	-4.086813	0.362927
C	-1.365863	-1.555027	-0.605068	C	-1.372412	-1.533506	-0.552255
C	-0.298020	-1.453938	-1.510924	C	-0.322433	-1.423103	-1.492901
H	-1.866676	-3.125007	0.878681	H	-1.842345	-3.129728	0.922984
H	1.455277	-2.779989	-1.810410	H	1.420307	-2.757473	-1.853970
C	1.077355	-1.482200	1.309714	C	1.106870	-1.451556	1.285477
C	1.594403	-1.569551	0.003149	C	1.591177	-1.547945	-0.039021
C	-0.292463	-1.741882	1.509338	C	-0.259345	-1.733142	1.513737
H	-2.363857	-1.150926	-0.745455	H	-2.389078	-1.163888	-0.684770
H	-0.342159	-1.043250	-2.513697	H	-0.414492	-1.046518	-2.510288
H	-0.745031	-1.570951	2.483666	H	-0.697558	-1.560008	2.499177
H	1.658387	-0.993541	2.091573	H	1.713429	-0.975727	2.061379
H	2.628424	-1.297454	-0.193096	H	2.622635	-1.270639	-0.263519
Cr	0.000000	0.000000	0.096058	Cr	0.000000	0.000000	0.100014

Table S15. Optimized coordinates for the**(bcod)$_2$Cr** structure **Cr-2T**

	M06-L				OPBE		
	x	y	z		x	y	z
C	0.000000	2.539917	1.180080	C	0.000000	2.548356	1.181068
C	0.000000	2.539917	-1.180080	C	0.000000	2.548356	-1.181068
C	-0.191497	3.502152	0.000000	C	-0.188876	3.511603	0.000000
H	0.600772	4.259265	0.000000	H	0.613631	4.264924	0.000000
H	-1.169861	3.995872	0.000000	H	-1.166648	4.015412	0.000000
C	1.174916	1.690751	0.701890	C	1.158158	1.675976	0.707426
C	1.174916	1.690751	-0.701890	C	1.158158	1.675976	-0.707426
H	0.157248	3.031430	2.144204	H	0.160407	3.039244	2.150591
H	0.157248	3.031430	-2.144204	H	0.160407	3.039244	-2.150591
C	-1.802530	1.269293	0.000000	C	-1.792651	1.253056	0.000000
C	-1.149647	1.541986	-1.216111	C	-1.136979	1.538733	-1.218244
C	-1.149647	1.541986	1.216111	C	-1.136979	1.538733	1.218244
H	1.969624	1.333654	1.351354	H	1.970908	1.353949	1.358996
H	1.969624	1.333654	-1.351354	H	1.970908	1.353949	-1.358996
H	-1.604496	1.253797	2.160363	H	-1.585408	1.243928	2.168847
H	-2.693069	0.639749	0.000000	H	-2.699682	0.642686	0.000000
H	-1.604496	1.253797	-2.160363	H	-1.585408	1.243928	-2.168847
C	0.000000	-2.539917	1.180080	C	0.000000	-2.548356	1.181068
C	0.000000	-2.539917	-1.180080	C	0.000000	-2.548356	-1.181068
C	0.191497	-3.502152	0.000000	C	0.188876	-3.511603	0.000000
H	-0.600772	-4.259265	0.000000	H	-0.613631	-4.264924	0.000000
H	1.169861	-3.995872	0.000000	H	1.166648	-4.015412	0.000000
C	-1.174916	-1.690751	0.701890	C	-1.158158	-1.675976	0.707426
C	-1.174916	-1.690751	-0.701890	C	-1.158158	-1.675976	-0.707426
H	-0.157248	-3.031430	2.144204	H	-0.160407	-3.039244	2.150591
H	-0.157248	-3.031430	-2.144204	H	-0.160407	-3.039244	-2.150591
C	1.802530	-1.269293	0.000000	C	1.792651	-1.253056	0.000000
C	1.149647	-1.541986	-1.216111	C	1.136979	-1.538733	-1.218244
C	1.149647	-1.541986	1.216111	C	1.136979	-1.538733	1.218244
H	-1.969624	-1.333654	1.351354	H	-1.970908	-1.353949	1.358996
H	-1.969624	-1.333654	-1.351354	H	-1.970908	-1.353949	-1.358996
H	1.604496	-1.253797	2.160363	H	1.585408	-1.243928	2.168847
H	2.693069	-0.639749	0.000000	H	2.699682	-0.642686	0.000000
H	1.604496	-1.253797	-2.160363	H	1.585408	-1.243928	-2.168847
Cr	0.000000	0.000000	0.000000	Cr	0.000000	0.000000	0.000000

Table S16. Optimized coordinates for the **(bcod)$_2$Cr** structure **Cr-3P.**

	M06-L				OPBE		
	x	y	z		x	y	z
C	0.000000	2.814473	1.176969	C	0.000000	2.838267	1.178734
C	0.000000	2.814473	-1.176969	C	0.000000	2.838267	-1.178734
C	-0.318716	3.749379	0.000000	C	-0.312210	3.775362	0.000000
H	0.363385	4.606825	0.000000	H	0.382666	4.628434	0.000000
H	-1.354602	4.102790	0.000000	H	-1.347710	4.141689	0.000000
C	1.296165	2.185748	0.676929	C	1.281181	2.179401	0.682647
C	1.296165	2.185748	-0.676929	C	1.281181	2.179401	-0.682647
H	0.091103	3.320907	2.142038	H	0.097766	3.346304	2.147978
H	0.091103	3.320907	-2.142038	H	0.097766	3.346304	-2.147978
C	-1.693125	1.402474	0.000000	C	-1.679957	1.403121	0.000000
C	-1.045790	1.699297	-1.217424	C	-1.038888	1.721127	-1.220527
C	-1.045790	1.699297	1.217424	C	-1.038888	1.721127	1.220527
H	2.025559	1.701170	1.323873	H	2.016336	1.707376	1.338452
H	2.025559	1.701170	-1.323873	H	2.016336	1.707376	-1.338452
H	-1.517662	1.441370	2.162861	H	-1.499254	1.446717	2.172311
H	-2.563654	0.741434	0.000000	H	-2.559825	0.749432	0.000000
H	-1.517662	1.441370	-2.162861	H	-1.499254	1.446717	-2.172311
C	0.000000	-2.814473	1.176969	C	0.000000	-2.838267	1.178734
C	0.000000	-2.814473	-1.176969	C	0.000000	-2.838267	-1.178734
C	0.318716	-3.749379	0.000000	C	0.312210	-3.775362	0.000000
H	-0.363385	-4.606825	0.000000	H	-0.382666	-4.628434	0.000000
H	1.354602	-4.102790	0.000000	H	1.347710	-4.141689	0.000000
C	-1.296165	-2.185748	0.676929	C	-1.281181	-2.179401	0.682647
C	-1.296165	-2.185748	-0.676929	C	-1.281181	-2.179401	-0.682647
H	-0.091103	-3.320907	2.142038	H	-0.097766	-3.346304	2.147978
H	-0.091103	-3.320907	-2.142038	H	-0.097766	-3.346304	-2.147978
C	1.693125	-1.402474	0.000000	C	1.679957	-1.403121	0.000000
C	1.045790	-1.699297	-1.217424	C	1.038888	-1.721127	-1.220527
C	1.045790	-1.699297	1.217424	C	1.038888	-1.721127	1.220527
H	-2.025559	-1.701170	1.323873	H	-2.016336	-1.707376	1.338452
H	-2.025559	-1.701170	-1.323873	H	-2.016336	-1.707376	-1.338452
H	1.517662	-1.441370	2.162861	H	1.499254	-1.446717	2.172311
H	2.563654	-0.741434	0.000000	H	2.559825	-0.749432	0.000000
H	1.517662	-1.441370	-2.162861	H	1.499254	-1.446717	-2.172311
Cr	0.000000	0.000000	0.000000	Cr	0.000000	0.000000	0.000000

Table S17. Optimized coordinates for the**(bcod)$_2$Cr** structure **Cr-4P.**

	M06-L				OPBE		
	x	y	z		x	y	z
C	0.000000	3.025112	-0.213787	C	0.000000	3.053644	-0.184890
C	-2.079068	1.992828	-0.608281	C	-2.100647	2.054595	-0.569052
C	-1.482591	3.390325	-0.389183	C	-1.483102	3.439163	-0.319587
H	-1.621292	4.006720	-1.284472	H	-1.631724	4.083057	-1.199433
H	-1.900924	3.906656	0.480468	H	-1.880726	3.938476	0.574268
C	0.159278	1.977766	-1.308789	C	0.135227	2.020702	-1.296116
C	-1.042051	1.398021	-1.552486	C	-1.089152	1.459154	-1.537697
H	0.686707	3.871682	-0.301504	H	0.698360	3.897842	-0.265467
H	-3.099600	1.995011	-1.001183	H	-3.133386	2.078323	-0.942747
C	-0.948121	1.585278	1.589065	C	-0.908026	1.530130	1.577962
C	-1.962137	1.184369	0.684149	C	-1.957507	1.193073	0.682308
C	0.171983	2.282086	1.103892	C	0.199864	2.260117	1.096178
H	1.118854	1.700999	-1.740760	H	1.085273	1.769193	-1.771205
H	-1.229631	0.552288	-2.210281	H	-1.313748	0.651369	-2.235448
H	0.992947	2.538698	1.768802	H	1.049226	2.476210	1.747935
H	-0.934067	1.174619	2.601251	H	-0.880024	1.086308	2.580185
H	-2.828243	0.637736	1.050221	H	-2.811164	0.609519	1.034611
C	0.000000	-3.025112	-0.213787	C	0.000000	-3.053644	-0.184890
C	2.079068	-1.992828	-0.608281	C	2.100647	-2.054595	-0.569052
C	1.482591	-3.390325	-0.389183	C	1.483102	-3.439163	-0.319587
H	1.621292	-4.006720	-1.284472	H	1.631724	-4.083057	-1.199433
H	1.900924	-3.906656	0.480468	H	1.880726	-3.938476	0.574268
C	-0.159278	-1.977766	-1.308789	C	-0.135227	-2.020702	-1.296116
C	1.042051	-1.398021	-1.552486	C	1.089152	-1.459154	-1.537697
H	-0.686707	-3.871682	-0.301504	H	-0.698360	-3.897842	-0.265467
H	3.099600	-1.995011	-1.001183	H	3.133386	-2.078323	-0.942747
C	0.948121	-1.585278	1.589065	C	0.908026	-1.530130	1.577962
C	1.962137	-1.184369	0.684149	C	1.957507	-1.193073	0.682308
C	-0.171983	-2.282086	1.103892	C	-0.199864	-2.260117	1.096178
H	-1.118854	-1.700999	-1.740760	H	-1.085273	-1.769193	-1.771205
H	1.229631	-0.552288	-2.210281	H	1.313748	-0.651369	-2.235448
H	-0.992947	-2.538698	1.768802	H	-1.049226	-2.476210	1.747935
H	0.934067	-1.174619	2.601251	H	0.880024	-1.086308	2.580185
H	2.828243	-0.637736	1.050221	H	2.811164	-0.609519	1.034611
Cr	0.000000	0.000000	0.400831	Cr	0.000000	0.000000	0.315222

Table S18. Optimized coordinates for the**(bcod)$_2$Cr** structure **Cr-5P.**

	M06-L				OPBE		
	x	y	z		x	y	z
C	-0.537503	-2.782493	1.178601	C	-0.498530	-2.828307	1.180197
C	-0.537503	-2.782493	-1.178601	C	-0.498530	-2.828307	-1.180197
C	-0.640939	-3.760048	0.000000	C	-0.573248	-3.808115	0.000000
H	-1.619477	-4.252864	0.000000	H	-1.543679	-4.326744	0.000000
H	0.150176	-4.516059	0.000000	H	0.239412	-4.547014	0.000000
C	-1.418280	-1.642242	0.682769	C	-1.390957	-1.695564	0.690462
C	-1.418280	-1.642242	-0.682769	C	-1.390957	-1.695564	-0.690462
H	-0.839763	-3.200398	2.142255	H	-0.790896	-3.255282	2.148626
H	-0.839763	-3.200398	-2.142255	H	-0.790896	-3.255282	-2.148626
C	1.568432	-2.129481	0.000000	C	1.577352	-2.062202	0.000000
C	0.861393	-2.180407	-1.217987	C	0.870074	-2.165521	-1.220480
C	0.861393	-2.180407	1.217987	C	0.870074	-2.165521	1.220480
H	-1.889869	-0.909795	1.335480	H	-1.917920	-1.004569	1.352314
H	-1.889869	-0.909795	-1.335480	H	-1.917920	-1.004569	-1.352314
H	1.385572	-2.085817	2.165242	H	1.382276	-2.023136	2.174318
H	2.618050	-1.829682	0.000000	H	2.617666	-1.717139	0.000000
H	1.385572	-2.085817	-2.165242	H	1.382276	-2.023136	-2.174318
C	-0.578175	2.517534	1.173125	C	-0.572848	2.565321	1.174367
C	-0.578175	2.517534	-1.173125	C	-0.572848	2.565321	-1.174367
C	-1.450439	2.049731	0.000000	C	-1.468279	2.144514	0.000000
H	-2.407649	2.583666	0.000000	H	-2.400196	2.730636	0.000000
H	-1.669124	0.973810	0.000000	H	-1.736273	1.077504	0.000000
C	-0.222933	3.907132	0.674045	C	-0.137486	3.934292	0.677940
C	-0.222933	3.907132	-0.674045	C	-0.137486	3.934292	-0.677940
H	-1.087217	2.488991	2.141470	H	-1.084155	2.564245	2.147236
H	-1.087217	2.488991	-2.141470	H	-1.084155	2.564245	-2.147236
C	1.470232	1.664586	0.000000	C	1.437919	1.608503	0.000000
C	0.735815	1.710022	-1.209363	C	0.701020	1.698162	-1.210577
C	0.735815	1.710022	1.209363	C	0.701020	1.698162	1.210577
H	0.140078	4.708785	1.312457	H	0.274427	4.716732	1.319935
H	0.140078	4.708785	-1.312457	H	0.274427	4.716732	-1.319935
H	1.281362	1.682092	2.151879	H	1.240507	1.633061	2.160094
H	2.535480	1.424779	0.000000	H	2.503294	1.349223	0.000000
H	1.281362	1.682092	-2.151879	H	1.240507	1.633061	-2.160094
Cr	0.443529	-0.210611	0.000000	Cr	0.358898	-0.217724	0.000000

Table S19. Optimized coordinates for the**(bcod)$_2$Cr** structure **Cr-6P.**

	M06-L				OPBE		
	x	y	z		x	y	z
C	-0.675101	2.710475	1.001363	C	-0.685558	2.695209	1.021254
C	0.973351	2.821313	-0.684228	C	0.969296	2.844026	-0.658396
C	0.000000	3.734855	0.084316	C	0.000000	3.742270	0.137126
H	0.549394	4.470687	0.682577	H	0.557826	4.454096	0.764382
H	-0.699411	4.252355	-0.579416	H	-0.694944	4.291187	-0.512768
C	0.528806	1.889403	1.447056	C	0.494522	1.829739	1.437355
C	1.457159	1.903637	0.435616	C	1.439125	1.873313	0.422519
H	-1.259242	3.146078	1.816093	H	-1.274300	3.109451	1.850291
H	1.782999	3.353564	-1.190969	H	1.789554	3.387367	-1.146959
C	-1.063217	1.516102	-1.181134	C	-1.061487	1.530286	-1.187858
C	0.172201	1.951881	-1.628757	C	0.173373	2.000719	-1.629185
C	-1.464919	1.685325	0.185197	C	-1.464793	1.685953	0.181029
H	0.601245	1.345794	2.387973	H	0.579633	1.297888	2.388958
H	2.403734	1.367244	0.417925	H	2.407043	1.368152	0.410080
H	-2.493835	1.467125	0.466444	H	-2.484109	1.423727	0.475021
H	-1.687693	0.910751	-1.840633	H	-1.694031	0.949142	-1.866896
H	0.531531	1.719520	-2.627342	H	0.529652	1.809369	-2.642688
C	0.675101	-2.710475	1.001363	C	0.685558	-2.695209	1.021254
C	-0.973351	-2.821313	-0.684228	C	-0.969296	-2.844026	-0.658396
C	0.000000	-3.734855	0.084316	C	0.000000	-3.742270	0.137126
H	-0.549394	-4.470687	0.682577	H	-0.557826	-4.454096	0.764382
H	0.699411	-4.252355	-0.579416	H	0.694944	-4.291187	-0.512768
C	-0.528806	-1.889403	1.447056	C	-0.494522	-1.829739	1.437355
C	-1.457159	-1.903637	0.435616	C	-1.439125	-1.873313	0.422519
H	1.259242	-3.146078	1.816093	H	1.274300	-3.109451	1.850291
H	-1.782999	-3.353564	-1.190969	H	-1.789554	-3.387367	-1.146959
C	1.063217	-1.516102	-1.181134	C	1.061487	-1.530286	-1.187858
C	-0.172201	-1.951881	-1.628757	C	-0.173373	-2.000719	-1.629185
C	1.464919	-1.685325	0.185197	C	1.464793	-1.685953	0.181029
H	-0.601245	-1.345794	2.387973	H	-0.579633	-1.297888	2.388958
H	-2.403734	-1.367244	0.417925	H	-2.407043	-1.368152	0.410080
H	2.493835	-1.467125	0.466444	H	2.484109	-1.423727	0.475021
H	1.687693	-0.910751	-1.840633	H	1.694031	-0.949142	-1.866896
H	-0.531531	-1.719520	-2.627342	H	-0.529652	-1.809369	-2.642688
Cr	0.000000	0.000000	0.209231	Cr	0.000000	0.000000	0.161459

Table S20. Optimized coordinates for the**(bcod)$_2$Cr** structure **Cr-7T.**

	M06-L				OPBE		
	x	y	z		x	y	z
C	2.570134	-0.541189	1.058225	C	2.535341	-0.507938	1.073995
C	2.642777	-0.157710	-1.265854	C	2.650318	-0.178617	-1.259100
C	3.589421	-0.350279	-0.073406	C	3.576124	-0.339654	-0.044967
H	4.178170	-1.264500	-0.207681	H	4.168116	-1.261356	-0.149554
H	4.262841	0.499694	0.086943	H	4.249354	0.516398	0.109149
C	1.549851	-1.488114	0.398673	C	1.520159	-1.468425	0.419368
C	1.575490	-1.215471	-0.991508	C	1.572166	-1.221594	-0.980198
H	2.994521	-0.923976	1.991126	H	2.942864	-0.874926	2.026561
H	3.128707	-0.241887	-2.242942	H	3.156401	-0.278762	-2.229922
C	1.725596	1.671368	0.179865	C	1.670196	1.678532	0.128714
C	1.898647	1.163295	-1.109275	C	1.867861	1.121993	-1.144771
C	1.812472	0.771565	1.279873	C	1.771669	0.807533	1.260102
H	1.160668	-2.386005	0.868940	H	1.150339	-2.376807	0.895218
H	1.157748	-1.855391	-1.767202	H	1.167057	-1.880501	-1.752916
H	1.643624	1.139317	2.289691	H	1.608881	1.205577	2.264122
H	1.296702	2.662739	0.321395	H	1.252189	2.682884	0.236516
H	1.684521	1.782225	-1.977810	H	1.628270	1.700194	-2.041256
C	-2.288089	-1.306520	-0.045471	C	-2.253626	-1.311486	-0.084267
C	-2.421779	0.901855	-0.858422	C	-2.397800	0.919746	-0.840270
C	-1.890463	-0.476223	-1.278087	C	-1.852814	-0.443559	-1.291106
H	-2.398362	-0.840415	-2.177699	H	-2.352560	-0.788941	-2.208867
H	-0.809390	-0.514795	-1.559220	H	-0.761988	-0.470105	-1.574528
C	-3.687490	-0.770339	0.175052	C	-3.655647	-0.788342	0.153394
C	-3.763066	0.493720	-0.287232	C	-3.738488	0.493896	-0.279479
H	-2.219904	-2.386727	-0.204818	H	-2.181181	-2.391181	-0.273700
H	-2.463641	1.624641	-1.678183	H	-2.440148	1.667465	-1.643988
C	-1.356204	0.533768	1.392651	C	-1.330479	0.497635	1.412764
C	-1.531014	1.409789	0.290118	C	-1.518407	1.400861	0.327739
C	-1.410180	-0.861356	1.139173	C	-1.384983	-0.894362	1.117981
H	-4.445292	-1.279945	0.764429	H	-4.412393	-1.317840	0.737180
H	-4.593606	1.178150	-0.135446	H	-4.574580	1.175327	-0.105267
H	-1.268171	-1.560550	1.959704	H	-1.240324	-1.619773	1.920769
H	-0.992576	0.909167	2.347356	H	-1.002881	0.852525	2.392485
H	-1.471184	2.484458	0.454643	H	-1.459024	2.475941	0.514753
Cr	0.210750	0.096035	0.035022	Cr	0.204669	0.099440	0.044327

Table S21. Optimized coordinates for the**(bcod)$_2$Cr** structure **Cr-8S.**

	M06-L				OPBE		
	x	y	z		x	y	z
C	-2.601556	-0.127700	-1.127427	C	-2.603471	-0.189878	-1.114837
C	-2.069374	-0.336228	1.146038	C	-2.037101	-0.276535	1.163049
C	-3.299607	-0.157449	0.228300	C	-3.284921	-0.152847	0.250317
H	-3.957703	-1.029562	0.300726	H	-3.935432	-1.030531	0.376292
H	-3.867278	0.751886	0.452104	H	-3.861242	0.764257	0.435505
C	-1.603367	-1.263874	-0.996535	C	-1.581942	-1.298463	-0.937709
C	-1.324001	-1.498680	0.374068	C	-1.292875	-1.468758	0.445389
H	-3.290901	-0.179659	-1.978317	H	-3.301057	-0.285524	-1.960621
H	-2.262358	-0.661989	2.172187	H	-2.219410	-0.553101	2.210863
C	-1.343205	1.772797	-0.020416	C	-1.323975	1.769469	-0.120388
C	-1.335562	1.036526	1.206889	C	-1.318584	1.103984	1.148744
C	-1.668191	1.066140	-1.185044	C	-1.649102	0.981597	-1.242173
H	-1.330721	-1.930331	-1.810586	H	-1.303282	-2.001869	-1.723816
H	-1.096888	-2.439284	0.876639	H	-1.100002	-2.396277	0.992416
H	-1.402341	1.477465	-2.158477	H	-1.389327	1.332363	-2.245182
H	-0.842497	2.740029	-0.069108	H	-0.848096	2.748765	-0.225439
H	-1.189614	1.505717	2.180099	H	-1.193740	1.631058	2.099719
C	2.388809	-1.133141	-0.580974	C	2.361350	-1.161464	-0.548903
C	2.527756	1.126014	0.043406	C	2.534645	1.115371	0.008981
C	3.431416	-0.090822	-0.165451	C	3.421459	-0.118024	-0.178322
H	4.134055	0.095694	-0.986164	H	4.113004	0.040209	-1.020654
H	3.986688	-0.374806	0.734850	H	3.993389	-0.383927	0.722349
C	1.495191	-0.316691	-1.511957	C	1.438156	-0.373818	-1.475481
C	1.570508	1.003303	-1.132079	C	1.534088	0.970454	-1.124895
H	2.808132	-2.041034	-1.026057	H	2.765144	-2.092501	-0.972447
H	3.058039	2.080890	0.113985	H	3.076075	2.071515	0.045234
C	1.293646	-0.444498	1.599405	C	1.251859	-0.386047	1.614093
C	1.582136	0.883024	1.204494	C	1.573459	0.923210	1.166479
C	1.465814	-1.427980	0.594632	C	1.434790	-1.403109	0.634860
H	0.934316	-0.712259	-2.351505	H	0.930690	-0.772327	-2.352531
H	1.069964	1.839862	-1.610490	H	1.091481	1.806632	-1.665344
H	1.201500	-2.463276	0.800528	H	1.168644	-2.435248	0.872769
H	0.851849	-0.677328	2.570141	H	0.848446	-0.588369	2.613152
H	1.343872	1.712721	1.867766	H	1.343881	1.785997	1.796764
Cr	-0.133774	-0.009966	0.077399	Cr	-0.121924	0.006168	0.077739

Table S22. Optimized coordinates for the**(bcod)$_2$Cr** structure **Cr-9S.**

	M06-L				OPBE		
	x	y	z		x	y	z
C	0.000000	2.364819	-1.145628	C	0.000000	2.340708	-1.141515
C	0.816552	2.523315	1.061253	C	0.855146	2.520291	1.052488
C	0.758896	3.341019	-0.234498	C	0.780915	3.323472	-0.252228
H	0.165149	4.249544	-0.079911	H	0.188270	4.238219	-0.095919
H	1.749124	3.612681	-0.618652	H	1.768701	3.590333	-0.656862
C	-1.093316	1.847979	-0.212010	C	-1.079025	1.827431	-0.186626
C	-0.573293	1.896901	1.087868	C	-0.528169	1.884205	1.111097
H	-0.362957	2.808053	-2.078298	H	-0.380559	2.778727	-2.075166
H	1.087109	3.106593	1.948109	H	1.149082	3.110993	1.932530
C	1.885605	0.827701	-0.451730	C	1.873240	0.770742	-0.455365
C	1.701359	1.301872	0.858851	C	1.704517	1.276442	0.852181
C	0.870189	1.134719	-1.389205	C	0.848621	1.095690	-1.389963
H	-2.144129	1.793007	-0.478865	H	-2.142709	1.845482	-0.420888
H	-1.151331	1.716899	1.994868	H	-1.094339	1.728464	2.034766
H	0.940850	0.728166	-2.394621	H	0.931225	0.708711	-2.406233
H	2.690061	0.140382	-0.695843	H	2.702401	0.114723	-0.717909
H	2.366698	0.963856	1.653591	H	2.349207	0.915893	1.659939
C	0.000000	-2.364819	-1.145628	C	0.000000	-2.340708	-1.141515
C	-0.816552	-2.523315	1.061253	C	-0.855146	-2.520291	1.052488
C	-0.758896	-3.341019	-0.234498	C	-0.780915	-3.323472	-0.252228
H	-0.165149	-4.249544	-0.079911	H	-0.188270	-4.238219	-0.095919
H	-1.749124	-3.612681	-0.618652	H	-1.768701	-3.590333	-0.656862
C	1.093316	-1.847979	-0.212010	C	1.079025	-1.827431	-0.186626
C	0.573293	-1.896901	1.087868	C	0.528169	-1.884205	1.111097
H	0.362957	-2.808053	-2.078298	H	0.380559	-2.778727	-2.075166
H	-1.087109	-3.106593	1.948109	H	-1.149082	-3.110993	1.932530
C	-1.885605	-0.827701	-0.451730	C	-1.873240	-0.770742	-0.455365
C	-1.701359	-1.301872	0.858851	C	-1.704517	-1.276442	0.852181
C	-0.870189	-1.134719	-1.389205	C	-0.848621	-1.095690	-1.389963
H	2.144129	-1.793007	-0.478865	H	2.142709	-1.845482	-0.420888
H	1.151331	-1.716899	1.994868	H	1.094339	-1.728464	2.034766
H	-0.940850	-0.728166	-2.394621	H	-0.931225	-0.708711	-2.406233
H	-2.690061	-0.140382	-0.695843	H	-2.702401	-0.114723	-0.717909
H	-2.366698	-0.963856	1.653591	H	-2.349207	-0.915893	1.659939
Cr	0.000000	0.000000	0.275018	Cr	0.000000	0.000000	0.267111

Table S23. Optimized coordinates for the **(bcod)$_2$Mn** structure **Mn-1D.**

	M06-L				OPBE		
	x	y	z		x	y	z
C	0.000000	2.509721	1.179844	C	0.000000	2.517141	1.182008
C	0.000000	2.509721	-1.179844	C	0.000000	2.517141	-1.182008
C	-0.221909	3.462503	0.000000	C	-0.223141	3.468754	0.000000
H	0.542805	4.247941	0.000000	H	0.547152	4.255682	0.000000
H	-1.216277	3.923296	0.000000	H	-1.219842	3.934495	0.000000
C	1.177569	1.672712	0.698037	C	1.157062	1.651724	0.705174
C	1.177569	1.672712	-0.698037	C	1.157062	1.651724	-0.705174
H	0.142068	3.007513	2.143637	H	0.143930	3.015014	2.150707
H	0.142068	3.007513	-2.143637	H	0.143930	3.015014	-2.150707
C	-1.762045	1.151431	0.000000	C	-1.743484	1.118715	0.000000
C	-1.092712	1.453738	-1.206913	C	-1.069590	1.438648	-1.209649
C	-1.092712	1.453738	1.206913	C	-1.069590	1.438648	1.209649
H	1.966834	1.299083	1.344521	H	1.970599	1.321755	1.351044
H	1.966834	1.299083	-1.344521	H	1.970599	1.321755	-1.351044
H	-1.511057	1.127840	2.157076	H	-1.479096	1.108107	2.166676
H	-2.663471	0.538289	0.000000	H	-2.669900	0.539243	0.000000
H	-1.511057	1.127840	-2.157076	H	-1.479096	1.108107	-2.166676
C	0.000000	-2.509721	1.179844	C	0.000000	-2.517141	1.182008
C	0.000000	-2.509721	-1.179844	C	0.000000	-2.517141	-1.182008
C	0.221909	-3.462503	0.000000	C	0.223141	-3.468754	0.000000
H	-0.542805	-4.247941	0.000000	H	-0.547152	-4.255682	0.000000
H	1.216277	-3.923296	0.000000	H	1.219842	-3.934495	0.000000
C	-1.177569	-1.672712	0.698037	C	-1.157062	-1.651724	0.705174
C	-1.177569	-1.672712	-0.698037	C	-1.157062	-1.651724	-0.705174
H	-0.142068	-3.007513	2.143637	H	-0.143930	-3.015014	2.150707
H	-0.142068	-3.007513	-2.143637	H	-0.143930	-3.015014	-2.150707
C	1.762045	-1.151431	0.000000	C	1.743484	-1.118715	0.000000
C	1.092712	-1.453738	-1.206913	C	1.069590	-1.438648	-1.209649
C	1.092712	-1.453738	1.206913	C	1.069590	-1.438648	1.209649
H	-1.966834	-1.299083	1.344521	H	-1.970599	-1.321755	1.351044
H	-1.966834	-1.299083	-1.344521	H	-1.970599	-1.321755	-1.351044
H	1.511057	-1.127840	2.157076	H	1.479096	-1.108107	2.166676
H	2.663471	-0.538289	0.000000	H	2.669900	-0.539243	0.000000
H	1.511057	-1.127840	-2.157076	H	1.479096	-1.108107	-2.166676
Mn	0.000000	0.000000	0.000000	Mn	0.000000	0.000000	0.000000

Table S24. Optimized coordinates for the **(bcod)$_2$Mn** structure **Mn-2D.**

	M06-L				OPBE		
	x	y	z		x	y	z
C	-1.050026	2.378672	-0.838099	C	-1.122564	2.318340	-0.907771
C	-2.545690	0.925328	0.266842	C	-2.535200	0.920587	0.368694
C	-2.456483	2.374675	-0.226739	C	-2.488169	2.342532	-0.207154
H	-3.203541	2.555809	-1.008310	H	-3.286938	2.474221	-0.953669
H	-2.583426	3.110760	0.575704	H	-2.571901	3.125641	0.561100
C	-1.000008	1.024546	-1.528140	C	-1.094067	0.925362	-1.523071
C	-1.887359	0.151269	-0.876553	C	-1.931457	0.084131	-0.760620
H	-0.839713	3.236560	-1.483377	H	-0.955674	3.145514	-1.611366
H	-3.556175	0.597313	0.527489	H	-3.529183	0.598629	0.708626
C	-0.408522	1.556125	1.443804	C	-0.311167	1.596163	1.367379
C	-1.549760	0.716262	1.400372	C	-1.462190	0.754224	1.436707
C	0.000000	2.185304	0.247740	C	0.000000	2.169475	0.108544
H	-0.539624	0.872901	-2.498846	H	-0.743543	0.736736	-2.535764
H	-2.235010	-0.805257	-1.253752	H	-2.317433	-0.883678	-1.078149
H	0.931688	2.743657	0.214940	H	0.925226	2.734612	-0.016313
H	0.247494	1.544212	2.311057	H	0.380968	1.677268	2.206468
H	-1.844441	0.160235	2.286932	H	-1.709843	0.258764	2.376914
C	1.050026	-2.378672	-0.838099	C	1.122564	-2.318340	-0.907771
C	2.545690	-0.925328	0.266842	C	2.535200	-0.920587	0.368694
C	2.456483	-2.374675	-0.226739	C	2.488169	-2.342532	-0.207154
H	3.203541	-2.555809	-1.008310	H	3.286938	-2.474221	-0.953669
H	2.583426	-3.110760	0.575704	H	2.571901	-3.125641	0.561100
C	1.000008	-1.024546	-1.528140	C	1.094067	-0.925362	-1.523071
C	1.887359	-0.151269	-0.876553	C	1.931457	-0.084131	-0.760620
H	0.839713	-3.236560	-1.483377	H	0.955674	-3.145514	-1.611366
H	3.556175	-0.597313	0.527489	H	3.529183	-0.598629	0.708626
C	0.408522	-1.556125	1.443804	C	0.311167	-1.596163	1.367379
C	1.549760	-0.716262	1.400372	C	1.462190	-0.754224	1.436707
C	0.000000	-2.185304	0.247740	C	0.000000	-2.169475	0.108544
H	0.539624	-0.872901	-2.498846	H	0.743543	-0.736736	-2.535764
H	2.235010	0.805257	-1.253752	H	2.317433	0.883678	-1.078149
H	-0.931688	-2.743657	0.214940	H	-0.925226	-2.734612	-0.016313
H	-0.247494	-1.544212	2.311057	H	-0.380968	-1.677268	2.206468
H	1.844441	-0.160235	2.286932	H	1.709843	-0.258764	2.376914
Mn	0.000000	0.000000	0.079424	Mn	0.000000	0.000000	0.083672

Table S25. Optimized coordinates for the**(bcod)$_2$Mn** structure **Mn-3Q.**

	M06-L				OPBE		
	x	y	z		x	y	z
C	2.630300	-0.501621	1.152647	C	2.654806	-0.516470	1.133974
C	2.735196	0.144141	-1.109586	C	2.729585	0.180020	-1.118455
C	3.629499	0.073878	0.137474	C	3.641162	0.076094	0.114707
H	4.453730	-0.629713	-0.024729	H	4.458930	-0.635040	-0.076995
H	4.031039	1.047823	0.433956	H	4.058501	1.042983	0.426754
C	1.956598	-1.565677	0.297485	C	1.938954	-1.545987	0.272239
C	2.011490	-1.194027	-1.001783	C	1.972211	-1.139146	-1.031506
H	3.087740	-0.882616	2.069870	H	3.125907	-0.925847	2.037936
H	3.278623	0.288203	-2.047430	H	3.261320	0.340313	-2.066140
C	1.354474	1.536701	0.455069	C	1.335184	1.517967	0.489961
C	1.669633	1.220246	-0.894560	C	1.658328	1.236125	-0.867815
C	1.560542	0.550132	1.443051	C	1.578717	0.515413	1.460987
H	1.396168	-2.403949	0.704986	H	1.403346	-2.407203	0.673901
H	1.509441	-1.683628	-1.833307	H	1.468506	-1.614008	-1.876221
H	1.252567	0.733754	2.468699	H	1.274572	0.671115	2.497499
H	0.758890	2.420096	0.684116	H	0.739206	2.397569	0.746264
H	1.487193	1.953909	-1.676593	H	1.437684	1.971600	-1.644209
C	-2.413016	-0.814167	-1.054333	C	-2.392127	-0.843153	-1.046364
C	-2.693294	-0.037221	1.151579	C	-2.733470	0.022128	1.119120
C	-3.527291	-0.557221	-0.039183	C	-3.536782	-0.543483	-0.076375
H	-4.018249	-1.503085	0.216745	H	-4.036739	-1.483702	0.202054
H	-4.279704	0.165939	-0.373340	H	-4.281193	0.169076	-0.459874
C	-1.376729	-1.536800	-0.192058	C	-1.382735	-1.536787	-0.132455
C	-1.476161	-0.979408	1.111427	C	-1.510079	-0.914482	1.145496
H	-2.726782	-1.360243	-1.948292	H	-2.682366	-1.415995	-1.937659
H	-3.221626	-0.071186	2.109067	H	-3.288211	0.016564	2.067954
C	-1.840091	1.596580	-0.480933	C	-1.799574	1.583868	-0.538499
C	-2.248934	1.370641	0.807119	C	-2.287935	1.418138	0.738095
C	-1.673265	0.489938	-1.403219	C	-1.607388	0.431856	-1.404965
H	-0.881297	-2.467161	-0.463514	H	-0.921361	-2.504121	-0.342408
H	-1.064484	-1.422281	2.015249	H	-1.131626	-1.325919	2.083181
H	-1.482310	0.718145	-2.450144	H	-1.361652	0.613315	-2.454792
H	-1.505160	2.590053	-0.782933	H	-1.468128	2.569887	-0.880252
H	-2.276472	2.168947	1.544850	H	-2.369660	2.254742	1.435986
Mn	-0.063720	0.062412	-0.117137	Mn	-0.049607	0.024483	-0.079274

Table S26. Optimized coordinates for the**(bcod)$_2$Mn** structure **Mn-4Q.**

	M06-L				OPBE		
	x	y	z		x	y	z
C	2.587963	0.784646	-0.889712	C	2.531143	0.876184	-0.829939
C	2.564191	-0.120713	1.286583	C	2.612743	-0.281941	1.223010
C	3.559933	0.335645	0.208671	C	3.556079	0.316768	0.164743
H	4.143263	1.190923	0.567120	H	4.140907	1.141210	0.599586
H	4.238052	-0.462446	-0.109729	H	4.236591	-0.427077	-0.272663
C	1.541201	1.516711	-0.056964	C	1.502948	1.492724	0.114834
C	1.514337	0.985013	1.202636	C	1.524381	0.788002	1.313020
H	3.043928	1.390402	-1.676941	H	2.946858	1.572108	-1.570844
H	2.999710	-0.252103	2.280518	H	3.094123	-0.514202	2.182576
C	1.710892	-1.543158	-0.578854	C	1.641174	-1.482334	-0.743963
C	1.866105	-1.370800	0.794419	C	1.911350	-1.482071	0.626074
C	1.830350	-0.420467	-1.448016	C	1.729350	-0.254406	-1.477801
H	0.898959	2.306286	-0.435391	H	0.930572	2.394694	-0.095418
H	0.841679	1.260591	2.009250	H	0.967710	1.022831	2.219384
H	1.746887	-0.557169	-2.523149	H	1.569680	-0.257571	-2.558219
H	1.284630	-2.472142	-0.957648	H	1.205740	-2.368221	-1.215922
H	1.605566	-2.166805	1.487476	H	1.696407	-2.360757	1.238030
C	-2.544272	-0.900756	-0.716622	C	-2.493063	-0.923387	-0.758457
C	-2.525763	0.492863	1.181473	C	-2.600540	0.440917	1.161064
C	-3.523358	-0.231897	0.247897	C	-3.534119	-0.294360	0.170346
H	-4.080914	-1.000024	0.796172	H	-4.095687	-1.089709	0.683726
H	-4.227415	0.458257	-0.230804	H	-4.236468	0.385758	-0.332706
C	-1.528892	-1.506741	0.257296	C	-1.484459	-1.483823	0.245041
C	-1.418864	-0.569934	1.328345	C	-1.468652	-0.585438	1.343696
H	-2.998076	-1.616523	-1.407739	H	-2.893977	-1.657947	-1.470053
H	-2.957959	0.780003	2.145225	H	-3.086236	0.709297	2.109835
C	-1.678942	1.493133	-0.890007	C	-1.639214	1.475497	-0.857619
C	-2.008629	1.695576	0.420855	C	-2.051778	1.655728	0.446576
C	-1.697233	0.155655	-1.461447	C	-1.639711	0.151596	-1.455462
H	-1.235252	-2.554816	0.284584	H	-1.098042	-2.504571	0.238307
H	-0.991237	-0.805139	2.301230	H	-1.042163	-0.804486	2.323625
H	-1.600390	0.064488	-2.542481	H	-1.474197	0.070751	-2.533285
H	-1.302167	2.317873	-1.496818	H	-1.246627	2.318349	-1.435620
H	-1.923124	2.673507	0.889005	H	-1.983197	2.627528	0.940794
Mn	-0.039210	-0.212953	-0.267968	Mn	-0.008711	-0.108636	-0.206484

Table S27. Optimized coordinates for the**(bcod)$_2$Mn** structure **Mn-5X.**

	M06-L				OPBE		
	x	y	z		x	y	z
C	0.010867	2.777665	-1.335819	C	0.000000	2.940224	-1.265239
C	0.000000	2.933111	1.020988	C	-0.052256	2.909213	1.098741
C	-0.242544	3.804216	-0.218905	C	-0.276178	3.875531	-0.074320
H	0.495285	4.612604	-0.269534	H	0.467069	4.686297	-0.047727
H	-1.250586	4.228363	-0.257349	H	-1.286665	4.305361	-0.096102
C	1.217141	2.036548	-0.782107	C	1.186822	2.141581	-0.755550
C	1.224967	2.143789	0.574872	C	1.166688	2.133812	0.619951
H	0.171354	3.216203	-2.324446	H	0.178096	3.456378	-2.218317
H	0.138790	3.496125	1.947610	H	0.069400	3.397961	2.074439
C	-1.665373	1.439666	-0.098238	C	-1.668244	1.466696	-0.161562
C	-1.081672	1.857276	1.148735	C	-1.115576	1.814412	1.118102
C	-1.112522	1.766228	-1.327184	C	-1.098186	1.907829	-1.357846
H	1.872246	1.410467	-1.385110	H	1.862891	1.580108	-1.403848
H	1.931028	1.673464	1.260300	H	1.886757	1.650327	1.287355
H	-1.471153	1.316967	-2.249732	H	-1.441240	1.534846	-2.324643
H	-2.522688	0.760842	-0.069281	H	-2.528846	0.788077	-0.199687
H	-1.699293	1.835388	2.045256	H	-1.717947	1.664998	2.018634
C	-0.010867	-2.777665	-1.335819	C	0.000000	-2.940224	-1.265239
C	0.000000	-2.933111	1.020988	C	0.052256	-2.909213	1.098741
C	0.242544	-3.804216	-0.218905	C	0.276178	-3.875531	-0.074320
H	-0.495285	-4.612604	-0.269534	H	-0.467069	-4.686297	-0.047727
H	1.250586	-4.228363	-0.257349	H	1.286665	-4.305361	-0.096102
C	-1.217141	-2.036548	-0.782107	C	-1.186822	-2.141581	-0.755550
C	-1.224967	-2.143789	0.574872	C	-1.166688	-2.133812	0.619951
H	-0.171354	-3.216203	-2.324446	H	-0.178096	-3.456378	-2.218317
H	-0.138790	-3.496125	1.947610	H	-0.069400	-3.397961	2.074439
C	1.665373	-1.439666	-0.098238	C	1.668244	-1.466696	-0.161562
C	1.081672	-1.857276	1.148735	C	1.115576	-1.814412	1.118102
C	1.112522	-1.766228	-1.327184	C	1.098186	-1.907829	-1.357846
H	-1.872246	-1.410467	-1.385110	H	-1.862891	-1.580108	-1.403848
H	-1.931028	-1.673464	1.260300	H	-1.886757	-1.650327	1.287355
H	1.471153	-1.316967	-2.249732	H	1.441240	-1.534846	-2.324643
H	2.522688	-0.760842	-0.069281	H	2.528846	-0.788077	-0.199687
H	1.699293	-1.835388	2.045256	H	1.717947	-1.664998	2.018634
Mn	0.000000	0.000000	0.592658	Mn	0.000000	0.000000	0.446099

Table S28. Optimized coordinates for the**(bcod)$_2$Mn** structure **Mn-6Q.**

	M06-L				OPBE		
	x	y	z		x	y	z
C	2.611613	0.494977	-1.110978	C	2.601217	0.529780	-1.102593
C	2.418773	-1.233259	0.464309	C	2.417136	-1.250703	0.416097
C	2.197966	-0.982273	-1.035460	C	2.201538	-0.952595	-1.076719
H	2.877471	-1.602704	-1.630637	H	2.892118	-1.551118	-1.690504
H	1.174652	-1.180377	-1.385140	H	1.176861	-1.140671	-1.434667
C	3.880563	0.434254	-0.276874	C	3.868155	0.459250	-0.264208
C	3.770805	-0.557734	0.626671	C	3.762304	-0.567710	0.611949
H	2.747003	0.863872	-2.131722	H	2.735317	0.936264	-2.114614
H	2.393608	-2.291105	0.743079	H	2.401125	-2.321785	0.661681
C	1.335719	0.973903	1.008173	C	1.319511	0.936628	1.037230
C	1.399085	-0.419070	1.286459	C	1.392791	-0.469768	1.266427
C	1.588430	1.357191	-0.341731	C	1.571680	1.357205	-0.304683
H	4.671975	1.178218	-0.316265	H	4.654726	1.217491	-0.274090
H	4.456601	-0.755474	1.446401	H	4.446844	-0.784430	1.435452
H	1.533128	2.414316	-0.599163	H	1.499610	2.423146	-0.539734
H	0.935113	1.679737	1.735395	H	0.951816	1.626004	1.802385
H	1.188435	-0.759832	2.298570	H	1.187300	-0.848486	2.270891
C	-2.608566	-0.153111	-1.294936	C	-2.598745	-0.142819	-1.305719
C	-2.755666	-0.680109	0.997717	C	-2.762025	-0.674226	0.987133
C	-3.660593	-0.482024	-0.232015	C	-3.659628	-0.467742	-0.247829
H	-4.168097	-1.418815	-0.487438	H	-4.168190	-1.407647	-0.509739
H	-4.403916	0.309536	-0.087469	H	-4.404874	0.328003	-0.106743
C	-1.532214	-1.196937	-0.986206	C	-1.519560	-1.180642	-0.990769
C	-1.583215	-1.464585	0.396711	C	-1.582672	-1.457048	0.397161
H	-2.979333	-0.174024	-2.323077	H	-2.964312	-0.161214	-2.341206
H	-3.240495	-1.194560	1.832152	H	-3.255909	-1.187064	1.823836
C	-1.947479	1.593829	0.410082	C	-1.914218	1.598090	0.402061
C	-2.218802	0.679619	1.407988	C	-2.198877	0.673968	1.401643
C	-1.899330	1.166104	-0.962068	C	-1.875244	1.166647	-0.969357
H	-0.999717	-1.777577	-1.736242	H	-0.998042	-1.774423	-1.744470
H	-1.091435	-2.284434	0.910968	H	-1.108786	-2.293927	0.910357
H	-1.751625	1.907550	-1.743274	H	-1.686341	1.898259	-1.757834
H	-1.582146	2.587484	0.671484	H	-1.551486	2.596187	0.667266
H	-2.110405	0.943584	2.457070	H	-2.096447	0.937091	2.456944
Mn	-0.225334	0.174798	-0.072070	Mn	-0.234060	0.166337	-0.042486

Table S29. Optimized coordinates for the**(bcod)$_2$Mn** structure **Mn-7X.**

	M06-L				OPBE		
	x	y	z		x	y	z
C	-2.664743	0.646013	1.201208	C	3.085777	0.456878	-0.973384
C	-2.779270	0.461825	-1.151182	C	2.617482	0.416971	1.345045
C	-3.690435	0.708575	0.058468	C	3.810841	0.500267	0.381400
H	-4.136805	1.707402	0.001032	H	4.329934	1.462629	0.502769
H	-4.482865	-0.039001	0.160518	H	4.527934	-0.321580	0.509680
C	-1.490011	1.392674	0.586448	C	1.870320	1.325615	-0.703232
C	-1.569026	1.301581	-0.773925	C	1.599827	1.309439	0.652282
H	-3.016134	1.061784	2.148849	H	3.696134	0.773650	-1.829188
H	-3.227920	0.715382	-2.114905	H	2.846943	0.695937	2.381585
C	-2.091578	-1.541673	0.174870	C	1.998617	-1.582467	-0.030559
C	-2.211065	-0.953831	-1.119580	C	1.926251	-0.930753	1.231844
C	-2.166535	-0.775911	1.337372	C	2.444500	-0.898310	-1.175740
H	-0.659354	1.801774	1.160630	H	1.284883	1.821410	-1.480729
H	-0.836854	1.667260	-1.493320	H	0.777503	1.820413	1.159951
H	-1.948499	-1.203549	2.311937	H	2.412631	-1.364893	-2.162041
H	-1.798836	-2.591914	0.250264	H	1.603909	-2.601113	-0.133317
H	-2.299152	-1.593150	-1.994512	H	1.648616	-1.488083	2.128951
C	2.818473	-0.648564	-0.895652	C	-2.748634	-1.186842	0.028762
C	2.874586	1.179934	0.596009	C	-3.144986	1.111087	0.409734
C	3.822351	0.169055	-0.071983	C	-3.903307	-0.172333	0.022307
H	4.529447	0.685647	-0.730669	H	-4.641400	-0.426341	0.797788
H	4.375802	-0.432615	0.655697	H	-4.406680	-0.091746	-0.950718
C	1.920821	0.462201	-1.427462	C	-1.977712	-0.745624	1.266732
C	1.939262	1.505127	-0.557758	C	-2.208904	0.584740	1.485267
H	3.273573	-1.269425	-1.672259	H	-3.070414	-2.237246	0.045756
H	3.376364	2.053392	1.022252	H	-3.791544	1.936106	0.739998
C	1.650164	-0.847273	1.311130	C	-1.665751	0.493672	-1.486511
C	2.032089	0.445221	1.612682	C	-2.244919	1.509101	-0.737770
C	1.885604	-1.452919	0.016384	C	-1.760757	-0.902912	-1.106293
H	1.310300	0.373349	-2.327178	H	-1.343893	-1.403909	1.868157
H	1.291184	2.380164	-0.583415	H	-1.708705	1.216101	2.223694
H	1.938860	-2.541393	-0.026092	H	-1.653082	-1.649895	-1.900925
H	1.091218	-1.418493	2.057132	H	-1.092389	0.754287	-2.385241
H	1.719846	0.927282	2.536016	H	-2.061544	2.561156	-0.967942
Mn	-0.087372	-0.583844	-0.269766	Mn	0.097972	-0.367522	-0.168301

Table S30. Optimized coordinates for the**(bcod)$_2$Mn** structure **Mn-8X.**

	M06-L				OPBE		
	x	y	z		x	y	z
C	3.049732	0.295321	-1.006831	C	3.085767	0.456873	-0.973384
C	2.457584	0.748657	1.235764	C	2.617482	0.416961	1.345046
C	3.696627	0.680944	0.332715	C	3.810837	0.500253	0.381397
H	4.166919	1.667517	0.257610	H	4.329937	1.462611	0.502767
H	4.436233	-0.050242	0.672642	H	4.527926	-0.321600	0.509670
C	1.797460	1.156642	-0.987258	C	1.870320	1.325624	-0.703223
C	1.461608	1.430830	0.308326	C	1.599833	1.309443	0.652291
H	3.690613	0.446491	-1.879098	H	3.696123	0.773642	-1.829190
H	2.619128	1.260462	2.187725	H	2.846950	0.695924	2.381585
C	2.061597	-1.548994	0.337153	C	1.998604	-1.582471	-0.030558
C	1.849925	-0.637211	1.406670	C	1.926246	-0.930760	1.231846
C	2.512267	-1.117516	-0.914655	C	2.444480	-0.898311	-1.175741
H	1.209157	1.401051	-1.870341	H	1.284883	1.821426	-1.480716
H	0.560506	1.946297	0.641581	H	0.777512	1.820418	1.159966
H	2.580210	-1.800509	-1.756164	H	2.412613	-1.364896	-2.162042
H	1.741067	-2.586921	0.456077	H	1.603887	-2.601113	-0.133317
H	1.598001	-1.006720	2.397691	H	1.648609	-1.488089	2.128952
C	-2.823781	-1.094610	0.231805	C	-2.748636	-1.186841	0.028734
C	-2.942563	1.262832	0.221183	C	-3.144974	1.111081	0.409761
C	-3.850415	0.032194	0.049796	C	-3.903303	-0.172326	0.022305
H	-4.602358	-0.000758	0.846089	H	-4.641397	-0.426347	0.797781
H	-4.349890	0.009149	-0.923915	H	-4.406677	-0.091713	-0.950717
C	-2.010313	-0.543184	1.395283	C	-1.977708	-0.745656	1.266713
C	-2.068901	0.810415	1.381822	C	-2.208893	0.584704	1.485280
H	-3.265396	-2.077571	0.419020	H	-3.070421	-2.237244	0.045704
H	-3.481795	2.196535	0.405752	H	-3.791528	1.936095	0.740045
C	-1.616663	0.169828	-1.560218	C	-1.665743	0.493701	-1.486499
C	-2.039428	1.353303	-0.988889	C	-2.244905	1.509117	-0.737734
C	-1.833739	-1.122901	-0.939913	C	-1.760760	-0.902890	-1.106315
H	-1.405023	-1.156341	2.062712	H	-1.343890	-1.403959	1.868120
H	-1.478725	1.483603	2.001029	H	-1.708687	1.216045	2.223719
H	-1.847298	-1.991922	-1.598853	H	-1.653082	-1.649857	-1.900961
H	-1.035254	0.207415	-2.486200	H	-1.092384	0.754335	-2.385226
H	-1.741296	2.317074	-1.396030	H	-2.061517	2.561176	-0.967877
Mn	0.095969	-0.540957	-0.138154	Mn	0.097971	-0.367514	-0.168311

Table S31. Optimized coordinates for the**(bcod)$_2$Mn** structure **Mn-9X.**

	M06-L				OPBE		
	x	y	z		x	y	z
C	-3.039862	1.114961	0.594951	C	-3.401620	0.772378	0.871471
C	-2.563670	-1.190151	0.383763	C	-2.458630	-1.238918	0.062412
C	-2.373137	-0.026881	1.372210	C	-2.530954	-0.397822	1.349934
H	-2.908188	-0.222715	2.307746	H	-3.042095	-0.959579	2.145977
H	-1.318772	0.177124	1.624026	H	-1.547682	-0.073220	1.726894
C	-4.259193	0.389996	0.046411	C	-4.434140	0.027858	0.037485
C	-3.981785	-0.924021	-0.069043	C	-3.891265	-1.127475	-0.415568
H	-3.261496	1.998947	1.200878	H	-3.816789	1.385789	1.683934
H	-2.409362	-2.174828	0.838892	H	-2.122263	-2.272903	0.234936
C	-1.634093	0.401321	-1.320543	C	-1.819067	0.935735	-1.036184
C	-1.617563	-0.975618	-0.815156	C	-1.552543	-0.513208	-0.957329
C	-2.206145	1.442672	-0.629330	C	-2.625618	1.593151	-0.142133
H	-5.135102	0.898189	-0.349451	H	-5.389633	0.457696	-0.273341
H	-4.604482	-1.659583	-0.573233	H	-4.340249	-1.793017	-1.157425
H	-2.172178	2.458489	-1.016274	H	-2.795249	2.670145	-0.221252
H	-1.189271	0.600248	-2.299952	H	-1.389893	1.498673	-1.875402
H	-1.671205	-1.741532	-1.596179	H	-1.526501	-0.995386	-1.950003
C	3.009877	-0.706767	1.045854	C	3.005007	-0.758955	1.128354
C	3.189415	0.697771	-0.847000	C	3.375235	0.454799	-0.869205
C	3.995137	0.268154	0.388270	C	4.114324	0.018683	0.404862
H	4.906002	-0.258848	0.084495	H	4.944529	-0.655960	0.148763
H	4.259747	1.110351	1.034432	H	4.497165	0.865636	0.989792
C	2.473821	-1.444092	-0.172392	C	2.342415	-1.495954	-0.024248
C	2.565830	-0.625655	-1.265863	C	2.557213	-0.784698	-1.191521
H	3.450359	-1.350419	1.810708	H	3.354052	-1.400860	1.947144
H	3.779067	1.186442	-1.626168	H	4.026644	0.801596	-1.681504
C	1.448581	1.234489	0.846259	C	1.685717	1.335267	0.750981
C	1.997463	1.522610	-0.407891	C	2.276207	1.441325	-0.528058
C	1.776023	0.037357	1.537613	C	1.885410	0.177767	1.544207
H	2.002999	-2.425744	-0.131647	H	1.758163	-2.414165	0.089460
H	2.165387	-0.821916	-2.259772	H	2.168418	-1.020351	-2.186674
H	1.393915	-0.138024	2.540026	H	1.422973	0.088681	2.529197
H	0.629483	1.855130	1.218207	H	0.954492	2.087858	1.069262
H	1.665734	2.382841	-0.981990	H	2.084370	2.307549	-1.164187
Mn	0.309327	-0.366841	-0.238137	Mn	0.383736	-0.128711	-0.318733

Table S32. Optimized coordinates for the **(bcod)$_2$Mn** structure **Mn-10X.**

	M06-L				OPBE		
	x	y	z		x	y	z
C	-2.501279	-0.731010	-0.970643	C	2.529261	-1.127984	0.387646
C	-3.008095	1.339655	0.049099	C	3.202755	1.123980	0.646112
C	-2.262665	0.775816	-1.167101	C	2.446097	0.024625	1.404900
H	-2.718025	1.122700	-2.101173	H	2.978529	-0.241752	2.330066
H	-1.197676	1.060970	-1.179424	H	1.415330	0.314555	1.667558
C	-3.953159	-0.717787	-0.547196	C	3.961679	-0.974942	-0.078820
C	-4.247422	0.458873	0.038699	C	4.350292	0.315782	0.058411
H	-2.298804	-1.322612	-1.871154	H	2.299273	-2.112474	0.822917
H	-3.206365	2.414639	-0.007335	H	3.507125	1.975057	1.271981
C	-1.703369	-0.298643	1.370784	C	1.713963	0.583270	-1.269119
C	-2.257131	0.951234	1.308789	C	2.394780	1.548933	-0.566094
C	-1.643548	-1.212634	0.218210	C	1.603090	-0.809149	-0.806259
H	-4.595353	-1.595439	-0.562330	H	4.516368	-1.752841	-0.609845
H	-5.160280	0.695908	0.579695	H	5.264964	0.760583	-0.341306
H	-1.795761	-2.264705	0.488518	H	1.650739	-1.545845	-1.625228
H	-1.298893	-0.648504	2.325047	H	1.286483	0.843730	-2.246377
H	-2.260684	1.608381	2.175419	H	2.453868	2.577188	-0.932293
C	2.992148	0.080434	-1.278263	C	-2.718985	0.665062	1.323542
C	2.751769	1.130169	0.825589	C	-3.327976	0.267846	-0.927800
C	3.819721	0.852570	-0.241440	C	-3.968843	0.561275	0.437188
H	4.182555	1.793209	-0.669314	H	-4.493136	1.527904	0.408534
H	4.666556	0.276776	0.143551	H	-4.664529	-0.223498	0.762988
C	1.693216	0.871870	-1.262338	C	-1.757466	1.414732	0.415031
C	1.551131	1.479020	-0.042520	C	-2.112138	1.179250	-0.900702
H	3.460734	-0.004888	-2.261322	H	-2.888370	1.132005	2.302170
H	3.023779	1.898766	1.552436	H	-3.994244	0.412989	-1.787785
C	2.419392	-1.337056	0.693106	C	-2.175054	-1.565233	0.323551
C	2.332606	-0.173981	1.478928	C	-2.667492	-1.096778	-0.915123
C	2.566869	-1.263047	-0.709572	C	-2.026181	-0.682021	1.422141
H	0.964157	0.858433	-2.072406	H	-0.900299	1.996320	0.766051
H	0.675372	2.019771	0.317020	H	-1.591491	1.536592	-1.793385
H	2.635910	-2.165773	-1.309121	H	-1.635412	-1.039498	2.376973
H	2.208980	-2.305414	1.153198	H	-1.779779	-2.586376	0.395371
H	2.167973	-0.232296	2.550787	H	-2.736795	-1.760461	-1.779219
Mn	0.369789	-0.657713	0.086525	Mn	-0.375012	-0.415442	-0.308672

Table S33. Optimized coordinates for the**(bcod)$_2$Mn** structure **Mn-11X.**

	M06-L				OPBE		
	x	y	z		x	y	z
C	-2.478274	-1.023275	0.711000	C	-2.524049	-1.102736	0.586880
C	-2.168707	1.263641	0.173943	C	-2.307201	1.249309	0.369775
C	-2.112977	0.309877	1.373113	C	-2.293069	0.150882	1.441482
H	-1.097258	0.265644	1.798727	H	-1.315161	0.105872	1.949933
H	-2.806376	0.592324	2.171106	H	-3.072949	0.293388	2.201740
C	-1.658982	-0.962503	-0.593296	C	-1.627221	-0.831766	-0.635958
C	-1.477393	0.432213	-0.925164	C	-1.496248	0.603378	-0.769425
H	-2.274718	-1.897144	1.337870	H	-2.319265	-2.045626	1.113475
H	-1.713090	2.242728	0.361422	H	-1.928893	2.220788	0.718700
C	-4.379792	0.227383	-0.285022	C	-4.413611	0.174156	-0.416104
C	-3.574664	1.366301	-0.322061	C	-3.670449	1.346581	-0.241374
C	-3.893805	-0.972674	0.229499	C	-3.895442	-1.060546	-0.014261
H	-1.879682	-1.698723	-1.372267	H	-1.752152	-1.472175	-1.519994
H	-1.555646	0.781356	-1.959438	H	-1.518683	1.085028	-1.756571
H	-4.480141	-1.886920	0.166090	H	-4.421990	-1.991609	-0.238936
H	-5.384539	0.266487	-0.702872	H	-5.385144	0.217779	-0.918006
H	-3.909670	2.271777	-0.823723	H	-4.019453	2.299380	-0.647612
C	3.189038	0.522409	-0.959891	C	3.273765	0.286654	-1.046300
C	2.731469	0.406870	1.355483	C	2.879713	0.474934	1.279265
C	3.918799	0.529583	0.390691	C	4.042304	0.378433	0.280321
H	4.431598	1.485831	0.540414	H	4.641378	1.300709	0.307069
H	4.637351	-0.289467	0.491322	H	4.693852	-0.487210	0.460485
C	1.986069	1.399656	-0.645992	C	2.142171	1.274534	-0.818017
C	1.721852	1.332523	0.693157	C	1.912063	1.385163	0.540926
H	3.793386	0.863620	-1.803725	H	3.880040	0.475913	-1.941397
H	2.963676	0.653066	2.394280	H	3.164461	0.817970	2.282154
C	2.208052	-1.584821	-0.054143	C	2.076322	-1.584869	0.105329
C	2.086411	-0.961752	1.205779	C	2.089367	-0.820625	1.297928
C	2.567938	-0.844828	-1.198854	C	2.501495	-1.017110	-1.118323
H	1.371394	1.890141	-1.398842	H	1.575690	1.758663	-1.618018
H	0.862423	1.765675	1.203763	H	1.132734	1.979413	1.025415
H	2.642566	-1.325618	-2.169919	H	2.452347	-1.587679	-2.047863
H	1.850388	-2.610206	-0.174990	H	1.600701	-2.573937	0.104088
H	1.787221	-1.532931	2.080035	H	1.742984	-1.249934	2.240147
Mn	0.350836	-0.419251	-0.361148	Mn	0.348402	-0.263399	-0.270707

Table S34. Optimized coordinates for the **(bcod)$_2$Fe**structure**Fe-1S.**

	M06-L				OPBE		
	x	y	z		x	y	z
C	0.836314	2.456376	-0.788547	C	-1.204396	2.206081	-1.002137
C	-1.300323	2.372242	0.210060	C	-2.506019	0.950361	0.513420
C	-0.239417	3.389865	-0.222731	C	-2.497185	2.313951	-0.185215
H	-0.630952	4.032817	-1.019864	H	-3.362927	2.396422	-0.861167
H	0.117122	4.013757	0.605025	H	-2.498694	3.162102	0.515660
C	0.000000	1.412742	-1.501353	C	-1.228237	0.759252	-1.480654
C	-1.272400	1.353311	-0.926006	C	-1.996667	0.011476	-0.573072
H	1.588718	2.955273	-1.406499	H	-1.093887	2.966368	-1.787759
H	-2.280316	2.803802	0.433523	H	-3.466814	0.675301	0.970082
C	0.653565	1.385245	1.463068	C	-0.177409	1.637288	1.240442
C	-0.748065	1.527139	1.341754	C	-1.326003	0.819326	1.458977
C	1.434957	1.585859	0.304769	C	0.000000	2.109442	-0.085245
H	0.314505	0.949317	-2.431194	H	-0.960454	0.453870	-2.490854
H	-2.145902	0.855358	-1.335991	H	-2.402602	-0.984040	-0.750043
H	2.503917	1.383358	0.323547	H	0.912521	2.650999	-0.346758
H	1.086941	0.932224	2.353559	H	0.585629	1.788960	2.007505
H	-1.391020	1.268473	2.181465	H	-1.474630	0.351278	2.435707
C	-0.836314	-2.456376	-0.788547	C	1.204396	-2.206081	-1.002137
C	1.300323	-2.372242	0.210060	C	2.506019	-0.950361	0.513420
C	0.239417	-3.389865	-0.222731	C	2.497185	-2.313951	-0.185215
H	0.630952	-4.032817	-1.019864	H	3.362927	-2.396422	-0.861167
H	-0.117122	-4.013757	0.605025	H	2.498694	-3.162102	0.515660
C	0.000000	-1.412742	-1.501353	C	1.228237	-0.759252	-1.480654
C	1.272400	-1.353311	-0.926006	C	1.996667	-0.011476	-0.573072
H	-1.588718	-2.955273	-1.406499	H	1.093887	-2.966368	-1.787759
H	2.280316	-2.803802	0.433523	H	3.466814	-0.675301	0.970082
C	-0.653565	-1.385245	1.463068	C	0.177409	-1.637288	1.240442
C	0.748065	-1.527139	1.341754	C	1.326003	-0.819326	1.458977
C	-1.434957	-1.585859	0.304769	C	0.000000	-2.109442	-0.085245
H	-0.314505	-0.949317	-2.431194	H	0.960454	-0.453870	-2.490854
H	2.145902	-0.855358	-1.335991	H	2.402602	0.984040	-0.750043
H	-2.503917	-1.383358	0.323547	H	-0.912521	-2.650999	-0.346758
H	-1.086941	-0.932224	2.353559	H	-0.585629	-1.788960	2.007505
H	1.391020	-1.268473	2.181465	H	1.474630	-0.351278	2.435707
Fe	0.000000	0.000000	0.077719	Fe	0.000000	0.000000	0.076040

Table S35. Optimized coordinates for the**(bcod)$_2$Fe**structure **Fe-2S.**

	M06-L				OPBE		
	x	y	z		x	y	z
C	0.000000	2.470520	1.183139	C	0.000000	2.482530	1.184761
C	0.000000	2.470520	-1.183139	C	0.000000	2.482530	-1.184761
C	-0.242029	3.416001	0.000000	C	-0.236622	3.428039	0.000000
H	0.505164	4.218406	0.000000	H	0.522239	4.226275	0.000000
H	-1.246026	3.855191	0.000000	H	-1.239745	3.879927	0.000000
C	1.177155	1.644780	0.695758	C	1.149121	1.616331	0.703709
C	1.177155	1.644780	-0.695758	C	1.149121	1.616331	-0.703709
H	0.144579	2.972258	2.143879	H	0.148945	2.982156	2.151244
H	0.144579	2.972258	-2.143879	H	0.148945	2.982156	-2.151244
C	-1.724860	1.098048	0.000000	C	-1.711877	1.078661	0.000000
C	-1.062868	1.387509	-1.217420	C	-1.044221	1.383475	-1.217608
C	-1.062868	1.387509	1.217420	C	-1.044221	1.383475	1.217608
H	1.951767	1.250602	1.346659	H	1.952594	1.274559	1.356049
H	1.951767	1.250602	-1.346659	H	1.952594	1.274559	-1.356049
H	-1.505054	1.083530	2.164217	H	-1.473652	1.068695	2.171932
H	-2.615414	0.468812	0.000000	H	-2.627423	0.481218	0.000000
H	-1.505054	1.083530	-2.164217	H	-1.473652	1.068695	-2.171932
C	0.000000	-2.470520	1.183139	C	0.000000	-2.482530	1.184761
C	0.000000	-2.470520	-1.183139	C	0.000000	-2.482530	-1.184761
C	0.242029	-3.416001	0.000000	C	0.236622	-3.428039	0.000000
H	-0.505164	-4.218406	0.000000	H	-0.522239	-4.226275	0.000000
H	1.246026	-3.855191	0.000000	H	1.239745	-3.879927	0.000000
C	-1.177155	-1.644780	0.695758	C	-1.149121	-1.616331	0.703709
C	-1.177155	-1.644780	-0.695758	C	-1.149121	-1.616331	-0.703709
H	-0.144579	-2.972258	2.143879	H	-0.148945	-2.982156	2.151244
H	-0.144579	-2.972258	-2.143879	H	-0.148945	-2.982156	-2.151244
C	1.724860	-1.098048	0.000000	C	1.711877	-1.078661	0.000000
C	1.062868	-1.387509	-1.217420	C	1.044221	-1.383475	-1.217608
C	1.062868	-1.387509	1.217420	C	1.044221	-1.383475	1.217608
H	-1.951767	-1.250602	1.346659	H	-1.952594	-1.274559	1.356049
H	-1.951767	-1.250602	-1.346659	H	-1.952594	-1.274559	-1.356049
H	1.505054	-1.083530	2.164217	H	1.473652	-1.068695	2.171932
H	2.615414	-0.468812	0.000000	H	2.627423	-0.481218	0.000000
H	1.505054	-1.083530	-2.164217	H	1.473652	-1.068695	-2.171932
Fe	0.000000	0.000000	0.000000	Fe	0.000000	0.000000	0.000000

Table S36. Optimized coordinates for the **(bcod)$_2$Fe**structure**Fe-3T.**

	M06-L				OPBE		
	x	y	z		x	y	z
C	0.000000	2.635903	1.175142	C	0.000000	2.634299	1.177335
C	0.000000	2.635903	-1.175142	C	0.000000	2.634299	-1.177335
C	-0.377254	3.550345	0.000000	C	-0.368683	3.551622	0.000000
H	0.250487	4.448956	0.000000	H	0.273970	4.445484	0.000000
H	-1.433112	3.838266	0.000000	H	-1.424439	3.854496	0.000000
C	1.338701	2.101978	0.675008	C	1.323762	2.066072	0.680795
C	1.338701	2.101978	-0.675008	C	1.323762	2.066072	-0.680795
H	0.055774	3.145391	2.141761	H	0.063702	3.145890	2.148002
H	0.055774	3.145391	-2.141761	H	0.063702	3.145890	-2.148002
C	-1.663367	1.163557	0.000000	C	-1.655350	1.149296	0.000000
C	-0.980123	1.456438	-1.212232	C	-0.972555	1.452513	-1.214730
C	-0.980123	1.456438	1.212232	C	-0.972555	1.452513	1.214730
H	2.102807	1.674217	1.320610	H	2.093162	1.651008	1.334321
H	2.102807	1.674217	-1.320610	H	2.093162	1.651008	-1.334321
H	-1.436457	1.192969	2.165122	H	-1.421026	1.179686	2.173887
H	-2.559323	0.540105	0.000000	H	-2.569855	0.548084	0.000000
H	-1.436457	1.192969	-2.165122	H	-1.421026	1.179686	-2.173887
C	0.000000	-2.635903	1.175142	C	0.000000	-2.634299	1.177335
C	0.000000	-2.635903	-1.175142	C	0.000000	-2.634299	-1.177335
C	0.377254	-3.550345	0.000000	C	0.368683	-3.551622	0.000000
H	-0.250487	-4.448956	0.000000	H	-0.273970	-4.445484	0.000000
H	1.433112	-3.838266	0.000000	H	1.424439	-3.854496	0.000000
C	-1.338701	-2.101978	0.675008	C	-1.323762	-2.066072	0.680795
C	-1.338701	-2.101978	-0.675008	C	-1.323762	-2.066072	-0.680795
H	-0.055774	-3.145391	2.141761	H	-0.063702	-3.145890	2.148002
H	-0.055774	-3.145391	-2.141761	H	-0.063702	-3.145890	-2.148002
C	1.663367	-1.163557	0.000000	C	1.655350	-1.149296	0.000000
C	0.980123	-1.456438	-1.212232	C	0.972555	-1.452513	-1.214730
C	0.980123	-1.456438	1.212232	C	0.972555	-1.452513	1.214730
H	-2.102807	-1.674217	1.320610	H	-2.093162	-1.651008	1.334321
H	-2.102807	-1.674217	-1.320610	H	-2.093162	-1.651008	-1.334321
H	1.436457	-1.192969	2.165122	H	1.421026	-1.179686	2.173887
H	2.559323	-0.540105	0.000000	H	2.569855	-0.548084	0.000000
H	1.436457	-1.192969	-2.165122	H	1.421026	-1.179686	-2.173887
Fe	0.000000	0.000000	0.000000	Fe	0.000000	0.000000	0.000000

Table S37. Optimized coordinates for the**(bcod)$_2$Fe**structure **Fe-4T.**

	M06-L				OPBE		
	x	y	z		x	y	z
C	2.542868	-0.975051	0.583261	C	2.465724	-1.002945	0.641281
C	2.502847	0.735229	-1.042572	C	2.569381	0.651765	-1.039681
C	3.504761	-0.084258	-0.203933	C	3.500639	-0.192377	-0.141758
H	4.137370	-0.702929	-0.851281	H	4.117255	-0.872381	-0.749913
H	4.140108	0.548230	0.426465	H	4.154482	0.428140	0.488277
C	1.551000	-1.393713	-0.498601	C	1.477571	-1.397268	-0.450465
C	1.456217	-0.322804	-1.406311	C	1.468504	-0.354393	-1.400282
H	3.021695	-1.794719	1.127107	H	2.878963	-1.832469	1.231667
H	2.950986	1.221647	-1.914210	H	3.070287	1.081560	-1.918336
C	1.431946	1.244014	1.116107	C	1.417627	1.278971	1.049129
C	1.824184	1.722086	-0.122597	C	1.920131	1.705923	-0.177898
C	1.609844	-0.138393	1.462185	C	1.525961	-0.103043	1.445888
H	1.183967	-2.406203	-0.658371	H	1.078183	-2.403125	-0.594920
H	0.991385	-0.373973	-2.388143	H	1.041528	-0.419222	-2.402140
H	1.426669	-0.444996	2.491200	H	1.296745	-0.366110	2.482742
H	0.936235	1.905760	1.826699	H	0.954139	1.994196	1.735448
H	1.590930	2.735892	-0.441577	H	1.782572	2.731183	-0.528393
C	-2.533911	0.725203	0.919672	C	-2.462340	0.785185	0.899934
C	-2.462732	-0.100382	-1.288119	C	-2.502414	-0.189892	-1.247543
C	-3.480858	0.277318	-0.201383	C	-3.466049	0.287758	-0.148951
H	-4.094310	1.122388	-0.533369	H	-4.068170	1.132261	-0.516722
H	-4.129956	-0.556626	0.084934	H	-4.130427	-0.507267	0.218044
C	-1.509747	1.526493	0.125843	C	-1.441445	1.506308	0.024215
C	-1.455621	1.040454	-1.152670	C	-1.441658	0.910015	-1.232676
H	-3.018148	1.282805	1.725744	H	-2.899611	1.404154	1.695218
H	-2.889100	-0.209121	-2.289133	H	-2.972042	-0.355107	-2.226849
C	-1.594338	-1.562982	0.539056	C	-1.545687	-1.542710	0.630352
C	-1.706313	-1.337107	-0.840889	C	-1.748766	-1.406326	-0.752119
C	-1.738214	-0.470684	1.436965	C	-1.650048	-0.384329	1.457871
H	-0.929758	2.348113	0.530274	H	-0.924986	2.420583	0.307556
H	-0.818799	1.398129	-1.955527	H	-0.908530	1.254671	-2.117997
H	-1.626324	-0.622925	2.507980	H	-1.483733	-0.462453	2.535417
H	-1.145946	-2.493095	0.892647	H	-1.098692	-2.460791	1.026361
H	-1.465349	-2.125051	-1.551123	H	-1.522853	-2.232780	-1.430280
Fe	0.003336	-0.236379	0.169754	Fe	-0.034150	-0.148112	0.131578

Table S38. Optimized coordinates for the **(bcod)$_2$Co**structure**Co-1D.**

	M06-L				OPBE		
	x	y	z		x	y	z
C	0.000000	2.561041	1.178181	C	0.000000	2.544508	1.180658
C	0.000000	2.561041	-1.178181	C	0.000000	2.544508	-1.180658
C	-0.323990	3.491310	0.000000	C	-0.288093	3.484390	0.000000
H	0.352597	4.353486	0.000000	H	0.428286	4.320115	0.000000
H	-1.362052	3.839575	0.000000	H	-1.313787	3.879407	0.000000
C	1.288267	1.917150	0.679181	C	1.240395	1.812098	0.688861
C	1.288267	1.917150	-0.679181	C	1.240395	1.812098	-0.688861
H	0.090477	3.070470	2.142016	H	0.113919	3.051397	2.148774
H	0.090477	3.070470	-2.142016	H	0.113919	3.051397	-2.148774
C	-1.687320	1.130561	0.000000	C	-1.700154	1.123176	0.000000
C	-1.019134	1.426522	-1.213570	C	-1.031694	1.427941	-1.214736
C	-1.019134	1.426522	1.213570	C	-1.031694	1.427941	1.214736
H	2.033054	1.467961	1.330317	H	2.000006	1.398726	1.351377
H	2.033054	1.467961	-1.330317	H	2.000006	1.398726	-1.351377
H	-1.466180	1.138748	2.163108	H	-1.466901	1.125924	2.170502
H	-2.568297	0.488740	0.000000	H	-2.602516	0.507601	0.000000
H	-1.466180	1.138748	-2.163108	H	-1.466901	1.125924	-2.170502
C	0.000000	-2.561041	1.178181	C	0.000000	-2.544508	1.180658
C	0.000000	-2.561041	-1.178181	C	0.000000	-2.544508	-1.180658
C	0.323990	-3.491310	0.000000	C	0.288093	-3.484390	0.000000
H	-0.352597	-4.353486	0.000000	H	-0.428286	-4.320115	0.000000
H	1.362052	-3.839575	0.000000	H	1.313787	-3.879407	0.000000
C	-1.288267	-1.917150	0.679181	C	-1.240395	-1.812098	0.688861
C	-1.288267	-1.917150	-0.679181	C	-1.240395	-1.812098	-0.688861
H	-0.090477	-3.070470	2.142016	H	-0.113919	-3.051397	2.148774
H	-0.090477	-3.070470	-2.142016	H	-0.113919	-3.051397	-2.148774
C	1.687320	-1.130561	0.000000	C	1.700154	-1.123176	0.000000
C	1.019134	-1.426522	-1.213570	C	1.031694	-1.427941	-1.214736
C	1.019134	-1.426522	1.213570	C	1.031694	-1.427941	1.214736
H	-2.033054	-1.467961	1.330317	H	-2.000006	-1.398726	1.351377
H	-2.033054	-1.467961	-1.330317	H	-2.000006	-1.398726	-1.351377
H	1.466180	-1.138748	2.163108	H	1.466901	-1.125924	2.170502
H	2.568297	-0.488740	0.000000	H	2.602516	-0.507601	0.000000
H	1.466180	-1.138748	-2.163108	H	1.466901	-1.125924	-2.170502
Co	0.000000	0.000000	0.000000	Co	0.000000	0.000000	0.000000

Table S39. Optimized coordinates for the **(bcod)$_2$Co**structure**Co-2D.**

	M06-L				OPBE		
	x	y	z		x	y	z
C	-2.375960	-0.870533	-1.005802	C	-2.309606	-0.972242	-0.924744
C	-2.619564	0.146918	1.109622	C	-2.649370	0.264214	1.061040
C	-3.473255	-0.379017	-0.058862	C	-3.451882	-0.440187	-0.057598
H	-4.091656	-1.225260	0.262372	H	-4.028576	-1.286440	0.347396
H	-4.114639	0.396000	-0.491718	H	-4.133481	0.246040	-0.580996
C	-1.420006	-1.538545	-0.033958	C	-1.335577	-1.492441	0.115288
C	-1.523623	-0.916275	1.196304	C	-1.469066	-0.696984	1.267717
H	-2.730994	-1.503686	-1.823565	H	-2.612308	-1.690669	-1.697975
H	-3.175051	0.290302	2.040784	H	-3.227034	0.446643	1.977636
C	-1.508622	1.472444	-0.670679	C	-1.478366	1.412327	-0.771188
C	-1.923369	1.410385	0.651416	C	-2.076426	1.529739	0.479313
C	-1.482752	0.276553	-1.468375	C	-1.402517	0.139631	-1.449043
H	-0.798497	-2.391205	-0.286779	H	-0.829678	-2.454072	0.034524
H	-1.033355	-1.211275	2.119078	H	-1.063076	-0.926203	2.253776
H	-1.197467	0.342007	-2.516757	H	-1.086816	0.119358	-2.495444
H	-1.052685	2.384636	-1.055976	H	-1.052092	2.296208	-1.254155
H	-1.821585	2.266765	1.313535	H	-2.077100	2.472853	1.029429
C	2.510815	-0.590729	1.105504	C	2.512623	-0.489142	1.135642
C	2.540622	0.071250	-1.153733	C	2.497833	0.033046	-1.166477
C	3.495144	-0.100507	0.036764	C	3.474492	-0.085795	0.010484
H	4.237268	-0.878428	-0.175868	H	4.191916	-0.900062	-0.173762
H	4.006290	0.828085	0.311258	H	4.021648	0.845870	0.215277
C	1.675658	-1.567746	0.292674	C	1.581093	-1.454283	0.422286
C	1.668178	-1.174707	-1.012885	C	1.558872	-1.151850	-0.942918
H	2.985459	-1.019670	1.992794	H	3.003137	-0.886716	2.034767
H	3.040123	0.168800	-2.122022	H	2.975453	0.078234	-2.154810
C	1.352310	1.551522	0.490526	C	1.294020	1.590771	0.427012
C	1.601226	1.232407	-0.864989	C	1.535926	1.182681	-0.917162
C	1.522478	0.518340	1.445016	C	1.538624	0.637296	1.438598
H	1.113881	-2.386370	0.732710	H	1.136305	-2.317759	0.915017
H	1.135292	-1.643251	-1.834703	H	1.127610	-1.756249	-1.740984
H	1.245082	0.688607	2.483122	H	1.237557	0.839894	2.469169
H	0.836028	2.472316	0.758156	H	0.748393	2.509812	0.648696
H	1.393402	1.963821	-1.644243	H	1.277564	1.850649	-1.742676
Co	-0.007873	0.118787	-0.015312	Co	0.054316	0.017479	-0.031644

Table S40. Optimized coordinates for the**(bcod)$_2$Co**structure **Co-3D.**

	M06-L				OPBE		
	x	y	z		x	y	z
C	-2.534724	0.707088	0.904967	C	-2.547057	0.707567	0.892564
C	-2.423503	-0.228648	-1.252208	C	-2.394579	-0.233383	-1.264205
C	-3.453728	0.127642	-0.173985	C	-3.445095	0.136811	-0.209831
H	-4.137906	0.902145	-0.539546	H	-4.109247	0.925912	-0.595211
H	-4.030429	-0.738444	0.167234	H	-4.047830	-0.722328	0.118008
C	-1.572244	1.533349	0.060821	C	-1.527646	1.503531	0.087717
C	-1.490526	0.983440	-1.192609	C	-1.419377	0.945376	-1.181485
H	-3.052944	1.260389	1.693415	H	-3.079010	1.270896	1.671404
H	-2.852006	-0.428590	-2.238600	H	-2.802472	-0.433256	-2.264647
C	-1.384053	-1.528871	0.645654	C	-1.357543	-1.519700	0.662669
C	-1.544870	-1.360775	-0.752117	C	-1.513582	-1.354020	-0.744975
C	-1.608457	-0.371908	1.442630	C	-1.624819	-0.363586	1.448133
H	-1.033726	2.403264	0.420248	H	-1.056903	2.421499	0.432788
H	-0.908666	1.359976	-2.027522	H	-0.887099	1.371194	-2.030933
H	-1.376277	-0.391909	2.506099	H	-1.392403	-0.364137	2.516316
H	-0.916631	-2.419818	1.061276	H	-0.903573	-2.414769	1.095156
H	-1.254028	-2.157647	-1.435044	H	-1.208699	-2.152980	-1.426037
C	2.492916	-0.995619	0.583936	C	2.458618	-1.000967	0.620692
C	2.496779	0.757499	-0.998079	C	2.514730	0.716355	-1.002385
C	3.474308	-0.087203	-0.154919	C	3.468649	-0.141116	-0.139233
H	4.123793	-0.690889	-0.799839	H	4.097868	-0.785340	-0.773293
H	4.094134	0.527330	0.507790	H	4.113574	0.470073	0.509515
C	1.508708	-1.365968	-0.511201	C	1.454563	-1.369573	-0.457151
C	1.448249	-0.284412	-1.408046	C	1.420448	-0.295019	-1.380878
H	2.952108	-1.832978	1.116041	H	2.890883	-1.837293	1.185765
H	2.967853	1.262572	-1.846277	H	3.001480	1.180141	-1.871381
C	1.340216	1.194549	1.133650	C	1.318883	1.222212	1.090555
C	1.794889	1.721169	-0.072590	C	1.856213	1.730078	-0.103522
C	1.523529	-0.193590	1.443738	C	1.484596	-0.160355	1.436753
H	1.105563	-2.363070	-0.668519	H	1.092621	-2.384309	-0.631199
H	1.001903	-0.313373	-2.398803	H	1.016369	-0.356637	-2.392545
H	1.264976	-0.555825	2.437035	H	1.203982	-0.497407	2.437443
H	0.811111	1.828594	1.845393	H	0.824652	1.889170	1.802490
H	1.565388	2.741879	-0.370256	H	1.700547	2.766343	-0.409360
Co	-0.027005	-0.149632	0.087853	Co	-0.049509	-0.129335	0.077526

Table S41. Optimized coordinates for the **(bcod)$_2$Co**structure**Co-4D.**

	M06-L				OPBE		
	x	y	z		x	y	z
C	-1.205259	2.422572	-0.977914	C	0.000000	2.677438	-1.008852
C	-2.416616	1.101357	0.556363	C	-1.626929	2.097604	0.601707
C	-2.478031	2.475492	-0.111903	C	-1.067104	3.331536	-0.109640
H	-3.371807	2.544316	-0.743001	H	-1.854943	3.796651	-0.722371
H	-2.469371	3.310206	0.597323	H	-0.644414	4.083158	0.572690
C	-1.227218	0.977756	-1.468590	C	-0.691978	1.388745	-1.445722
C	-1.995948	0.208854	-0.606115	C	-1.696165	1.073348	-0.524385
H	-1.183277	3.161338	-1.783985	H	0.336202	3.309918	-1.841637
H	-3.333210	0.801807	1.071572	H	-2.561775	2.266425	1.152628
C	-0.061812	1.849683	1.138291	C	0.827163	1.620709	1.085092
C	-1.165925	0.964545	1.416856	C	-0.557223	1.388037	1.421596
C	0.000000	2.521877	-0.070901	C	1.144509	2.195966	-0.149028
H	-0.859047	0.675564	-2.444232	H	-0.580296	0.965748	-2.443311
H	-2.323245	-0.813680	-0.762847	H	-2.495187	0.345897	-0.658685
H	0.879440	3.093222	-0.356911	H	2.181051	2.291560	-0.479200
H	0.764276	1.918878	1.844941	H	1.621169	1.330540	1.778532
H	-1.248216	0.524548	2.410199	H	-0.805885	1.039005	2.427516
C	1.205259	-2.422572	-0.977914	C	0.000000	-2.677438	-1.008852
C	2.416616	-1.101357	0.556363	C	1.626929	-2.097604	0.601707
C	2.478031	-2.475492	-0.111903	C	1.067104	-3.331536	-0.109640
H	3.371807	-2.544316	-0.743001	H	1.854943	-3.796651	-0.722371
H	2.469371	-3.310206	0.597323	H	0.644414	-4.083158	0.572690
C	1.227218	-0.977756	-1.468590	C	0.691978	-1.388745	-1.445722
C	1.995948	-0.208854	-0.606115	C	1.696165	-1.073348	-0.524385
H	1.183277	-3.161338	-1.783985	H	-0.336202	-3.309918	-1.841637
H	3.333210	-0.801807	1.071572	H	2.561775	-2.266425	1.152628
C	0.061812	-1.849683	1.138291	C	-0.827163	-1.620709	1.085092
C	1.165925	-0.964545	1.416856	C	0.557223	-1.388037	1.421596
C	0.000000	-2.521877	-0.070901	C	-1.144509	-2.195966	-0.149028
H	0.859047	-0.675564	-2.444232	H	0.580296	-0.965748	-2.443311
H	2.323245	0.813680	-0.762847	H	2.495187	-0.345897	-0.658685
H	-0.879440	-3.093222	-0.356911	H	-2.181051	-2.291560	-0.479200
H	-0.764276	-1.918878	1.844941	H	-1.621169	-1.330540	1.778532
H	1.248216	-0.524548	2.410199	H	0.805885	-1.039005	2.427516
Co	0.000000	0.000000	0.067438	Co	0.000000	0.000000	0.073276

Table S42. Optimized coordinates for the**(bcod)$_2$Co**structure **Co-5D.**

	M06-L				OPBE		
	x	y	z		x	y	z
C	-2.483753	0.710943	0.999399	C	-2.458817	0.577049	1.110697
C	-2.335003	-1.300584	-0.191746	C	-2.320236	-1.274907	-0.318587
C	-2.064370	-0.747549	1.216650	C	-2.059791	-0.902832	1.148176
H	-2.710442	-1.239233	1.953670	H	-2.722366	-1.471340	1.819609
H	-1.022434	-0.847679	1.554616	H	-1.018190	-1.057919	1.465709
C	-3.780574	0.483796	0.238996	C	-3.751238	0.467875	0.314676
C	-3.697073	-0.672532	-0.443929	C	-3.670257	-0.601639	-0.511709
H	-2.587015	1.284313	1.925283	H	-2.561575	1.036963	2.103374
H	-2.313493	-2.393432	-0.249792	H	-2.313060	-2.357016	-0.511681
C	-1.262726	0.745244	-1.209031	C	-1.239882	0.882000	-1.086962
C	-1.337240	-0.673872	-1.186987	C	-1.299513	-0.543409	-1.218537
C	-1.471198	1.376579	0.047948	C	-1.452234	1.354900	0.240335
H	-4.579348	1.216610	0.160061	H	-4.540365	1.223543	0.314510
H	-4.413263	-1.038558	-1.174874	H	-4.382925	-0.862528	-1.297754
H	-1.363000	2.459283	0.114417	H	-1.347507	2.425365	0.442433
H	-0.892440	1.288779	-2.077103	H	-0.943906	1.538270	-1.909879
H	-1.148019	-1.222723	-2.109329	H	-1.113570	-0.985329	-2.202039
C	2.512388	-0.198381	1.339827	C	2.642462	0.080056	1.271526
C	2.756350	-0.510967	-0.989254	C	2.572671	-0.817640	-0.915817
C	3.607349	-0.319480	0.275945	C	3.584302	-0.379215	0.153697
H	4.217433	-1.210067	0.466405	H	4.172882	-1.243564	0.497852
H	4.256222	0.560698	0.218006	H	4.264293	0.410204	-0.197102
C	1.530429	-1.272036	0.886493	C	1.540447	-0.965081	1.211882
C	1.654571	-1.437285	-0.484372	C	1.487998	-1.510517	-0.081364
H	2.868146	-0.294656	2.369179	H	3.122298	0.214067	2.250173
H	3.310140	-0.896552	-1.849742	H	2.998926	-1.430241	-1.722203
C	1.667849	1.597700	-0.219400	C	1.656619	1.512350	-0.563797
C	2.024382	0.782290	-1.295218	C	1.819249	0.399436	-1.430368
C	1.660863	1.043575	1.103551	C	1.800018	1.265369	0.834167
H	0.893201	-1.851622	1.549061	H	1.002934	-1.316386	2.093780
H	1.155020	-2.182014	-1.094793	H	0.956913	-2.411970	-0.387566
H	1.371807	1.668284	1.945718	H	1.548983	2.044889	1.557140
H	1.219819	2.574282	-0.400633	H	1.253184	2.460630	-0.928407
H	1.913537	1.129561	-2.319264	H	1.604326	0.500082	-2.497529
Co	0.219654	0.124077	-0.056079	Co	0.255849	0.148870	-0.068093

Table S43. Optimized coordinates for the **(bcod)$_2$Ni** structure **Ni-1S.**

	M06-L				OPBE		
	x	y	z		x	y	z
C	-2.550712	0.554233	1.177971	C	2.569210	0.531382	-1.180123
C	-2.550694	0.554216	-1.177984	C	2.569207	0.531361	1.180138
C	-3.523203	0.679681	-0.000015	C	3.542539	0.646738	0.000009
H	-3.990980	1.670521	-0.000029	H	4.016730	1.639880	0.000019
H	-4.300567	-0.091371	-0.000015	H	4.319159	-0.131056	0.000003
C	-1.373705	1.395372	0.688535	C	1.384400	1.367573	-0.696523
C	-1.373697	1.395359	-0.688545	C	1.384398	1.367560	0.696550
H	-2.965153	0.860982	2.142136	H	2.988466	0.835223	-2.148817
H	-2.965124	0.860950	-2.142159	H	2.988462	0.835185	2.148837
C	-1.925316	-1.582110	0.000018	C	1.877550	-1.593442	-0.000013
C	-1.962979	-0.847678	-1.207777	C	1.949185	-0.856767	1.210806
C	-1.963019	-0.847666	1.207792	C	1.949188	-0.856745	-1.210818
H	-0.679096	1.911013	1.344845	H	0.739302	1.944224	-1.358969
H	-0.679084	1.911010	-1.344844	H	0.739300	1.944200	1.359006
H	-1.807093	-1.349083	2.159781	H	1.772646	-1.353057	-2.167931
H	-1.637202	-2.631779	0.000027	H	1.574865	-2.643906	-0.000022
H	-1.807088	-1.349135	-2.159751	H	1.772641	-1.353096	2.167910
C	2.386182	0.555138	1.165548	C	-2.412079	0.549792	-1.166157
C	2.386168	0.555111	-1.165554	C	-2.412082	0.549765	1.166165
C	2.051835	1.493502	-0.000012	C	-2.110321	1.499315	0.000015
H	2.725960	2.358413	-0.000030	H	-2.813622	2.346553	0.000024
H	1.019457	1.847303	-0.000004	H	-1.084087	1.875862	0.000021
C	3.732137	0.032918	0.671885	C	-3.741196	-0.021472	-0.675439
C	3.732132	0.032904	-0.671892	C	-3.741198	-0.021488	0.675430
H	2.418975	1.052800	2.140338	H	-2.462783	1.047396	-2.145286
H	2.418949	1.052754	-2.140354	H	-2.462788	1.047347	2.145306
C	1.316931	-1.426677	0.000029	C	-1.279366	-1.401756	-0.000017
C	1.401013	-0.630408	-1.186584	C	-1.390852	-0.604536	1.187057
C	1.401011	-0.630371	1.186611	C	-1.390850	-0.604509	-1.187073
H	4.498883	-0.390134	1.315552	H	-4.496365	-0.471871	-1.323714
H	4.498874	-0.390158	-1.315557	H	-4.496367	-0.471902	1.323693
H	1.272666	-1.127629	2.149010	H	-1.245212	-1.095287	-2.154929
H	1.115392	-2.497900	0.000034	H	-1.076448	-2.476843	-0.000029
H	1.272691	-1.127703	-2.148967	H	-1.245216	-1.095336	2.154902
Ni	-0.268392	-0.366857	-0.000006	Ni	0.285176	-0.318576	-0.000003

Table S44. Optimized coordinates for the **(bcod)$_2$Ni** structure **Ni-2S.**

	M06-L				OPBE		
	x	y	z		x	y	z
C	-0.413357	2.520019	1.169707	C	-0.436565	2.502279	1.168453
C	-0.413357	2.520019	-1.169707	C	-0.436565	2.502279	-1.168453
C	-1.383667	2.305274	0.000000	C	-1.409149	2.296293	0.000000
H	-2.157257	3.082722	0.000000	H	-2.183315	3.079277	0.000000
H	-1.859360	1.320844	0.000000	H	-1.877269	1.308171	0.000000
C	0.288768	3.777950	0.672414	C	0.269845	3.764129	0.675589
C	0.288768	3.777950	-0.672414	C	0.269845	3.764129	-0.675589
H	-0.905987	2.623510	2.141351	H	-0.929490	2.605175	2.145654
H	-0.905987	2.623510	-2.141351	H	-0.929490	2.605175	-2.145654
C	1.373859	1.179608	0.000000	C	1.370355	1.169558	0.000000
C	0.635246	1.390532	-1.197191	C	0.611416	1.373698	-1.193043
C	0.635246	1.390532	1.197191	C	0.611416	1.373698	1.193043
H	0.819451	4.476983	1.313624	H	0.798355	4.467943	1.322739
H	0.819451	4.476983	-1.313624	H	0.798355	4.467943	-1.322739
H	1.123052	1.193233	2.151674	H	1.092016	1.177254	2.156555
H	2.364010	0.722690	0.000000	H	2.400049	0.800324	0.000000
H	1.123052	1.193233	-2.151674	H	1.092016	1.177254	-2.156555
C	0.060344	-2.743943	-1.175247	C	0.045025	-2.720422	-1.179956
C	0.060344	-2.743943	1.175247	C	0.045025	-2.720422	1.179956
C	-0.277661	-3.670508	0.000000	C	-0.254313	-3.654802	0.000000
H	0.389885	-4.539305	0.000000	H	0.455204	-4.496066	0.000000
H	-1.319753	-4.006041	0.000000	H	-1.283820	-4.039718	0.000000
C	1.372024	-2.137688	-0.677283	C	1.308695	-2.010993	-0.690481
C	1.372024	-2.137688	0.677283	C	1.308695	-2.010993	0.690481
H	0.133654	-3.251054	-2.141816	H	0.142885	-3.229223	-2.148923
H	0.133654	-3.251054	2.141816	H	0.142885	-3.229223	2.148923
C	-1.634282	-1.295346	0.000000	C	-1.642957	-1.251798	0.000000
C	-0.948922	-1.599574	1.205599	C	-0.971955	-1.588803	1.209397
C	-0.948922	-1.599574	-1.205599	C	-0.971955	-1.588803	-1.209397
H	2.119179	-1.687330	-1.325272	H	2.081281	-1.610769	-1.347667
H	2.119179	-1.687330	1.325272	H	2.081281	-1.610769	1.347667
H	-1.367619	-1.286157	-2.158936	H	-1.369333	-1.243037	-2.166546
H	-2.519979	-0.661898	0.000000	H	-2.529955	-0.615474	0.000000
H	-1.367619	-1.286157	2.158936	H	-1.369333	-1.243037	2.166546
Ni	0.030724	-0.202111	0.000000	Ni	0.110233	-0.270191	0.000000

Table S45. Optimized coordinates for the **(bcod)$_2$Ni** structure **Ni-3S.**

	M06-L				OPBE		
	x	y	z		x	y	z
C	2.617368	0.366473	1.089992	C	2.637042	0.315085	1.092030
C	2.342323	-0.832125	-0.908833	C	2.316600	-0.833674	-0.928965
C	3.466970	-0.338205	-0.006367	C	3.462923	-0.401200	-0.020067
H	4.013357	-1.197804	0.401420	H	3.975249	-1.294774	0.371183
H	4.175644	0.345910	-0.485143	H	4.201391	0.265971	-0.486420
C	1.445738	-0.636711	1.225022	C	1.428101	-0.649789	1.212430
C	1.432704	-1.509962	0.107882	C	1.385888	-1.502282	0.073093
H	3.145276	0.479866	2.042594	H	3.170773	0.390562	2.050729
H	2.660832	-1.447956	-1.754418	H	2.609846	-1.436772	-1.798796
C	1.679127	1.634070	-0.733194	C	1.733812	1.649826	-0.704203
C	1.398652	0.323937	-1.322985	C	1.391515	0.353605	-1.298043
C	2.230282	1.698536	0.501178	C	2.316992	1.672348	0.523453
H	1.082914	-0.917907	2.212222	H	1.081460	-0.952915	2.203160
H	1.124794	-2.554514	0.094843	H	1.076950	-2.550110	0.051701
H	2.458082	2.635448	1.002332	H	2.612064	2.593819	1.030091
H	1.373397	2.535946	-1.265934	H	1.478127	2.573391	-1.234659
H	1.089032	0.320400	-2.369482	H	1.056894	0.372501	-2.340279
C	-2.427142	0.147885	1.302200	C	-2.474195	0.062039	1.287623
C	-2.528850	0.671819	-0.994165	C	-2.506769	0.741083	-0.973971
C	-3.457959	0.437360	0.204320	C	-3.470377	0.437085	0.182366
H	-4.011787	1.354077	0.435423	H	-4.018318	1.349802	0.461512
H	-4.162613	-0.386420	0.050084	H	-4.185816	-0.365704	-0.045314
C	-1.356594	1.195931	0.988331	C	-1.361973	1.090560	1.072848
C	-1.422271	1.494099	-0.345289	C	-1.391409	1.489754	-0.252488
H	-2.824303	0.189245	2.319813	H	-2.899882	0.041690	2.299725
H	-3.009942	1.149789	-1.851758	H	-2.960674	1.283790	-1.814056
C	-1.672801	-1.593159	-0.352504	C	-1.639217	-1.561701	-0.457313
C	-1.826619	-0.625519	-1.365322	C	-1.786053	-0.525361	-1.409644
C	-1.730517	-1.163936	0.994643	C	-1.761997	-1.223644	0.916440
H	-0.640168	1.594079	1.702099	H	-0.706948	1.477414	1.853654
H	-0.788403	2.191165	-0.881486	H	-0.783217	2.266579	-0.708489
H	-1.492476	-1.856492	1.798734	H	-1.534391	-1.965218	1.685498
H	-1.303439	-2.587624	-0.596026	H	-1.270746	-2.544836	-0.760312
H	-1.691328	-0.894040	-2.409693	H	-1.610413	-0.721468	-2.469592
Ni	-0.083619	-0.306290	-0.098395	Ni	-0.106345	-0.266647	-0.080102

Table S46. Optimized coordinates for the **(bcod)$_2$Ni** structure **Ni-4S.**

	M06-L				OPBE		
	x	y	z		x	y	z
C	2.717997	-0.912139	0.590244	C	2.722403	-0.933032	0.551482
C	2.469999	0.946952	-0.837523	C	2.459564	0.975190	-0.814066
C	3.535098	0.251928	0.022811	C	3.537922	0.239294	-0.002631
H	4.346414	-0.129638	-0.607166	H	4.327448	-0.137149	-0.670704
H	3.949995	0.905347	0.797188	H	3.987799	0.865135	0.781104
C	1.915625	-1.339372	-0.633938	C	1.852980	-1.310342	-0.642514
C	1.758620	-0.252980	-1.457829	C	1.693938	-0.186208	-1.445190
H	3.313814	-1.703151	1.052920	H	3.320272	-1.749478	0.977436
H	2.870255	1.662007	-1.561171	H	2.852192	1.710426	-1.529210
C	1.184857	0.958480	1.313412	C	1.181385	0.914148	1.349743
C	1.416689	1.562801	0.067948	C	1.423291	1.569298	0.126318
C	1.621066	-0.383999	1.496093	C	1.633821	-0.434080	1.481795
H	1.513823	-2.334754	-0.791713	H	1.493877	-2.317202	-0.853869
H	1.245951	-0.233606	-2.413316	H	1.235210	-0.155564	-2.432199
H	1.366430	-0.922746	2.405423	H	1.371031	-1.018466	2.365864
H	0.503910	1.418411	2.028415	H	0.518831	1.357530	2.097347
H	0.999024	2.541102	-0.154463	H	1.016250	2.564958	-0.054978
C	-2.186263	-0.876774	-1.057132	C	-2.178018	-0.857561	-1.073930
C	-2.768904	0.137773	0.976075	C	-2.765484	0.105163	0.983309
C	-3.435815	-0.563273	-0.242586	C	-3.430776	-0.583987	-0.247444
H	-3.927524	-1.498922	0.052245	H	-3.902925	-1.539494	0.032354
H	-4.162163	0.084467	-0.744812	H	-4.175691	0.061627	-0.733398
C	-1.315892	-1.553639	0.001281	C	-1.288438	-1.541914	-0.038229
C	-1.517020	-0.759528	1.152594	C	-1.494713	-0.772142	1.135405
H	-2.361149	-1.449857	-1.972290	H	-2.346547	-1.408953	-2.008987
H	-3.385899	0.117327	1.880686	H	-3.379284	0.054731	1.894817
C	-1.792372	1.629031	-0.638257	C	-1.812894	1.645691	-0.601654
C	-2.473315	1.544520	0.528055	C	-2.510331	1.525865	0.558772
C	-1.341422	0.400056	-1.294152	C	-1.338804	0.430851	-1.273213
H	-0.929133	-2.570699	-0.034242	H	-0.911864	-2.566269	-0.090686
H	-1.194632	-1.054905	2.150782	H	-1.186213	-1.102122	2.130807
H	-0.959616	0.519670	-2.310195	H	-0.959493	0.577576	-2.289413
H	-1.506551	2.590656	-1.066235	H	-1.556365	2.622848	-1.023937
H	-2.830119	2.410542	1.078075	H	-2.906168	2.376923	1.116535
Ni	0.086196	-0.181796	0.010260	Ni	0.110234	-0.175517	0.000122

Table S47. Optimized coordinates for the**(bcod)$_2$Cu**structure **Cu-1D.**

	M06-L				OPBE		
	x	y	z		x	y	z
C	3.195192	-0.055001	1.014065	C	3.369029	-0.171604	0.899110
C	2.579829	0.303171	-1.234796	C	2.528954	0.472048	-1.211332
C	3.788213	-0.161037	-0.403942	C	3.807484	-0.113382	-0.578672
H	4.626121	0.534858	-0.518793	H	4.650445	0.583371	-0.696162
H	4.120133	-1.174495	-0.653059	H	4.084498	-1.096188	-0.985300
C	2.447393	1.268079	0.899132	C	2.658958	1.172038	1.027222
C	2.104393	1.474314	-0.386543	C	2.181960	1.537854	-0.183753
H	3.941859	-0.076807	1.813813	H	4.197849	-0.310368	1.608331
H	2.824458	0.569775	-2.267144	H	2.673824	0.864689	-2.227751
C	1.418680	-1.514307	0.048136	C	1.446130	-1.469620	-0.038121
C	1.489797	-0.769406	-1.177523	C	1.431511	-0.593926	-1.182735
C	2.174050	-1.155199	1.172854	C	2.327791	-1.254507	1.037196
H	2.124947	1.855070	1.756218	H	2.464559	1.666762	1.981648
H	1.472748	2.273633	-0.769002	H	1.557402	2.405588	-0.403289
H	2.035565	-1.662298	2.124406	H	2.274747	-1.872105	1.936734
H	0.798629	-2.412066	0.091434	H	0.858297	-2.394963	-0.054243
H	1.194574	-1.261572	-2.103159	H	1.105960	-1.007291	-2.142551
C	-2.882154	-0.453156	1.105956	C	-2.951544	-0.596806	0.992338
C	-2.820316	0.377312	-1.100920	C	-2.818530	0.590515	-1.046416
C	-3.775372	0.292324	0.101544	C	-3.813475	0.302521	0.092010
H	-4.652526	-0.313707	-0.149033	H	-4.676485	-0.262084	-0.290745
H	-4.100204	1.273613	0.461754	H	-4.164782	1.212105	0.597914
C	-2.254563	-1.500370	0.196061	C	-2.253485	-1.470056	-0.040950
C	-2.215681	-1.023392	-1.071566	C	-2.171771	-0.780618	-1.225738
H	-3.418648	-0.864401	1.965395	H	-3.515926	-1.149946	1.754894
H	-3.308501	0.635456	-2.044577	H	-3.277441	0.997965	-1.957196
C	-1.323267	1.436066	0.605260	C	-1.339207	1.320756	0.845683
C	-1.685614	1.336826	-0.765175	C	-1.689489	1.466246	-0.525852
C	-1.749397	0.464720	1.527871	C	-1.813665	0.213260	1.584491
H	-1.788201	-2.413699	0.557915	H	-1.827087	-2.450947	0.178276
H	-1.728804	-1.490337	-1.924493	H	-1.696077	-1.115099	-2.149469
H	-1.409484	0.492117	2.559024	H	-1.490880	0.051305	2.614523
H	-0.604010	2.194164	0.918359	H	-0.608896	1.998580	1.297225
H	-1.401237	2.117444	-1.465194	H	-1.346635	2.328415	-1.099849
Cu	-0.126707	-0.075945	-0.121943	Cu	-0.229906	-0.144762	-0.090686

Table S48. Optimized coordinates for the**(bcod)$_2$Cu**structure **Cu-2D.**

	M06-L				OPBE		
	x	y	z		x	y	z
C	2.460766	0.466252	-1.252256	C	2.469898	0.499996	-1.235012
C	3.188441	0.185908	0.972908	C	3.344901	0.050603	0.910771
C	3.746930	0.161922	-0.464273	C	3.787103	0.054610	-0.568025
H	4.482200	0.962058	-0.601431	H	4.573660	0.806973	-0.726698
H	4.199922	-0.799146	-0.729792	H	4.141648	-0.926276	-0.914429
C	1.877511	1.571915	-0.385850	C	2.046043	1.601731	-0.275806
C	2.277742	1.404607	0.886776	C	2.537909	1.343514	0.955858
H	2.635901	0.759643	-2.291762	H	2.590246	0.837630	-2.274266
H	3.956001	0.260915	1.749486	H	4.177601	0.019240	1.628346
C	1.612864	-1.508462	0.046346	C	1.549086	-1.459478	0.043398
C	2.335298	-1.046887	1.153183	C	2.395697	-1.105732	1.109276
C	1.525549	-0.743787	-1.165574	C	1.459347	-0.647004	-1.141804
H	1.146160	2.295890	-0.739407	H	1.369745	2.415253	-0.543576
H	1.923664	1.955257	1.755486	H	2.310488	1.885085	1.877014
H	1.274240	-1.266775	-2.087150	H	1.155244	-1.130625	-2.075232
H	1.143232	-2.493033	0.094187	H	1.044966	-2.432446	0.076196
H	2.318622	-1.586025	2.096836	H	2.399108	-1.682191	2.037046
C	-2.502583	0.569847	1.279554	C	-2.607006	0.472891	1.298954
C	-2.867552	0.485935	-1.050641	C	-2.868963	0.542674	-1.048456
C	-3.648031	0.660170	0.265233	C	-3.707484	0.625987	0.241687
H	-4.114237	1.650539	0.307806	H	-4.178648	1.616297	0.329276
H	-4.414034	-0.108603	0.406353	H	-4.479684	-0.153132	0.298546
C	-1.429197	1.395964	0.585534	C	-1.492360	1.328012	0.713456
C	-1.627932	1.329564	-0.767915	C	-1.636789	1.358046	-0.665135
H	-2.761343	0.904970	2.286948	H	-2.912310	0.740592	2.318855
H	-3.417513	0.793083	-1.944065	H	-3.383325	0.906597	-1.947889
C	-1.997201	-1.563999	0.052741	C	-1.998355	-1.569308	-0.045769
C	-2.380886	-0.942841	-1.137994	C	-2.346837	-0.868566	-1.211822
C	-1.886033	-0.821468	1.260664	C	-1.961883	-0.901507	1.212897
H	-0.596672	1.872067	1.098636	H	-0.716811	1.817463	1.305268
H	-0.991816	1.748050	-1.543630	H	-1.007297	1.880536	-1.386055
H	-1.638262	-1.321653	2.192579	H	-1.704710	-1.446066	2.123408
H	-1.667822	-2.603072	0.034629	H	-1.655654	-2.606449	-0.117427
H	-2.380440	-1.480218	-2.081252	H	-2.309001	-1.345941	-2.192320
Cu	-0.179721	-0.385234	-0.057761	Cu	-0.249556	-0.315909	-0.054582

Table S49. Optimized coordinates for the **(bcod)$_2$Cu**structure**Cu-3D.**

	M06-L				OPBE		
	x	y	z		x	y	z
C	-0.432274	-2.657938	1.177775	C	0.434721	2.680601	1.177054
C	-0.432274	-2.657938	-1.177775	C	0.434721	2.680601	-1.177054
C	-0.677683	-3.621872	0.000000	C	0.723798	3.637387	0.000000
H	-1.717078	-3.969070	0.000000	H	1.783119	3.935497	0.000000
H	-0.007317	-4.488452	0.000000	H	0.092472	4.537621	0.000000
C	-1.239930	-1.436327	0.704242	C	1.202736	1.430534	0.706600
C	-1.239930	-1.436327	-0.704242	C	1.202736	1.430534	-0.706600
H	-0.782034	-3.038042	2.141875	H	0.799762	3.046097	2.147177
H	-0.782034	-3.038042	-2.141875	H	0.799762	3.046097	-2.147177
C	1.715826	-2.195603	0.000000	C	-1.735920	2.314504	0.000000
C	1.040574	-2.328604	-1.213729	C	-1.049168	2.414711	-1.214305
C	1.040574	-2.328604	1.213729	C	-1.049168	2.414711	1.214305
H	-1.997476	-0.973540	1.333260	H	1.972247	0.979063	1.337332
H	-1.997476	-0.973540	-1.333260	H	1.972247	0.979063	-1.337332
H	1.547388	-2.167616	2.162268	H	-1.562394	2.284285	2.169452
H	2.776292	-1.944946	0.000000	H	-2.813384	2.122272	0.000000
H	1.547388	-2.167616	-2.162268	H	-1.562394	2.284285	-2.169452
C	-0.062005	2.796445	-1.179382	C	0.047793	-2.823530	-1.181742
C	-0.062005	2.796445	1.179382	C	0.047793	-2.823530	1.181742
C	0.296101	3.714713	0.000000	C	-0.285536	-3.749197	0.000000
H	-0.347138	4.601534	0.000000	H	0.387238	-4.619767	0.000000
H	1.346230	4.023858	0.000000	H	-1.329548	-4.090996	0.000000
C	-1.372679	2.202730	-0.677478	C	1.327852	-2.162485	-0.686114
C	-1.372679	2.202730	0.677478	C	1.327852	-2.162485	0.686114
H	-0.138598	3.311503	-2.141107	H	0.142046	-3.338440	-2.147344
H	-0.138598	3.311503	2.141107	H	0.142046	-3.338440	2.147344
C	1.532991	1.273209	0.000000	C	-1.539993	-1.283158	0.000000
C	0.929117	1.639861	1.226519	C	-0.946408	-1.673703	1.228687
C	0.929117	1.639861	-1.226519	C	-0.946408	-1.673703	-1.228687
H	-2.110054	1.732034	-1.323657	H	2.071191	-1.705774	-1.342218
H	-2.110054	1.732034	1.323657	H	2.071191	-1.705774	1.342218
H	1.380806	1.342101	-2.168489	H	-1.377435	-1.351748	-2.177989
H	2.352322	0.552639	0.000000	H	-2.357962	-0.557629	0.000000
H	1.380806	1.342101	2.168489	H	-1.377435	-1.351748	2.177989
Cu	-0.129670	0.110168	0.000000	Cu	0.171132	-0.174646	0.000000

Table S50. Optimized coordinates for the**(bcod)$_2$Cu**structure **Cu-4D.**

	M06-L				OPBE		
	x	y	z		x	y	z
C	1.083526	2.457257	1.261399	C	-1.034288	2.480618	-1.271083
C	0.844150	3.140703	-0.986798	C	-0.892005	3.307400	0.940929
C	0.000000	2.926238	0.276576	C	0.000000	3.043837	-0.281267
H	-0.441755	3.872348	0.606699	H	0.415755	3.989829	-0.657920
H	-0.811506	2.193325	0.140246	H	0.833348	2.353047	-0.074156
C	2.200092	3.420362	0.904271	C	-2.197447	3.421093	-1.009405
C	2.068531	3.810874	-0.378440	C	-2.123315	3.891435	0.259531
H	0.767529	2.486899	2.308411	H	-0.683762	2.457193	-2.312451
H	0.343158	3.718691	-1.768430	H	-0.434547	3.951716	1.704374
C	1.785269	0.868626	-0.551653	C	-1.752940	0.978978	0.617972
C	1.345421	1.804002	-1.492061	C	-1.386962	1.995714	1.509791
C	1.545840	1.054974	0.856873	C	-1.488209	1.097099	-0.799239
H	3.054788	3.621784	1.545138	H	-3.042991	3.548944	-1.689558
H	2.795965	4.374847	-0.956285	H	-2.894398	4.459489	0.784839
H	2.168533	0.498892	1.556719	H	-2.102478	0.502997	-1.483812
H	2.358763	0.003045	-0.889279	H	-2.347109	0.135025	0.989890
H	1.519940	1.643772	-2.552987	H	-1.594242	1.898134	2.577974
C	-1.083526	-2.457257	1.261399	C	1.034288	-2.480618	-1.271083
C	-0.844150	-3.140703	-0.986798	C	0.892005	-3.307400	0.940929
C	0.000000	-2.926238	0.276576	C	0.000000	-3.043837	-0.281267
H	0.441755	-3.872348	0.606699	H	-0.415755	-3.989829	-0.657920
H	0.811506	-2.193325	0.140246	H	-0.833348	-2.353047	-0.074156
C	-2.200092	-3.420362	0.904271	C	2.197447	-3.421093	-1.009405
C	-2.068531	-3.810874	-0.378440	C	2.123315	-3.891435	0.259531
H	-0.767529	-2.486899	2.308411	H	0.683762	-2.457193	-2.312451
H	-0.343158	-3.718691	-1.768430	H	0.434547	-3.951716	1.704374
C	-1.785269	-0.868626	-0.551653	C	1.752940	-0.978978	0.617972
C	-1.345421	-1.804002	-1.492061	C	1.386962	-1.995714	1.509791
C	-1.545840	-1.054974	0.856873	C	1.488209	-1.097099	-0.799239
H	-3.054788	-3.621784	1.545138	H	3.042991	-3.548944	-1.689558
H	-2.795965	-4.374847	-0.956285	H	2.894398	-4.459489	0.784839
H	-2.168533	-0.498892	1.556719	H	2.102478	-0.502997	-1.483812
H	-2.358763	-0.003045	-0.889279	H	2.347109	-0.135025	0.989890
H	-1.519940	-1.643772	-2.552987	H	1.594242	-1.898134	2.577974
Cu	0.000000	0.000000	0.046122	Cu	0.000000	0.000000	0.024652

Table S51. Optimized coordinates for the**(bcod)$_2$Cu**structure **Cu-5D.**

	M06-L				OPBE		
	x	y	z		x	y	z
C	-0.479268	2.481531	-0.728325	C	-0.039396	2.768506	-0.503896
C	1.884615	2.525688	-0.742424	C	2.234780	2.296321	-0.960073
C	0.715239	1.830841	-1.450312	C	0.834442	2.020032	-1.525627
H	0.701743	2.078189	-2.517030	H	0.730658	2.472494	-2.522629
H	0.761000	0.734774	-1.349031	H	0.612027	0.945698	-1.603623
C	0.000000	3.919603	-0.669968	C	0.783862	4.031565	-0.322619
C	1.346194	3.948943	-0.671575	C	2.088203	3.763385	-0.573092
H	-1.433483	2.336017	-1.245378	H	-1.070992	2.935703	-0.844836
H	2.845022	2.422705	-1.255172	H	3.056020	2.080350	-1.657277
C	0.738714	1.888392	1.377163	C	1.304269	1.568094	1.245083
C	1.942293	2.043912	0.689490	C	2.395774	1.585443	0.363958
C	-0.535424	1.960483	0.712020	C	0.000000	2.033748	0.839355
H	-0.653744	4.768786	-0.487340	H	0.394272	4.956579	0.109390
H	1.970439	4.819232	-0.487125	H	2.935099	4.423915	-0.373972
H	-1.405876	2.219661	1.314256	H	-0.675875	2.387218	1.626050
H	0.765466	1.746434	2.459401	H	1.481729	1.296727	2.293868
H	2.892561	1.953428	1.209092	H	3.373140	1.216165	0.682876
C	0.479268	-2.481531	-0.728325	C	0.039396	-2.768506	-0.503896
C	-1.884615	-2.525688	-0.742424	C	-2.234780	-2.296321	-0.960073
C	-0.715239	-1.830841	-1.450312	C	-0.834442	-2.020032	-1.525627
H	-0.701743	-2.078189	-2.517030	H	-0.730658	-2.472494	-2.522629
H	-0.761000	-0.734774	-1.349031	H	-0.612027	-0.945698	-1.603623
C	0.000000	-3.919603	-0.669968	C	-0.783862	-4.031565	-0.322619
C	-1.346194	-3.948943	-0.671575	C	-2.088203	-3.763385	-0.573092
H	1.433483	-2.336017	-1.245378	H	1.070992	-2.935703	-0.844836
H	-2.845022	-2.422705	-1.255172	H	-3.056020	-2.080350	-1.657277
C	-0.738714	-1.888392	1.377163	C	-1.304269	-1.568094	1.245083
C	-1.942293	-2.043912	0.689490	C	-2.395774	-1.585443	0.363958
C	0.535424	-1.960483	0.712020	C	0.000000	-2.033748	0.839355
H	0.653744	-4.768786	-0.487340	H	-0.394272	-4.956579	0.109390
H	-1.970439	-4.819232	-0.487125	H	-2.935099	-4.423915	-0.373972
H	1.405876	-2.219661	1.314256	H	0.675875	-2.387218	1.626050
H	-0.765466	-1.746434	2.459401	H	-1.481729	-1.296727	2.293868
H	-2.892561	-1.953428	1.209092	H	-3.373140	-1.216165	0.682876
Cu	0.000000	0.000000	0.776684	Cu	0.000000	0.000000	0.752526

Table S52 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$(bcod)_2Ti$** structure **Ti-1S.**

M06-L			OPBE		
77(0)	841(0)	1277(0)	61(0)	840(1)	1245(2)
89(20)	847(5)	1293(1)	93(0)	847(2)	1265(0)
97(0)	861(5)	1295(0)	111(4)	853(10)	1268(1)
130(0)	864(4)	1311(0)	137(1)	861(6)	1280(1)
175(1)	896(16)	1312(0)	169(0)	879(24)	1280(0)
178(0)	898(1)	1336(14)	175(1)	882(0)	1307(18)
237(1)	923(14)	1337(15)	237(1)	920(9)	1307(21)
309(35)	933(3)	1420(41)	313(18)	924(1)	1399(48)
342(3)	943(8)	1424(4)	334(1)	931(8)	1406(1)
367(0)	945(0)	1430(38)	352(0)	936(0)	1411(13)
368(15)	945(3)	1437(0)	365(20)	942(4)	1413(0)
405(0)	948(2)	1472(3)	398(0)	945(2)	1443(4)
440(12)	988(5)	1472(1)	447(17)	980(5)	1444(1)
469(15)	988(10)	1558(18)	450(5)	981(9)	1541(16)
471(3)	1000(0)	1558(20)	456(2)	990(0)	1541(21)
476(0)	1000(1)	3045(143)	461(0)	990(0)	3055(64)
479(1)	1034(17)	3045(3)	480(0)	1011(5)	3056(2)
593(4)	1035(3)	3083(54)	581(4)	1012(15)	3092(40)
596(0)	1068(13)	3083(103)	582(0)	1050(7)	3092(20)
618(8)	1081(0)	3092(130)	604(1)	1061(0)	3095(60)
621(2)	1098(3)	3093(9)	605(16)	1086(2)	3096(1)
632(2)	1098(10)	3116(20)	622(5)	1086(3)	3128(8)
646(15)	1115(3)	3116(51)	629(3)	1102(4)	3128(20)
646(7)	1117(0)	3127(9)	651(5)	1104(1)	3140(2)
696(2)	1158(1)	3127(25)	685(17)	1131(1)	3140(7)
696(22)	1160(1)	3171(11)	698(0)	1133(1)	3176(7)
716(19)	1203(1)	3172(18)	701(13)	1177(1)	3176(0)
724(12)	1206(1)	3173(23)	724(10)	1181(1)	3192(4)
740(27)	1238(22)	3173(36)	735(30)	1213(11)	3192(3)
762(0)	1241(3)	3181(0)	755(1)	1216(2)	3197(10)
767(34)	1255(4)	3182(30)	763(32)	1223(6)	3197(0)
828(10)	1258(0)	3205(14)	827(15)	1227(2)	3218(5)
831(2)	1277(11)	3206(27)	830(3)	1245(7)	3222(7)

Table S53 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$(bcod)_2Ti$** structure **Ti-2S.**

M06-L			OPBE		
59(0)	857(5)	1278(3)	37(0)	829(1)	1246(4)
67(0)	859(3)	1293(1)	53(0)	849(4)	1256(2)
103(0)	870(2)	1303(5)	105(0)	855(5)	1276(5)
145(2)	878(10)	1315(8)	138(2)	857(8)	1291(7)
173(1)	888(7)	1317(6)	167(1)	875(6)	1292(10)
217(2)	896(3)	1323(4)	210(2)	877(10)	1299(5)
251(4)	908(5)	1328(5)	252(4)	884(4)	1314(3)
296(10)	912(6)	1364(6)	294(5)	904(4)	1333(9)
317(9)	928(12)	1420(3)	301(12)	914(11)	1396(3)
343(1)	941(6)	1423(6)	340(1)	930(5)	1405(11)
382(3)	951(1)	1470(4)	368(5)	947(1)	1438(3)
400(2)	965(3)	1472(3)	389(2)	961(4)	1441(4)
432(1)	977(7)	1527(14)	415(2)	966(10)	1513(9)
452(3)	992(13)	1549(16)	442(2)	984(11)	1533(16)
465(2)	997(2)	1580(14)	450(3)	988(0)	1535(9)
470(2)	1015(8)	3042(79)	460(0)	998(8)	3055(32)
499(3)	1026(0)	3051(64)	479(2)	1016(5)	3059(28)
586(5)	1045(2)	3071(104)	554(4)	1021(0)	3077(54)
595(9)	1061(3)	3098(76)	577(6)	1041(2)	3107(32)
601(10)	1084(4)	3103(76)	593(7)	1058(3)	3110(31)
631(1)	1093(4)	3106(37)	616(1)	1080(4)	3112(13)
639(1)	1107(0)	3114(36)	626(1)	1092(1)	3128(13)
642(1)	1112(8)	3123(29)	633(1)	1098(1)	3134(9)
655(6)	1118(1)	3131(18)	643(11)	1102(6)	3150(4)
677(5)	1147(1)	3139(19)	662(8)	1123(0)	3151(9)
694(24)	1162(1)	3140(23)	682(20)	1135(1)	3165(2)
707(7)	1169(9)	3161(7)	697(17)	1146(7)	3172(1)
714(21)	1199(4)	3165(37)	700(12)	1179(4)	3181(7)
729(52)	1226(0)	3171(27)	704(43)	1201(2)	3184(8)
750(41)	1228(2)	3173(32)	742(37)	1205(0)	3186(9)
784(0)	1261(0)	3188(12)	763(1)	1230(0)	3192(1)
807(6)	1268(4)	3202(15)	804(7)	1243(3)	3211(4)
848(3)	1276(1)	3229(4)	824(4)	1245(3)	3245(1)

Table S54 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$(bcod)_2Ti$** structure **Ti-3S.**

M06-L			OPBE		
45(0)	842(3)	1277(3)	42(0)	822(3)	1250(2)
64(0)	856(2)	1293(2)	64(0)	849(0)	1256(2)
106(0)	858(3)	1303(3)	102(0)	852(10)	1278(5)
138(1)	876(9)	1315(12)	136(1)	856(5)	1289(16)
154(2)	889(4)	1317(4)	166(3)	871(6)	1292(2)
202(0)	894(13)	1325(4)	199(2)	874(14)	1300(2)
250(13)	910(6)	1331(5)	256(13)	883(2)	1328(10)
266(7)	912(3)	1363(9)	267(4)	899(6)	1330(13)
293(7)	927(10)	1417(2)	294(3)	912(6)	1390(4)
326(4)	949(3)	1432(4)	319(5)	931(8)	1410(8)
384(8)	951(5)	1471(6)	374(7)	946(0)	1439(5)
402(5)	967(2)	1471(3)	385(7)	965(1)	1440(3)
430(1)	976(7)	1541(24)	413(1)	965(13)	1504(21)
445(3)	988(9)	1549(11)	428(1)	976(10)	1523(25)
462(6)	995(1)	1554(31)	446(4)	988(1)	1529(5)
470(0)	1012(12)	3042(77)	457(0)	999(10)	3055(32)
488(3)	1025(1)	3050(65)	469(1)	1016(7)	3057(29)
581(1)	1046(3)	3070(109)	557(2)	1019(0)	3077(56)
588(6)	1059(2)	3098(74)	576(4)	1038(2)	3105(31)
607(17)	1083(1)	3101(80)	594(9)	1053(1)	3109(35)
614(4)	1089(5)	3109(39)	604(5)	1075(5)	3116(13)
631(2)	1107(0)	3114(38)	614(2)	1091(1)	3128(12)
644(2)	1115(8)	3123(29)	627(3)	1099(1)	3132(10)
666(7)	1120(1)	3133(19)	651(9)	1102(6)	3152(5)
672(5)	1144(3)	3156(24)	661(14)	1122(1)	3172(5)
688(39)	1164(4)	3167(2)	670(12)	1136(1)	3182(4)
692(14)	1164(9)	3170(7)	690(23)	1142(10)	3184(2)
710(8)	1199(5)	3172(35)	702(5)	1181(5)	3185(5)
717(17)	1225(1)	3175(31)	707(9)	1202(0)	3187(5)
745(27)	1226(1)	3181(10)	738(28)	1203(1)	3190(1)
781(0)	1261(0)	3185(24)	752(1)	1230(0)	3193(5)
804(6)	1270(4)	3195(15)	798(3)	1244(4)	3205(3)
834(2)	1273(2)	3210(9)	800(8)	1244(3)	3227(6)

Table S55 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$(bcod)_2Ti$** structure **Ti-4T.**

M06-L			OPBE		
34(0)	855(0)	1289(0)	37(0)	848(7)	1252(1)
49(0)	856(8)	1308(1)	65(0)	848(2)	1280(6)
88(0)	862(0)	1308(11)	107(0)	853(10)	1281(1)
156(0)	862(18)	1313(1)	134(0)	854(18)	1289(7)
170(2)	881(6)	1315(11)	150(0)	860(5)	1290(1)
196(6)	881(1)	1352(12)	211(0)	865(1)	1316(4)
224(4)	906(8)	1353(0)	217(1)	897(0)	1318(19)
259(1)	910(0)	1420(12)	272(0)	898(4)	1405(0)
267(6)	943(0)	1422(0)	311(1)	939(0)	1406(17)
322(3)	945(0)	1469(19)	330(1)	941(0)	1436(0)
329(0)	946(0)	1469(0)	345(3)	943(1)	1437(16)
369(0)	953(0)	1509(2)	369(0)	949(2)	1479(4)
410(4)	980(0)	1513(52)	408(3)	972(15)	1479(65)
431(0)	980(27)	1521(103)	419(1)	972(1)	1508(33)
436(0)	1014(1)	1525(0)	428(0)	1002(0)	1508(11)
446(2)	1014(0)	3049(129)	446(0)	1004(0)	3057(54)
470(1)	1041(11)	3049(2)	447(1)	1014(2)	3057(1)
577(1)	1044(0)	3090(19)	557(3)	1016(16)	3091(45)
584(9)	1078(0)	3090(144)	562(3)	1049(8)	3092(39)
598(17)	1079(5)	3092(172)	581(1)	1049(1)	3098(54)
598(0)	1108(32)	3093(9)	592(15)	1092(2)	3098(19)
631(5)	1109(1)	3121(0)	620(7)	1092(2)	3132(3)
631(13)	1112(0)	3121(61)	625(0)	1100(15)	3132(19)
645(2)	1112(0)	3128(0)	632(14)	1100(0)	3161(3)
650(5)	1157(3)	3128(30)	643(4)	1130(4)	3161(2)
660(16)	1157(0)	3169(7)	672(0)	1130(0)	3173(4)
673(10)	1214(0)	3172(2)	691(14)	1190(0)	3174(0)
696(19)	1217(1)	3172(49)	694(15)	1190(0)	3178(2)
710(1)	1259(0)	3173(7)	716(21)	1224(0)	3178(13)
745(2)	1260(0)	3182(19)	717(0)	1224(0)	3198(4)
758(0)	1267(11)	3183(22)	719(2)	1238(2)	3200(7)
799(0)	1269(0)	3204(1)	786(0)	1239(8)	3221(1)
800(0)	1289(4)	3204(26)	788(0)	1251(5)	3221(10)

Table S56 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$(bcod)_2Ti$** structure **Ti-5T.**

M06-L			OPBE		
38(0)	853(6)	1290(2)	19(0)	846(13)	1252(4)
48(0)	855(8)	1306(5)	32(0)	849(2)	1282(5)
83(0)	858(5)	1310(3)	85(0)	852(2)	1284(0)
139(0)	860(5)	1311(7)	138(0)	857(5)	1292(5)
166(0)	888(4)	1316(2)	159(2)	859(21)	1292(1)
204(2)	891(7)	1347(11)	171(0)	860(1)	1318(7)
214(1)	912(2)	1351(5)	202(0)	882(1)	1318(19)
280(2)	920(2)	1423(4)	295(2)	888(5)	1401(16)
288(2)	941(1)	1428(7)	306(1)	941(0)	1402(0)
322(1)	941(0)	1467(16)	327(0)	942(0)	1436(1)
337(2)	945(1)	1468(21)	329(0)	945(0)	1436(15)
372(1)	951(2)	1496(54)	364(1)	951(0)	1481(40)
414(0)	980(13)	1498(37)	397(2)	969(6)	1481(23)
433(1)	984(11)	1519(35)	418(1)	971(19)	1506(29)
439(1)	1009(1)	1525(22)	424(2)	1007(0)	1509(8)
449(2)	1012(1)	3048(127)	439(1)	1007(0)	3057(57)
458(1)	1040(8)	3049(5)	445(0)	1013(11)	3058(1)
576(4)	1043(6)	3088(76)	553(7)	1014(6)	3098(48)
578(4)	1075(5)	3088(87)	557(3)	1051(3)	3098(16)
589(13)	1077(5)	3091(157)	583(16)	1051(2)	3100(79)
600(7)	1107(21)	3092(19)	584(5)	1091(2)	3100(3)
618(12)	1109(2)	3120(30)	614(22)	1094(0)	3133(6)
635(4)	1111(1)	3121(32)	616(4)	1094(16)	3133(15)
641(11)	1116(5)	3130(12)	625(6)	1097(0)	3153(1)
645(2)	1158(2)	3141(11)	636(11)	1132(2)	3154(3)
654(6)	1159(1)	3165(9)	669(16)	1133(0)	3186(5)
677(17)	1210(1)	3173(8)	670(0)	1191(0)	3186(3)
699(13)	1214(1)	3175(27)	687(20)	1192(0)	3189(2)
712(2)	1256(0)	3177(27)	704(3)	1225(0)	3190(1)
718(7)	1259(0)	3184(23)	708(0)	1225(0)	3191(4)
730(3)	1261(9)	3186(14)	713(2)	1238(3)	3193(5)
795(0)	1266(8)	3194(13)	777(0)	1239(6)	3211(17)
800(0)	1288(3)	3207(12)	788(0)	1252(1)	3215(0)

Table S57 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$(bcod)_2Ti$** structure **Ti-6T.**

M06-L			OPBE		
38(0)	853(6)	1290(2)	19(0)	846(13)	1252(4)
48(0)	855(8)	1306(5)	32(0)	849(2)	1282(5)
83(0)	858(5)	1310(3)	85(0)	852(2)	1284(0)
139(0)	860(5)	1311(7)	138(0)	857(5)	1292(5)
166(0)	888(4)	1316(2)	159(2)	859(21)	1292(1)
204(2)	891(7)	1347(11)	171(0)	860(1)	1318(7)
214(1)	912(2)	1351(5)	202(0)	882(1)	1318(19)
280(2)	920(2)	1423(4)	295(2)	888(5)	1401(16)
288(2)	941(1)	1428(7)	306(1)	941(0)	1402(0)
322(1)	941(0)	1467(16)	327(0)	942(0)	1436(1)
337(2)	945(1)	1468(21)	329(0)	945(0)	1436(15)
372(1)	951(2)	1496(54)	364(1)	951(0)	1481(40)
414(0)	980(13)	1498(37)	397(2)	969(6)	1481(23)
433(1)	984(11)	1519(35)	418(1)	971(19)	1506(29)
439(1)	1009(1)	1525(22)	424(2)	1007(0)	1509(8)
449(2)	1012(1)	3048(127)	439(1)	1007(0)	3057(57)
458(1)	1040(8)	3049(5)	445(0)	1013(11)	3058(1)
576(4)	1043(6)	3088(76)	553(7)	1014(6)	3098(49)
578(4)	1075(5)	3088(87)	557(3)	1051(3)	3098(16)
589(13)	1077(5)	3091(157)	583(16)	1051(2)	3100(79)
600(7)	1107(21)	3092(19)	584(5)	1091(2)	3100(3)
618(12)	1109(2)	3120(30)	614(22)	1094(0)	3133(6)
635(4)	1111(1)	3121(32)	616(4)	1094(16)	3133(15)
641(11)	1116(5)	3130(12)	625(6)	1097(0)	3153(1)
645(2)	1158(2)	3141(11)	636(11)	1132(2)	3154(3)
654(6)	1159(1)	3165(9)	669(16)	1133(0)	3186(5)
677(17)	1210(1)	3173(8)	670(0)	1191(0)	3186(3)
699(13)	1214(1)	3175(27)	687(20)	1192(0)	3189(2)
712(2)	1256(0)	3177(27)	704(3)	1225(0)	3190(1)
718(7)	1259(0)	3184(23)	708(0)	1225(0)	3191(4)
730(3)	1261(9)	3186(14)	713(2)	1238(3)	3193(5)
795(0)	1266(8)	3194(13)	777(0)	1239(6)	3211(17)
800(0)	1288(3)	3207(12)	788(0)	1252(1)	3215(0)

Table S58 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the**$(bcod)_2V$** structure **V-1Q.**

M06-L			OPBE		
54(0)	858(0)	1291(4)	36(0)	851(14)	1254(5)
65(0)	859(7)	1313(8)	74(0)	851(0)	1289(4)
102(0)	868(19)	1313(0)	111(0)	867(27)	1289(0)
147(0)	869(0)	1319(0)	145(0)	868(16)	1296(0)
185(0)	896(15)	1321(12)	179(0)	869(0)	1298(7)
224(2)	898(0)	1356(16)	207(2)	872(0)	1325(25)
227(9)	927(4)	1358(0)	222(9)	894(3)	1327(0)
259(0)	936(0)	1428(5)	260(0)	904(0)	1408(10)
315(5)	948(0)	1430(0)	324(4)	945(0)	1409(0)
336(1)	949(0)	1470(11)	326(0)	948(0)	1438(11)
357(0)	958(3)	1471(0)	345(0)	958(2)	1439(0)
367(0)	962(0)	1523(0)	354(0)	963(0)	1497(35)
412(6)	985(21)	1525(55)	400(6)	973(21)	1499(0)
433(0)	986(0)	1538(48)	415(0)	975(0)	1514(33)
446(2)	1019(1)	1540(0)	430(3)	1013(1)	1514(0)
464(2)	1019(0)	3049(132)	454(1)	1014(0)	3057(57)
468(0)	1045(6)	3049(0)	461(0)	1016(13)	3058(0)
587(0)	1047(0)	3093(0)	563(0)	1018(0)	3101(0)
597(2)	1083(0)	3093(155)	572(2)	1059(0)	3101(63)
607(22)	1086(2)	3096(162)	592(0)	1062(2)	3103(73)
607(0)	1112(18)	3097(0)	593(17)	1097(0)	3103(0)
642(8)	1114(1)	3119(0)	624(5)	1099(0)	3132(0)
647(0)	1116(0)	3119(34)	628(0)	1100(11)	3132(21)
657(0)	1116(0)	3121(0)	648(42)	1104(0)	3141(11)
671(49)	1159(3)	3122(69)	670(0)	1132(2)	3142(0)
677(32)	1161(0)	3174(0)	677(0)	1135(0)	3181(0)
690(0)	1219(0)	3175(63)	697(14)	1198(0)	3181(14)
717(23)	1221(1)	3178(20)	710(31)	1201(0)	3186(0)
723(0)	1261(0)	3178(0)	714(0)	1229(0)	3186(12)
769(0)	1262(1)	3179(44)	731(0)	1229(0)	3197(2)
773(0)	1272(4)	3180(0)	744(0)	1245(7)	3197(0)
817(1)	1273(0)	3201(0)	793(0)	1246(0)	3218(13)
820(0)	1291(0)	3202(25)	794(0)	1254(0)	3218(0)

Table S59 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$(bcod)_2V$** structure **V-2Q.**

M06-L			OPBE		
20(0)	858(3)	1290(1)	34(0)	851(9)	1255(4)
60(0)	859(2)	1311(7)	82(0)	852(1)	1287(4)
99(0)	865(15)	1312(1)	109(0)	863(9)	1287(0)
139(0)	866(4)	1318(9)	137(0)	863(18)	1296(4)
181(0)	893(13)	1319(1)	174(0)	865(12)	1296(1)
200(4)	895(0)	1356(13)	191(3)	868(0)	1324(9)
228(1)	919(2)	1357(3)	219(0)	893(1)	1324(19)
287(6)	923(1)	1431(0)	310(4)	903(0)	1409(11)
307(3)	945(0)	1431(5)	314(2)	943(0)	1409(0)
344(1)	947(0)	1470(1)	336(0)	944(0)	1439(11)
348(0)	955(2)	1470(11)	343(0)	955(3)	1439(0)
378(1)	959(0)	1522(38)	383(0)	959(0)	1499(18)
404(1)	984(6)	1525(7)	405(2)	973(6)	1500(21)
433(0)	984(14)	1534(31)	422(1)	973(11)	1512(20)
437(2)	1017(1)	1534(25)	428(3)	1011(0)	1515(7)
464(1)	1017(1)	3049(126)	454(1)	1011(0)	3057(55)
465(0)	1045(3)	3049(1)	459(0)	1016(8)	3057(0)
587(2)	1046(3)	3089(125)	567(2)	1017(5)	3097(45)
592(3)	1081(0)	3089(36)	569(1)	1054(2)	3097(22)
603(17)	1083(2)	3094(166)	592(3)	1056(1)	3099(76)
606(7)	1113(16)	3094(1)	593(15)	1096(1)	3100(1)
640(5)	1114(1)	3121(12)	625(2)	1099(0)	3132(7)
644(5)	1114(2)	3121(51)	626(2)	1101(11)	3132(15)
660(38)	1117(0)	3134(19)	645(35)	1102(0)	3153(2)
666(14)	1158(3)	3135(7)	669(25)	1132(2)	3155(1)
686(8)	1159(0)	3172(24)	707(0)	1135(1)	3178(12)
691(16)	1218(1)	3172(36)	711(19)	1196(0)	3178(6)
718(15)	1218(0)	3176(24)	717(8)	1198(0)	3184(6)
729(2)	1260(1)	3176(12)	732(3)	1227(0)	3185(10)
766(0)	1262(0)	3179(13)	734(1)	1228(0)	3195(2)
767(0)	1272(3)	3179(33)	744(0)	1243(3)	3198(2)
814(0)	1272(2)	3201(7)	794(0)	1243(5)	3216(10)
819(1)	1290(3)	3202(18)	812(1)	1254(2)	3219(1)

Table S60 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$(bcod)_2V$** structure **V-3D.**

M06-L			OPBE		
33(0)	832(2)	1285(3)	49(0)	819(2)	1254(2)
87(0)	862(2)	1292(2)	91(0)	854(6)	1262(1)
109(0)	864(3)	1314(6)	122(1)	859(6)	1288(8)
161(3)	870(5)	1317(4)	162(4)	863(4)	1289(0)
174(1)	885(6)	1319(11)	175(1)	866(10)	1292(14)
224(7)	892(11)	1323(3)	229(9)	870(1)	1295(2)
296(4)	892(2)	1358(9)	303(2)	877(6)	1323(14)
304(13)	918(0)	1388(15)	317(7)	902(0)	1384(10)
311(3)	921(1)	1416(3)	325(10)	918(1)	1394(8)
344(0)	939(9)	1442(2)	343(1)	933(7)	1418(5)
396(2)	949(0)	1473(8)	389(0)	945(0)	1442(7)
412(1)	960(1)	1474(3)	414(3)	956(2)	1444(3)
431(2)	975(8)	1525(27)	424(2)	966(7)	1481(21)
451(0)	986(6)	1530(10)	444(1)	975(5)	1514(6)
466(1)	1001(0)	1532(17)	459(1)	993(1)	1523(10)
477(1)	1018(0)	3047(48)	469(0)	1005(6)	3056(28)
502(4)	1025(10)	3049(63)	493(6)	1009(1)	3058(21)
578(3)	1046(4)	3063(147)	563(3)	1017(8)	3074(68)
590(1)	1060(4)	3090(81)	574(1)	1040(3)	3094(34)
601(11)	1081(2)	3094(84)	592(8)	1054(2)	3096(40)
630(3)	1083(5)	3110(38)	614(1)	1075(5)	3113(14)
638(8)	1110(1)	3119(32)	623(2)	1095(1)	3129(12)
642(3)	1116(0)	3120(33)	631(5)	1098(0)	3132(11)
659(3)	1120(8)	3130(16)	656(6)	1108(5)	3145(5)
680(4)	1143(4)	3141(10)	693(2)	1122(1)	3159(2)
699(1)	1159(2)	3156(27)	703(2)	1132(1)	3171(7)
716(5)	1164(10)	3163(41)	715(4)	1141(14)	3175(11)
733(5)	1209(6)	3172(35)	736(1)	1189(4)	3182(7)
747(14)	1221(0)	3182(27)	740(18)	1196(0)	3189(10)
756(13)	1235(0)	3185(30)	751(19)	1209(0)	3194(8)
762(3)	1263(0)	3187(23)	764(2)	1229(0)	3200(7)
798(3)	1272(5)	3200(10)	796(3)	1243(6)	3215(3)
807(2)	1282(1)	3235(8)	803(2)	1248(2)	3241(4)

Table S61 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the**$(bcod)_2V$** structure **V-4D.**

M06-L			OPBE		
44(0)	834(1)	1283(2)	31(0)	827(1)	1256(2)
75(0)	861(3)	1293(1)	103(0)	854(3)	1258(2)
129(1)	866(3)	1312(8)	107(1)	855(6)	1281(4)
164(0)	875(6)	1317(4)	147(2)	860(4)	1288(18)
169(1)	887(3)	1319(9)	176(2)	865(11)	1290(1)
225(1)	891(4)	1327(3)	211(4)	877(5)	1295(1)
276(10)	914(5)	1360(8)	274(22)	891(2)	1325(13)
300(6)	916(4)	1387(10)	312(5)	898(7)	1378(7)
317(9)	919(1)	1415(1)	330(2)	914(3)	1392(4)
339(1)	943(8)	1440(4)	354(4)	935(5)	1419(6)
403(2)	952(0)	1472(5)	389(1)	945(0)	1441(7)
408(2)	965(0)	1476(3)	412(3)	955(2)	1444(4)
434(1)	974(7)	1531(11)	424(3)	966(7)	1475(14)
443(1)	987(7)	1539(19)	442(2)	977(6)	1516(8)
462(1)	1001(1)	1544(13)	451(2)	991(0)	1521(7)
469(2)	1022(0)	3047(51)	464(2)	1005(6)	3055(29)
507(3)	1026(9)	3049(64)	483(1)	1010(1)	3059(18)
584(2)	1046(3)	3063(146)	564(3)	1016(7)	3073(69)
591(3)	1061(2)	3093(78)	573(3)	1043(2)	3095(36)
608(8)	1083(2)	3096(84)	596(3)	1054(2)	3098(39)
635(1)	1084(3)	3109(34)	616(1)	1078(3)	3114(11)
641(1)	1111(1)	3119(32)	624(2)	1091(1)	3128(12)
651(6)	1117(1)	3120(33)	647(4)	1097(1)	3133(11)
670(5)	1121(7)	3138(15)	663(7)	1108(4)	3151(4)
675(23)	1143(4)	3142(35)	702(1)	1123(1)	3164(1)
700(2)	1160(1)	3142(18)	706(4)	1133(0)	3166(11)
725(5)	1164(9)	3168(38)	721(4)	1144(9)	3179(5)
728(6)	1207(6)	3173(37)	730(6)	1183(3)	3180(11)
735(11)	1224(0)	3179(32)	744(19)	1197(0)	3187(8)
755(19)	1232(0)	3180(18)	750(18)	1207(0)	3194(1)
769(1)	1263(0)	3187(20)	758(4)	1229(0)	3198(12)
796(4)	1275(3)	3192(8)	797(2)	1240(7)	3219(3)
823(1)	1281(3)	3245(8)	817(2)	1244(3)	3239(3)

Table S62 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the**$(bcod)_2V$** structure **V-5D.**

M06-L			OPBE		
39(0)	853(6)	1291(2)	46(0)	845(8)	1253(1)
63(21)	854(8)	1304(1)	83(0)	847(10)	1280(2)
100(28)	859(4)	1311(4)	91(29)	855(1)	1280(2)
161(7)	865(7)	1314(0)	174(1)	856(14)	1292(2)
164(7)	892(7)	1321(2)	176(6)	863(10)	1292(1)
201(35)	895(8)	1349(7)	213(54)	868(2)	1315(2)
247(2)	933(7)	1353(12)	244(1)	912(0)	1317(28)
291(5)	937(1)	1413(35)	292(20)	914(0)	1411(4)
313(13)	940(3)	1434(3)	329(9)	934(0)	1411(8)
342(1)	948(6)	1442(3)	343(0)	935(8)	1430(55)
357(2)	956(1)	1469(14)	349(0)	944(8)	1432(1)
403(1)	960(1)	1475(2)	394(1)	953(0)	1450(22)
425(1)	986(2)	1506(41)	419(1)	974(18)	1454(4)
437(1)	987(17)	1530(26)	420(1)	974(0)	1516(22)
442(6)	1006(1)	1535(16)	422(5)	1004(0)	1520(7)
459(1)	1016(1)	3040(73)	444(1)	1005(0)	3052(58)
483(1)	1032(22)	3047(62)	472(1)	1011(28)	3053(0)
582(0)	1044(4)	3079(84)	562(0)	1014(1)	3087(27)
591(0)	1069(4)	3082(111)	571(1)	1045(7)	3088(51)
612(3)	1077(3)	3087(80)	590(3)	1048(1)	3092(70)
615(15)	1107(7)	3090(83)	596(9)	1089(6)	3092(15)
626(0)	1111(7)	3110(36)	608(0)	1092(2)	3126(6)
640(14)	1115(4)	3118(31)	623(10)	1102(0)	3126(17)
646(0)	1117(3)	3141(9)	631(0)	1102(9)	3161(4)
675(5)	1155(2)	3153(19)	671(1)	1128(2)	3161(1)
696(1)	1157(0)	3158(5)	699(4)	1130(0)	3170(1)
710(2)	1207(1)	3160(40)	707(0)	1188(1)	3172(8)
720(8)	1216(1)	3169(7)	723(1)	1188(0)	3177(8)
736(18)	1250(0)	3171(33)	739(6)	1223(0)	3178(2)
751(9)	1252(15)	3179(35)	740(23)	1223(0)	3193(7)
761(1)	1257(1)	3182(22)	750(1)	1231(14)	3195(7)
827(0)	1265(6)	3187(19)	819(1)	1231(0)	3213(10)
836(2)	1288(2)	3211(12)	820(0)	1252(5)	3213(3)

Table S63 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the**$(bcod)_2V$** structure **V-6Q.**

M06-L			OPBE		
35(0)	857(3)	1289(2)	27(0)	849(6)	1252(3)
52(0)	862(0)	1310(4)	58(0)	853(2)	1284(2)
87(0)	865(10)	1315(3)	95(0)	863(14)	1288(4)
136(0)	890(6)	1316(4)	133(1)	871(24)	1292(0)
160(0)	897(10)	1321(6)	148(0)	873(2)	1294(9)
221(3)	898(17)	1354(11)	211(5)	874(6)	1321(16)
226(6)	927(1)	1356(6)	215(3)	908(0)	1322(10)
276(0)	928(4)	1425(1)	267(0)	911(3)	1402(3)
321(0)	938(2)	1429(2)	321(3)	915(2)	1407(4)
330(5)	946(0)	1470(6)	328(1)	943(0)	1438(7)
348(0)	956(2)	1513(21)	335(0)	955(1)	1481(15)
370(10)	964(11)	1524(32)	368(7)	957(11)	1502(19)
414(15)	983(11)	1526(22)	408(14)	972(12)	1514(16)
438(3)	1004(1)	1584(7)	427(4)	993(1)	1535(13)
452(7)	1009(0)	1628(18)	435(7)	997(0)	1595(13)
468(1)	1016(1)	2877(53)	459(1)	1009(1)	2846(35)
514(1)	1045(4)	3050(66)	479(0)	1015(8)	3058(29)
577(4)	1060(2)	3083(11)	555(4)	1024(4)	3082(7)
583(28)	1084(2)	3092(67)	567(22)	1057(2)	3101(28)
594(1)	1088(6)	3094(83)	570(1)	1070(1)	3102(33)
605(12)	1105(1)	3097(80)	593(9)	1085(0)	3103(37)
645(5)	1113(10)	3098(53)	625(5)	1095(0)	3104(12)
654(1)	1114(1)	3119(22)	630(0)	1098(9)	3126(9)
663(3)	1122(6)	3122(27)	669(17)	1105(1)	3132(10)
688(22)	1123(1)	3123(25)	678(1)	1106(7)	3145(5)
699(44)	1159(2)	3166(34)	710(22)	1132(2)	3175(6)
722(19)	1216(1)	3171(24)	711(16)	1195(0)	3180(9)
726(39)	1224(6)	3177(26)	712(61)	1203(3)	3181(9)
760(21)	1253(1)	3179(1)	734(1)	1222(2)	3182(6)
768(0)	1262(0)	3182(35)	753(21)	1228(0)	3187(5)
785(7)	1270(2)	3186(20)	763(9)	1242(3)	3195(1)
822(0)	1275(0)	3202(14)	796(0)	1243(1)	3206(16)
851(1)	1289(2)	3205(54)	847(1)	1251(3)	3215(5)

Table S64 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the**$(bcod)_2V$** structure **V-7D.**

M06-L			OPBE		
47(0)	853(2)	1281(2)	53(0)	847(0)	1253(3)
78(0)	860(3)	1291(2)	85(0)	856(4)	1256(1)
84(0)	866(0)	1310(7)	95(0)	859(2)	1283(8)
156(0)	886(3)	1315(10)	153(0)	866(16)	1287(6)
169(1)	893(16)	1316(4)	171(1)	873(5)	1287(13)
209(3)	899(6)	1322(3)	212(3)	881(3)	1292(5)
293(13)	909(6)	1357(8)	288(8)	882(5)	1323(11)
296(2)	916(2)	1373(12)	299(5)	909(2)	1365(10)
334(0)	929(2)	1410(1)	338(0)	912(4)	1383(3)
342(2)	934(3)	1431(1)	349(1)	917(2)	1405(2)
400(9)	940(9)	1474(3)	390(2)	932(8)	1443(4)
401(6)	966(8)	1518(11)	400(12)	957(9)	1504(6)
446(4)	975(8)	1542(14)	439(4)	964(9)	1524(10)
462(1)	998(0)	1605(9)	453(1)	989(1)	1558(14)
469(3)	1003(1)	1632(12)	458(2)	993(1)	1600(8)
511(3)	1016(2)	2820(12)	482(6)	1001(7)	2727(4)
514(2)	1024(8)	3049(41)	500(2)	1008(2)	3059(14)
578(3)	1057(3)	3063(146)	558(3)	1035(3)	3071(73)
587(2)	1067(1)	3080(10)	570(1)	1037(3)	3080(6)
591(23)	1081(4)	3090(71)	576(22)	1069(4)	3101(29)
635(1)	1091(8)	3095(51)	620(1)	1071(3)	3103(14)
651(1)	1106(1)	3114(35)	628(1)	1085(1)	3116(12)
653(4)	1110(1)	3121(33)	651(7)	1092(1)	3134(11)
674(2)	1124(10)	3142(10)	684(2)	1105(2)	3156(3)
698(2)	1128(3)	3149(5)	700(0)	1108(12)	3159(1)
719(7)	1139(5)	3162(18)	715(62)	1117(2)	3171(8)
730(45)	1162(10)	3165(47)	724(3)	1135(10)	3173(8)
755(21)	1204(7)	3167(35)	747(26)	1183(5)	3178(1)
762(16)	1228(4)	3173(34)	761(6)	1204(0)	3180(5)
777(9)	1230(1)	3177(0)	767(12)	1206(2)	3181(18)
792(7)	1256(1)	3177(45)	789(7)	1226(2)	3186(8)
801(2)	1276(0)	3180(34)	798(1)	1246(3)	3188(13)
834(2)	1280(3)	3205(58)	820(2)	1246(1)	3205(18)

Table S65 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$(bcod)_2Cr$** structure **Cr-1T.**

M06-L			OPBE		
54(0)	857(9)	1290(1)	49(0)	851(11)	1253(2)
79(51)	858(0)	1310(0)	94(1)	855(3)	1282(0)
107(18)	863(4)	1311(1)	111(0)	856(9)	1283(1)
112(0)	863(7)	1317(0)	169(0)	861(3)	1288(2)
171(3)	896(19)	1317(2)	169(5)	871(21)	1288(0)
175(0)	897(0)	1353(11)	213(38)	874(1)	1321(15)
219(1)	934(1)	1353(9)	219(2)	909(0)	1321(12)
320(2)	938(2)	1440(10)	322(2)	916(0)	1417(0)
338(1)	942(6)	1441(0)	335(2)	941(5)	1417(3)
364(0)	947(0)	1445(48)	360(0)	943(0)	1420(39)
374(2)	948(1)	1450(7)	378(1)	944(1)	1423(3)
407(1)	954(2)	1477(1)	409(2)	950(2)	1447(0)
425(1)	985(4)	1477(1)	421(2)	975(5)	1447(1)
434(2)	985(6)	1526(16)	442(4)	975(4)	1514(9)
450(2)	1011(0)	1531(12)	451(3)	1003(0)	1520(8)
473(1)	1012(1)	3044(141)	465(1)	1004(0)	3052(62)
483(1)	1037(13)	3044(0)	472(0)	1010(8)	3053(0)
589(0)	1037(5)	3085(142)	577(1)	1011(10)	3092(58)
593(1)	1071(2)	3085(38)	581(0)	1047(1)	3092(19)
612(2)	1071(3)	3090(130)	595(1)	1048(2)	3095(60)
613(18)	1111(4)	3091(29)	597(12)	1093(1)	3095(11)
633(0)	1112(0)	3113(29)	621(3)	1095(0)	3124(12)
642(1)	1114(0)	3113(43)	624(1)	1101(0)	3124(14)
649(8)	1114(8)	3147(7)	668(2)	1102(7)	3160(1)
707(7)	1156(1)	3148(7)	701(1)	1129(1)	3163(1)
725(6)	1158(1)	3173(46)	716(2)	1132(1)	3181(4)
726(4)	1212(0)	3174(21)	736(13)	1190(0)	3183(11)
738(3)	1213(0)	3182(12)	742(27)	1190(0)	3191(10)
742(5)	1254(0)	3182(44)	753(1)	1221(0)	3191(3)
752(23)	1256(1)	3190(22)	759(3)	1223(0)	3200(7)
757(4)	1259(18)	3192(21)	761(7)	1232(9)	3202(7)
824(1)	1262(3)	3209(24)	826(2)	1234(5)	3218(6)
843(1)	1290(1)	3214(12)	844(4)	1253(2)	3220(6)

Table S66 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$(bcod)_2Cr$** structure **Cr-2T.**

M06-L			OPBE		
64(0)	860(0)	1290(2)	52(0)	852(0)	1254(3)
86(0)	862(6)	1316(0)	90(0)	853(11)	1289(0)
138(5)	865(21)	1316(0)	116(0)	863(28)	1290(2)
140(0)	867(0)	1316(3)	144(2)	864(0)	1290(0)
169(74)	900(19)	1317(0)	186(0)	876(20)	1290(1)
190(0)	901(0)	1356(19)	210(41)	877(0)	1326(26)
282(13)	941(5)	1357(0)	276(10)	916(8)	1328(0)
304(0)	948(0)	1440(9)	304(0)	923(0)	1417(10)
322(16)	951(0)	1443(0)	328(3)	948(0)	1418(41)
334(1)	952(0)	1448(64)	331(21)	949(11)	1418(0)
355(0)	953(15)	1450(0)	346(0)	952(0)	1422(0)
398(0)	961(0)	1478(2)	388(0)	958(0)	1446(2)
433(3)	985(16)	1478(0)	422(6)	976(13)	1447(0)
445(0)	985(0)	1531(44)	438(0)	976(0)	1521(26)
447(4)	1015(1)	1532(0)	442(1)	1008(1)	1524(0)
471(0)	1016(0)	3045(146)	459(0)	1009(0)	3053(65)
488(2)	1038(18)	3045(0)	474(1)	1010(18)	3053(0)
582(0)	1044(0)	3091(0)	565(0)	1016(0)	3098(0)
593(0)	1073(0)	3091(158)	578(0)	1052(0)	3098(64)
610(23)	1078(4)	3093(171)	593(17)	1056(2)	3100(75)
613(0)	1112(13)	3095(0)	597(0)	1096(0)	3100(0)
637(4)	1113(0)	3114(0)	620(4)	1098(0)	3124(0)
643(0)	1114(0)	3114(70)	624(0)	1101(8)	3124(25)
656(8)	1115(0)	3139(27)	666(4)	1103(0)	3162(3)
676(0)	1158(2)	3140(0)	670(0)	1130(2)	3162(0)
698(0)	1160(0)	3178(0)	704(0)	1133(0)	3187(0)
706(14)	1215(0)	3179(46)	712(0)	1192(0)	3187(7)
709(0)	1220(1)	3181(46)	721(4)	1198(0)	3193(0)
739(36)	1257(0)	3181(0)	728(3)	1226(0)	3193(12)
744(0)	1259(0)	3185(50)	734(45)	1227(0)	3193(0)
745(0)	1263(23)	3186(0)	740(0)	1236(15)	3194(12)
819(0)	1266(0)	3199(0)	815(0)	1238(0)	3211(0)
820(0)	1290(0)	3201(29)	817(0)	1254(0)	3211(13)

Table S67 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$(bcod)_2Cr$** structure **Cr-3P.**

M06-L			OPBE		
16(0)	858(0)	1291(5)	19(0)	852(0)	1256(6)
42(1)	859(4)	1311(5)	54(0)	852(7)	1285(2)
48(0)	866(26)	1311(0)	55(2)	861(28)	1285(0)
123(0)	866(0)	1317(0)	102(1)	862(0)	1293(0)
125(0)	899(16)	1319(12)	109(0)	875(18)	1296(10)
127(3)	901(0)	1358(17)	118(6)	878(0)	1326(28)
153(8)	922(3)	1359(0)	119(0)	898(3)	1327(0)
180(0)	929(0)	1430(3)	162(0)	905(0)	1408(7)
243(27)	948(0)	1431(0)	220(24)	945(0)	1409(0)
307(0)	949(0)	1472(9)	291(0)	946(0)	1441(10)
332(3)	952(13)	1472(0)	322(2)	951(12)	1441(0)
360(0)	955(0)	1521(0)	346(0)	954(0)	1512(39)
409(6)	992(25)	1522(55)	391(5)	980(22)	1513(0)
435(0)	993(0)	1604(23)	414(2)	982(0)	1563(22)
435(0)	1015(0)	1605(0)	414(0)	1011(0)	1565(0)
441(0)	1015(1)	3052(123)	425(0)	1011(1)	3061(52)
458(0)	1045(8)	3052(0)	438(0)	1017(13)	3061(0)
576(0)	1046(0)	3091(0)	550(0)	1018(0)	3098(0)
581(11)	1092(0)	3091(162)	552(10)	1069(0)	3098(68)
610(0)	1092(7)	3094(159)	593(0)	1070(3)	3100(71)
613(18)	1117(1)	3095(0)	596(16)	1102(1)	3100(0)
640(7)	1118(0)	3117(30)	620(3)	1103(0)	3135(0)
645(0)	1119(11)	3118(0)	625(0)	1105(9)	3135(24)
660(0)	1121(0)	3123(0)	675(0)	1107(0)	3137(6)
688(44)	1158(3)	3123(68)	695(133)	1134(2)	3138(0)
714(135)	1159(0)	3164(0)	698(26)	1135(0)	3181(8)
718(34)	1215(0)	3165(20)	701(0)	1196(0)	3181(0)
718(0)	1217(1)	3175(0)	707(59)	1198(0)	3184(0)
731(0)	1262(0)	3175(64)	718(0)	1229(0)	3185(7)
784(0)	1262(2)	3179(51)	762(0)	1230(1)	3186(0)
784(0)	1273(1)	3179(0)	762(0)	1244(4)	3186(16)
853(0)	1273(0)	3192(0)	827(0)	1245(0)	3210(0)
856(0)	1291(0)	3193(27)	832(4)	1256(0)	3210(11)

Table S68 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) forthe**$(bcod)_2Cr$** structure **Cr-4P.**

M06-L			OPBE		
41(0)	859(4)	1292(0)	18(1)	852(6)	1256(5)
45(1)	859(1)	1312(4)	36(0)	853(0)	1287(2)
53(0)	866(0)	1314(2)	60(0)	864(0)	1288(0)
80(0)	867(20)	1319(12)	92(0)	864(24)	1295(10)
126(0)	896(9)	1320(0)	119(0)	872(13)	1295(0)
138(5)	898(1)	1358(17)	131(3)	874(0)	1327(28)
149(0)	914(2)	1359(0)	141(0)	890(2)	1327(1)
220(0)	920(2)	1431(4)	215(0)	901(1)	1408(10)
232(20)	948(1)	1432(0)	222(20)	945(0)	1410(0)
315(1)	949(0)	1473(9)	299(0)	946(0)	1441(9)
322(0)	957(6)	1473(0)	318(0)	956(6)	1441(0)
376(8)	959(3)	1519(1)	368(6)	958(2)	1509(31)
394(1)	990(21)	1520(48)	381(0)	978(16)	1509(1)
438(0)	993(6)	1592(4)	421(2)	982(9)	1549(7)
441(0)	1018(0)	1597(27)	422(1)	1013(0)	1555(24)
442(0)	1019(1)	3051(124)	424(0)	1014(1)	3060(54)
443(1)	1045(2)	3052(3)	427(1)	1017(1)	3060(1)
576(1)	1047(3)	3091(2)	548(1)	1019(9)	3099(1)
583(9)	1088(8)	3091(163)	553(9)	1064(3)	3099(68)
602(7)	1092(0)	3094(145)	588(8)	1071(1)	3101(66)
605(7)	1116(11)	3095(15)	593(5)	1099(0)	3102(5)
638(1)	1117(0)	3120(2)	620(0)	1101(1)	3130(1)
642(3)	1118(2)	3121(35)	624(2)	1102(9)	3135(1)
662(1)	1120(2)	3122(3)	667(86)	1105(1)	3135(29)
688(56)	1159(0)	3122(58)	672(0)	1132(0)	3135(0)
693(57)	1159(3)	3174(2)	691(30)	1133(2)	3181(0)
715(26)	1219(0)	3174(0)	707(16)	1199(0)	3181(11)
719(51)	1221(1)	3176(69)	707(46)	1200(0)	3187(3)
724(21)	1262(1)	3176(4)	712(34)	1230(0)	3188(11)
782(0)	1263(0)	3184(41)	760(0)	1230(0)	3194(0)
786(0)	1275(0)	3184(8)	763(0)	1245(1)	3199(3)
840(2)	1275(0)	3201(12)	809(3)	1245(4)	3220(10)
853(2)	1292(4)	3203(16)	827(3)	1255(0)	3225(1)

Table S69 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$(bcod)_2Cr$** structure **Cr-5P.**

M06-L			OPBE		
37(0)	861(3)	1298(0)	40(0)	852(6)	1259(1)
53(0)	863(0)	1316(4)	49(0)	856(1)	1290(6)
70(0)	872(11)	1318(3)	73(0)	858(8)	1291(3)
144(1)	882(10)	1322(6)	134(0)	869(14)	1291(0)
149(0)	896(8)	1323(0)	141(0)	872(10)	1297(2)
159(4)	899(6)	1358(15)	168(4)	882(7)	1323(18)
175(3)	917(2)	1361(3)	178(3)	894(2)	1328(11)
239(7)	923(0)	1426(1)	239(6)	901(0)	1400(2)
276(4)	935(3)	1437(2)	269(2)	924(1)	1414(4)
322(5)	950(0)	1473(5)	309(5)	946(0)	1442(6)
328(0)	963(5)	1491(5)	316(0)	958(9)	1443(8)
377(1)	967(9)	1501(21)	365(0)	961(6)	1487(17)
414(23)	989(13)	1522(25)	402(21)	976(13)	1510(14)
430(1)	999(2)	1560(17)	415(3)	987(1)	1514(16)
450(5)	1023(1)	1630(21)	435(5)	1010(7)	1599(18)
458(1)	1033(0)	3041(38)	451(0)	1016(0)	3041(26)
474(2)	1046(4)	3053(64)	456(3)	1018(6)	3062(27)
580(0)	1051(3)	3084(84)	556(1)	1024(0)	3094(38)
584(9)	1089(5)	3086(33)	560(7)	1064(4)	3095(10)
598(18)	1091(4)	3098(78)	583(15)	1072(1)	3101(48)
600(6)	1113(2)	3098(85)	585(6)	1095(1)	3106(31)
635(1)	1118(1)	3101(63)	612(0)	1100(1)	3108(30)
643(2)	1118(8)	3121(9)	623(3)	1103(7)	3129(3)
670(4)	1124(7)	3125(31)	676(55)	1108(7)	3137(10)
697(58)	1148(0)	3131(16)	687(0)	1120(0)	3142(4)
712(24)	1161(2)	3156(39)	703(34)	1134(1)	3162(10)
726(46)	1224(3)	3162(25)	711(53)	1202(0)	3168(11)
734(47)	1225(5)	3172(5)	732(27)	1203(4)	3178(8)
775(11)	1259(1)	3174(25)	753(0)	1228(2)	3187(3)
780(0)	1264(1)	3186(27)	763(15)	1232(1)	3189(1)
785(9)	1271(0)	3190(21)	765(15)	1239(1)	3192(5)
832(0)	1275(1)	3196(9)	801(0)	1244(3)	3205(22)
847(2)	1293(2)	3203(63)	840(3)	1256(2)	3211(4)

Table S70 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the**$(bcod)_2Cr$** structure **Cr-6P.**

M06-L			OPBE		
35(0)	856(0)	1291(1)	39(0)	849(9)	1254(2)
64(8)	856(7)	1312(2)	53(11)	849(0)	1287(1)
71(0)	869(13)	1313(5)	74(0)	861(22)	1287(1)
71(5)	870(6)	1318(5)	83(4)	861(9)	1291(1)
130(0)	895(17)	1318(3)	130(0)	874(17)	1292(3)
177(0)	896(0)	1356(11)	171(0)	875(0)	1324(17)
210(4)	907(0)	1356(8)	204(7)	887(0)	1324(14)
242(0)	907(9)	1421(1)	247(0)	888(5)	1400(1)
258(15)	940(1)	1421(1)	256(6)	934(3)	1400(1)
325(3)	941(0)	1470(21)	319(3)	935(0)	1438(24)
334(1)	961(6)	1471(0)	329(1)	959(5)	1438(0)
371(0)	963(1)	1531(37)	357(0)	960(3)	1492(29)
390(5)	981(4)	1534(13)	383(3)	970(7)	1495(11)
420(1)	981(10)	1549(32)	408(2)	970(5)	1529(32)
420(1)	1021(1)	1555(27)	408(2)	1012(1)	1535(16)
467(1)	1021(0)	3050(142)	459(1)	1013(6)	3058(63)
468(3)	1043(1)	3050(1)	459(2)	1016(3)	3058(1)
578(46)	1044(8)	3095(106)	559(6)	1016(6)	3101(54)
582(9)	1078(3)	3095(53)	562(4)	1052(2)	3101(14)
584(38)	1079(1)	3099(131)	566(70)	1052(2)	3107(50)
595(7)	1105(13)	3100(27)	581(4)	1093(11)	3107(19)
632(6)	1106(5)	3122(32)	616(2)	1094(3)	3134(10)
638(0)	1117(2)	3122(28)	620(0)	1097(2)	3134(10)
643(21)	1118(0)	3134(14)	634(42)	1099(0)	3152(3)
653(5)	1162(1)	3134(7)	646(7)	1134(1)	3152(1)
671(66)	1165(1)	3162(0)	653(51)	1138(1)	3172(5)
676(23)	1220(2)	3162(47)	666(21)	1196(0)	3173(0)
702(11)	1220(1)	3166(20)	700(7)	1196(1)	3175(10)
709(16)	1257(2)	3168(14)	706(12)	1223(0)	3179(2)
772(2)	1257(0)	3193(3)	743(4)	1223(1)	3199(4)
772(0)	1271(4)	3193(38)	745(0)	1242(6)	3201(9)
817(10)	1271(0)	3196(6)	794(9)	1243(2)	3208(9)
825(0)	1291(2)	3197(17)	806(0)	1254(2)	3209(0)

Table S71 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the**$(bcod)_2Cr$** structure **Cr-7T.**

M06-L			OPBE		
49(0)	854(7)	1290(1)	54(0)	848(2)	1252(3)
79(0)	858(4)	1301(1)	83(0)	852(7)	1274(1)
92(0)	864(0)	1312(8)	94(0)	856(2)	1284(9)
161(0)	885(16)	1314(0)	157(0)	859(15)	1287(1)
173(1)	891(4)	1319(3)	181(0)	866(2)	1288(5)
219(3)	902(4)	1347(9)	214(3)	886(4)	1315(13)
277(7)	923(4)	1357(7)	268(5)	901(2)	1322(11)
304(8)	934(5)	1417(24)	298(2)	907(2)	1394(10)
314(12)	935(1)	1421(3)	315(14)	919(2)	1398(4)
350(1)	936(3)	1432(7)	344(0)	931(4)	1406(15)
377(5)	945(2)	1472(2)	376(2)	940(2)	1441(2)
397(6)	961(9)	1500(7)	392(9)	953(10)	1486(4)
434(0)	982(6)	1534(14)	437(1)	970(7)	1518(8)
451(3)	1001(2)	1582(9)	441(2)	991(1)	1543(15)
469(5)	1007(1)	1634(10)	462(5)	1000(4)	1602(6)
488(1)	1018(1)	2841(20)	473(3)	1002(5)	2743(10)
505(5)	1032(12)	3044(71)	483(3)	1010(4)	3053(31)
582(3)	1065(0)	3077(14)	560(3)	1033(2)	3077(8)
592(0)	1068(6)	3081(93)	574(0)	1044(3)	3087(43)
596(18)	1087(12)	3088(66)	579(20)	1068(5)	3093(35)
616(5)	1104(4)	3089(90)	602(1)	1085(1)	3099(30)
639(3)	1106(1)	3093(51)	624(3)	1089(3)	3101(14)
648(2)	1112(1)	3113(37)	627(2)	1095(1)	3125(13)
676(6)	1121(11)	3149(3)	684(4)	1103(1)	3161(0)
714(3)	1127(0)	3152(8)	709(3)	1104(12)	3165(5)
731(3)	1156(1)	3155(25)	717(56)	1130(1)	3165(4)
732(48)	1206(1)	3166(36)	737(13)	1182(1)	3173(9)
754(12)	1225(2)	3168(38)	753(10)	1204(1)	3177(5)
769(7)	1246(14)	3179(16)	763(3)	1217(5)	3181(7)
779(14)	1251(0)	3179(24)	774(14)	1222(3)	3185(12)
796(6)	1256(0)	3180(44)	789(4)	1226(1)	3190(11)
833(1)	1277(0)	3195(19)	828(2)	1247(0)	3202(6)
852(1)	1287(1)	3207(58)	846(7)	1251(1)	3207(18)

Table S72 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the**bcod)$_2$Cr** structure **Cr-8S.**

M06-L			OPBE		
51(0)	848(4)	1293(4)	58(0)	838(4)	1258(1)
118(0)	853(0)	1294(1)	120(0)	840(3)	1267(1)
141(0)	867(3)	1319(5)	149(0)	860(5)	1291(4)
205(1)	870(6)	1320(8)	201(2)	864(10)	1295(11)
214(2)	876(2)	1323(11)	224(2)	871(1)	1296(7)
241(8)	890(6)	1326(3)	240(13)	877(7)	1299(3)
316(20)	897(10)	1360(5)	321(17)	890(7)	1327(9)
339(14)	917(3)	1414(6)	347(11)	904(5)	1393(2)
372(1)	929(2)	1419(8)	372(2)	923(2)	1402(7)
380(2)	946(0)	1442(5)	383(3)	940(0)	1417(8)
407(1)	947(8)	1471(6)	402(2)	943(8)	1441(4)
421(3)	965(1)	1477(3)	411(8)	962(3)	1446(4)
436(7)	977(6)	1510(6)	439(8)	968(3)	1488(12)
459(4)	983(4)	1527(10)	450(5)	972(2)	1495(3)
477(4)	1004(0)	1530(18)	477(9)	995(0)	1509(4)
491(1)	1022(0)	3044(57)	485(5)	1004(3)	3050(25)
519(11)	1029(4)	3048(25)	513(18)	1015(0)	3059(14)
570(2)	1046(3)	3060(170)	560(3)	1017(4)	3073(74)
595(2)	1059(3)	3078(87)	576(2)	1042(2)	3083(42)
606(4)	1078(2)	3081(119)	588(2)	1052(2)	3086(55)
639(1)	1083(6)	3088(52)	624(2)	1076(5)	3092(19)
648(2)	1112(2)	3112(51)	632(3)	1097(1)	3119(20)
659(13)	1114(0)	3115(34)	653(5)	1098(0)	3124(12)
667(12)	1128(12)	3120(53)	664(14)	1117(5)	3133(11)
737(3)	1140(6)	3121(21)	731(3)	1120(3)	3137(19)
748(8)	1152(2)	3124(26)	744(12)	1125(2)	3138(13)
758(2)	1162(14)	3139(44)	749(3)	1138(21)	3154(11)
771(2)	1211(4)	3154(55)	774(9)	1190(4)	3166(23)
773(7)	1226(0)	3158(50)	779(6)	1203(0)	3168(25)
781(7)	1238(1)	3161(30)	788(5)	1210(1)	3169(10)
808(2)	1263(0)	3183(33)	809(2)	1234(0)	3194(9)
819(1)	1273(3)	3198(11)	822(1)	1245(6)	3211(3)
827(4)	1283(1)	3228(10)	831(1)	1249(3)	3233(4)

Table S73 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) forthe**$(bcod)_2Cr$** structure **Cr-9S.**

M06-L			OPBE		
64(0)	860(10)	1292(0)	78(0)	853(1)	1255(0)
106(0)	862(0)	1312(3)	119(0)	854(15)	1285(1)
165(0)	862(1)	1313(0)	153(1)	855(1)	1286(0)
211(1)	863(4)	1319(5)	207(0)	858(9)	1291(4)
212(0)	890(4)	1320(0)	217(1)	866(4)	1293(0)
225(1)	898(1)	1354(2)	242(1)	887(0)	1320(3)
325(5)	935(0)	1356(10)	331(1)	919(0)	1323(18)
350(3)	942(3)	1441(1)	338(1)	932(1)	1414(5)
379(33)	947(6)	1442(2)	380(3)	940(2)	1414(0)
384(3)	950(5)	1454(1)	388(1)	942(3)	1426(0)
398(4)	963(1)	1456(53)	399(22)	945(6)	1427(37)
422(1)	969(0)	1479(4)	419(3)	957(3)	1449(5)
438(2)	979(0)	1480(1)	426(4)	968(0)	1450(1)
447(0)	981(13)	1521(11)	444(1)	970(8)	1505(4)
452(8)	1013(1)	1523(11)	452(7)	1003(3)	1506(8)
460(3)	1015(0)	3040(114)	474(0)	1008(2)	3048(55)
485(0)	1036(1)	3040(6)	476(11)	1008(0)	3048(3)
585(3)	1038(16)	3069(151)	562(4)	1013(15)	3079(74)
594(0)	1067(6)	3069(90)	577(0)	1042(4)	3080(37)
614(2)	1070(0)	3080(117)	592(0)	1046(1)	3089(51)
616(0)	1108(6)	3081(65)	592(0)	1090(2)	3089(30)
631(4)	1109(1)	3109(7)	623(0)	1091(1)	3119(3)
638(0)	1117(0)	3109(65)	626(2)	1101(0)	3119(24)
650(8)	1119(10)	3143(8)	638(5)	1106(6)	3151(2)
692(0)	1152(1)	3143(4)	695(0)	1125(1)	3152(2)
728(1)	1154(0)	3146(2)	723(4)	1127(0)	3156(2)
748(1)	1215(0)	3148(56)	739(2)	1190(0)	3159(10)
763(2)	1216(0)	3169(8)	746(3)	1191(0)	3179(1)
769(4)	1254(2)	3172(25)	761(3)	1222(2)	3185(6)
810(8)	1254(0)	3186(102)	813(6)	1223(1)	3194(0)
811(1)	1262(1)	3186(41)	827(1)	1234(2)	3195(1)
853(0)	1263(11)	3187(1)	843(0)	1235(8)	3201(41)
855(8)	1292(2)	3188(21)	848(9)	1255(3)	3201(17)

Table S74 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the**$(bcod)_2Mn$** structure **Mn-1D.**

M06-L			OPBE		
51(0)	862(0)	1294(1)	42(0)	851(0)	1257(2)
91(0)	865(6)	1321(7)	88(0)	853(14)	1295(3)
160(4)	872(18)	1322(0)	167(1)	866(0)	1296(0)
218(0)	873(0)	1325(0)	221(0)	867(26)	1297(0)
221(0)	892(0)	1326(0)	223(0)	868(6)	1298(0)
261(56)	894(5)	1361(10)	270(20)	871(0)	1328(16)
274(15)	926(4)	1365(0)	300(0)	899(3)	1334(0)
289(0)	936(0)	1442(5)	308(50)	912(0)	1413(5)
343(4)	949(0)	1444(0)	347(11)	943(0)	1416(0)
358(0)	951(0)	1462(35)	364(0)	949(0)	1426(26)
387(0)	962(6)	1464(0)	395(0)	959(8)	1430(0)
406(0)	968(0)	1484(0)	404(0)	962(0)	1450(0)
421(3)	980(0)	1485(7)	407(6)	970(0)	1450(1)
436(0)	983(11)	1519(0)	436(0)	971(9)	1498(9)
445(1)	1023(1)	1519(21)	448(3)	1010(10)	1499(0)
471(0)	1024(0)	3043(135)	460(0)	1016(0)	3050(65)
491(4)	1040(8)	3043(0)	478(3)	1017(0)	3050(0)
590(0)	1047(0)	3084(0)	572(0)	1017(0)	3094(0)
593(0)	1073(0)	3084(172)	575(0)	1054(0)	3095(73)
611(14)	1079(1)	3087(208)	590(10)	1059(1)	3096(94)
613(0)	1112(0)	3088(0)	593(0)	1094(0)	3097(0)
647(6)	1115(0)	3111(0)	625(0)	1097(0)	3120(0)
649(0)	1117(15)	3111(70)	629(4)	1103(0)	3120(26)
697(15)	1118(0)	3133(43)	703(12)	1104(8)	3157(9)
709(0)	1155(1)	3134(0)	704(0)	1126(1)	3157(0)
724(0)	1158(0)	3167(0)	714(0)	1130(0)	3179(14)
732(9)	1226(0)	3167(73)	726(3)	1202(0)	3179(0)
737(0)	1230(0)	3171(0)	741(0)	1208(0)	3183(0)
758(0)	1260(0)	3171(63)	753(36)	1232(0)	3185(19)
763(28)	1261(0)	3181(30)	754(0)	1233(1)	3198(0)
765(0)	1272(9)	3181(0)	758(1)	1243(12)	3198(8)
836(0)	1274(0)	3201(0)	838(0)	1245(0)	3216(0)
838(0)	1294(0)	3202(37)	840(0)	1257(0)	3217(13)

Table S75 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the**$(bcod)_2Mn$** structure **Mn-2D.**

M06-L			OPBE		
34(0)	859(5)	1292(1)	49(0)	851(0)	1255(2)
79(0)	863(1)	1315(6)	91(0)	853(2)	1288(4)
167(1)	865(10)	1317(0)	150(1)	856(4)	1290(0)
203(1)	866(2)	1318(1)	205(0)	860(3)	1291(1)
224(0)	877(7)	1319(0)	226(1)	861(13)	1291(0)
242(7)	885(1)	1355(8)	231(5)	866(2)	1322(6)
315(8)	919(1)	1356(3)	317(7)	899(0)	1322(14)
330(14)	921(3)	1430(3)	373(6)	907(4)	1404(7)
357(11)	946(0)	1432(1)	374(10)	943(1)	1405(0)
378(0)	949(2)	1447(8)	386(1)	944(1)	1425(2)
383(3)	955(2)	1450(34)	393(0)	951(1)	1427(24)
416(2)	963(2)	1475(1)	430(7)	957(3)	1447(2)
427(3)	977(4)	1475(1)	437(8)	965(3)	1449(2)
444(1)	983(13)	1510(8)	440(0)	971(11)	1492(3)
455(2)	1017(0)	1520(1)	460(0)	1008(3)	1502(0)
467(0)	1018(1)	3041(147)	462(6)	1008(6)	3048(68)
481(2)	1035(5)	3041(0)	472(1)	1011(0)	3048(0)
589(0)	1037(3)	3086(37)	573(1)	1012(2)	3093(21)
590(2)	1073(0)	3086(126)	577(0)	1048(0)	3093(50)
606(12)	1075(2)	3088(187)	589(0)	1049(0)	3095(87)
607(1)	1106(3)	3089(4)	590(8)	1085(2)	3096(2)
623(4)	1107(0)	3109(16)	610(4)	1093(0)	3119(8)
639(1)	1107(12)	3109(57)	628(2)	1095(5)	3120(19)
667(1)	1111(0)	3162(1)	685(2)	1095(0)	3174(1)
682(5)	1154(1)	3164(5)	691(3)	1126(1)	3180(0)
721(3)	1155(0)	3177(32)	712(3)	1129(0)	3184(9)
734(9)	1218(0)	3178(44)	730(12)	1195(0)	3187(7)
753(1)	1221(0)	3189(30)	747(11)	1198(0)	3199(8)
754(6)	1255(0)	3189(19)	766(3)	1224(0)	3203(13)
765(0)	1257(0)	3190(39)	786(1)	1226(0)	3206(7)
772(2)	1265(5)	3192(9)	792(2)	1236(3)	3210(3)
837(1)	1266(5)	3211(31)	830(6)	1238(7)	3225(3)
852(1)	1291(0)	3211(7)	840(3)	1254(1)	3230(8)

Table S76 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the**$(bcod)_2Mn$** structure **Mn-3Q.**

M06-L			OPBE		
45(1)	856(7)	1294(1)	45(1)	846(4)	1258(2)
67(0)	858(2)	1295(1)	65(0)	848(10)	1268(1)
87(1)	864(4)	1314(1)	102(1)	851(3)	1283(1)
130(5)	879(9)	1314(3)	115(5)	864(6)	1287(1)
140(3)	890(3)	1320(4)	136(1)	865(10)	1295(4)
162(1)	896(7)	1342(11)	156(1)	878(7)	1311(17)
195(4)	912(1)	1361(7)	187(3)	892(1)	1329(12)
267(4)	926(3)	1401(17)	257(1)	916(2)	1376(8)
271(2)	939(2)	1414(11)	266(4)	926(2)	1391(14)
344(1)	947(8)	1425(3)	337(1)	943(6)	1404(6)
383(0)	952(0)	1471(6)	371(0)	947(1)	1439(7)
386(5)	956(1)	1471(3)	381(5)	955(1)	1440(3)
414(15)	983(4)	1507(7)	405(11)	974(3)	1496(5)
442(1)	994(16)	1586(14)	426(1)	981(14)	1562(8)
445(5)	1009(0)	1609(9)	431(3)	1000(3)	1566(12)
448(0)	1020(0)	3043(79)	438(2)	1006(6)	3052(37)
494(4)	1027(9)	3052(61)	484(4)	1015(0)	3060(26)
583(3)	1044(3)	3086(85)	554(3)	1016(5)	3092(38)
591(4)	1064(4)	3093(80)	577(3)	1045(2)	3100(33)
605(8)	1092(7)	3094(103)	590(11)	1069(3)	3101(38)
612(6)	1095(2)	3096(52)	598(3)	1084(2)	3103(30)
632(2)	1115(0)	3112(36)	616(2)	1097(0)	3124(14)
640(3)	1118(7)	3123(31)	622(2)	1102(0)	3135(10)
657(1)	1120(1)	3134(17)	671(3)	1104(7)	3147(4)
691(21)	1159(1)	3151(6)	678(39)	1133(1)	3165(8)
699(21)	1160(1)	3160(12)	693(19)	1134(1)	3170(0)
726(63)	1205(2)	3163(43)	710(82)	1180(1)	3172(6)
731(28)	1220(0)	3176(16)	724(4)	1200(0)	3187(4)
739(2)	1239(4)	3178(22)	734(3)	1210(2)	3188(13)
760(11)	1259(9)	3183(33)	758(5)	1231(0)	3193(4)
789(0)	1265(1)	3186(18)	771(0)	1235(6)	3196(2)
826(1)	1275(2)	3191(22)	823(2)	1245(4)	3198(6)
849(6)	1285(2)	3204(10)	840(9)	1250(1)	3222(3)

Table S77 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the**$(bcod)_2Mn$** structure **Mn-4Q.**

M06-L			OPBE		
56(0)	851(5)	1290(1)	52(2)	844(5)	1257(2)
68(0)	859(1)	1295(2)	72(0)	849(14)	1270(1)
93(0)	861(7)	1311(1)	96(13)	850(3)	1284(1)
117(3)	872(6)	1317(2)	105(4)	862(11)	1287(1)
139(6)	895(6)	1324(1)	138(2)	874(11)	1293(0)
151(0)	897(6)	1336(11)	159(2)	877(2)	1312(17)
224(3)	919(5)	1360(11)	191(1)	899(2)	1324(18)
265(2)	922(1)	1390(19)	245(1)	911(2)	1381(4)
280(1)	940(2)	1407(5)	266(3)	925(1)	1406(27)
332(1)	942(5)	1436(1)	336(1)	939(1)	1407(1)
373(0)	947(1)	1469(5)	359(3)	942(6)	1438(12)
397(3)	964(1)	1471(7)	386(3)	956(2)	1440(4)
424(6)	982(6)	1538(9)	409(3)	971(10)	1486(22)
434(1)	987(11)	1550(23)	417(1)	973(3)	1527(5)
447(14)	1006(1)	1592(18)	430(6)	1002(4)	1555(16)
463(0)	1021(0)	3041(82)	458(0)	1007(5)	3052(37)
498(2)	1024(9)	3053(65)	478(2)	1012(1)	3059(29)
583(3)	1045(4)	3080(86)	556(6)	1015(7)	3092(38)
599(1)	1061(6)	3095(85)	578(3)	1045(4)	3102(41)
603(5)	1084(2)	3097(74)	583(7)	1053(1)	3102(27)
616(14)	1091(1)	3101(70)	592(16)	1082(2)	3105(31)
633(3)	1112(6)	3110(36)	614(2)	1095(4)	3125(13)
642(1)	1114(0)	3123(29)	620(1)	1097(0)	3131(10)
669(19)	1122(1)	3131(18)	640(9)	1104(2)	3148(5)
678(46)	1159(1)	3148(4)	668(46)	1134(1)	3160(1)
700(23)	1163(0)	3151(14)	692(17)	1137(0)	3164(10)
707(5)	1199(3)	3154(55)	704(14)	1182(1)	3181(3)
720(22)	1223(0)	3171(27)	712(16)	1197(0)	3183(7)
735(2)	1235(6)	3182(27)	726(4)	1211(2)	3189(8)
775(4)	1255(7)	3182(26)	751(1)	1226(1)	3194(5)
782(1)	1262(0)	3189(17)	766(1)	1235(6)	3203(4)
820(2)	1270(3)	3202(6)	797(3)	1240(5)	3221(1)
827(5)	1279(3)	3225(6)	825(3)	1251(2)	3241(3)

Table S78 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the**$(bcod)_2Mn$** structure **Mn-5X.**

M06-L			OPBE		
40(0)	853(4)	1291(0)	26(4)	847(6)	1253(0)
51(3)	854(0)	1311(5)	28(0)	847(2)	1289(3)
62(0)	877(18)	1311(9)	62(0)	868(20)	1289(1)
77(2)	877(3)	1320(6)	74(1)	869(12)	1294(0)
111(1)	894(15)	1320(1)	92(0)	875(14)	1294(11)
142(0)	895(0)	1357(14)	136(0)	875(5)	1326(25)
179(1)	904(7)	1359(0)	167(1)	886(7)	1327(0)
190(9)	907(5)	1414(0)	186(8)	890(1)	1396(2)
265(33)	948(8)	1415(2)	252(35)	942(9)	1397(1)
309(0)	949(0)	1470(10)	291(0)	943(0)	1438(13)
313(4)	963(18)	1470(1)	298(2)	960(17)	1438(1)
369(1)	965(2)	1541(0)	363(1)	961(1)	1520(8)
391(15)	987(24)	1547(48)	382(14)	977(27)	1523(19)
416(0)	987(0)	1573(0)	402(0)	977(0)	1530(21)
422(2)	1024(0)	1574(30)	409(2)	1013(8)	1530(21)
458(0)	1025(0)	3052(131)	445(0)	1014(1)	3062(57)
458(4)	1041(5)	3052(0)	446(2)	1018(2)	3062(0)
576(1)	1043(2)	3095(18)	550(3)	1018(0)	3103(18)
580(10)	1083(0)	3095(142)	552(11)	1059(0)	3103(51)
589(63)	1084(6)	3099(132)	580(40)	1062(4)	3107(50)
600(0)	1106(4)	3100(13)	587(0)	1093(4)	3107(14)
635(18)	1107(3)	3111(0)	620(7)	1094(2)	3133(10)
640(9)	1119(0)	3111(39)	622(3)	1099(0)	3133(0)
650(39)	1120(0)	3123(0)	635(50)	1100(1)	3136(0)
657(5)	1164(1)	3123(64)	643(1)	1136(2)	3136(20)
697(82)	1166(0)	3155(9)	678(136)	1138(0)	3164(5)
709(1)	1223(0)	3155(7)	689(1)	1200(0)	3164(5)
712(89)	1225(0)	3160(45)	698(41)	1202(0)	3172(4)
717(58)	1261(0)	3161(20)	699(66)	1228(0)	3172(3)
783(0)	1261(1)	3187(25)	759(0)	1228(0)	3196(4)
783(1)	1270(1)	3187(14)	760(4)	1242(0)	3196(7)
851(6)	1270(0)	3191(10)	817(9)	1242(4)	3207(10)
851(5)	1291(4)	3192(23)	819(3)	1253(5)	3208(2)

Table S79 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the**$(bcod)_2Mn$** structure **Mn-6Q.**

M06-L			OPBE		
34(0)	851(7)	1296(0)	40(0)	846(6)	1260(0)
66(1)	860(8)	1302(1)	65(0)	850(15)	1277(1)
77(0)	863(0)	1312(10)	87(0)	853(8)	1286(8)
139(0)	873(11)	1315(0)	136(0)	854(0)	1286(1)
170(1)	896(8)	1317(1)	163(1)	875(9)	1287(3)
186(14)	903(6)	1348(11)	189(9)	888(7)	1317(16)
213(3)	914(1)	1356(8)	207(2)	897(0)	1322(13)
242(9)	931(3)	1414(3)	247(6)	913(4)	1391(5)
283(2)	935(2)	1418(7)	277(3)	924(0)	1398(2)
347(1)	941(1)	1434(29)	338(0)	935(1)	1412(26)
377(6)	947(8)	1472(3)	370(6)	943(7)	1441(4)
387(8)	961(10)	1481(3)	382(5)	954(10)	1446(10)
404(5)	983(6)	1485(8)	400(4)	973(5)	1466(3)
437(5)	996(5)	1560(10)	431(6)	984(3)	1537(8)
467(2)	1011(0)	1636(16)	454(2)	1003(3)	1604(11)
469(1)	1028(2)	3027(29)	456(1)	1009(9)	3029(21)
485(2)	1033(9)	3048(73)	473(2)	1015(5)	3057(31)
584(2)	1049(2)	3085(45)	562(3)	1022(0)	3093(14)
587(3)	1067(4)	3090(43)	570(4)	1044(2)	3096(36)
602(17)	1086(18)	3092(99)	585(18)	1070(5)	3099(44)
605(2)	1102(3)	3094(85)	588(1)	1090(2)	3099(26)
631(1)	1109(1)	3099(77)	614(1)	1094(1)	3104(32)
635(5)	1117(1)	3117(34)	618(5)	1100(1)	3129(12)
655(2)	1120(13)	3141(8)	664(3)	1105(16)	3153(1)
704(11)	1143(0)	3142(11)	696(4)	1118(0)	3156(2)
714(27)	1161(1)	3157(44)	708(57)	1135(1)	3167(13)
727(33)	1212(1)	3169(26)	714(29)	1189(0)	3178(8)
734(5)	1222(2)	3173(9)	729(1)	1201(2)	3180(7)
775(36)	1247(3)	3178(23)	762(2)	1216(2)	3181(2)
780(2)	1260(1)	3178(30)	769(30)	1229(1)	3183(6)
801(17)	1261(10)	3187(21)	796(12)	1234(7)	3192(6)
824(0)	1271(0)	3206(18)	817(0)	1240(1)	3207(22)
846(2)	1288(2)	3206(60)	840(2)	1253(2)	3215(3)

Table S80 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) forthe**$(bcod)_2$Mn** structure **Mn-7X.**

M06-L			OPBE		
31(1)	852(4)	1292(2)	14(0)	844(2)	1254(2)
51(1)	857(2)	1309(7)	38(4)	850(5)	1284(5)
66(0)	875(10)	1315(4)	51(1)	867(22)	1290(5)
80(2)	879(10)	1320(3)	70(1)	869(8)	1292(1)
93(1)	890(7)	1322(4)	73(1)	872(7)	1296(4)
142(1)	895(8)	1357(11)	123(2)	875(12)	1325(11)
167(1)	896(7)	1360(6)	156(3)	884(4)	1327(16)
210(2)	911(4)	1406(1)	206(1)	887(2)	1382(1)
263(29)	947(2)	1427(1)	251(27)	940(9)	1410(2)
306(2)	948(7)	1469(6)	290(5)	941(1)	1437(7)
319(3)	961(8)	1472(5)	306(2)	955(6)	1440(5)
366(10)	968(11)	1535(25)	353(7)	965(11)	1508(19)
395(14)	986(20)	1553(22)	386(18)	975(14)	1516(22)
416(1)	988(7)	1559(21)	403(1)	975(14)	1536(17)
419(1)	1025(1)	1582(16)	407(2)	1010(5)	1551(14)
459(2)	1025(0)	3050(69)	443(3)	1016(2)	3060(30)
460(5)	1040(3)	3054(61)	455(0)	1017(3)	3063(27)
576(6)	1045(2)	3090(80)	549(9)	1018(1)	3096(36)
581(8)	1082(4)	3094(82)	556(13)	1054(4)	3099(36)
591(29)	1085(3)	3099(76)	575(22)	1058(2)	3108(32)
601(28)	1104(3)	3102(64)	593(16)	1089(4)	3111(29)
634(18)	1111(3)	3115(15)	618(11)	1096(1)	3122(5)
636(14)	1118(0)	3120(16)	624(4)	1099(1)	3131(4)
645(4)	1123(1)	3121(33)	629(10)	1103(1)	3133(12)
657(41)	1163(2)	3124(29)	652(57)	1135(2)	3137(9)
685(70)	1166(1)	3140(32)	671(122)	1139(1)	3138(9)
696(62)	1224(0)	3150(18)	679(53)	1199(0)	3171(4)
710(61)	1224(0)	3165(8)	695(29)	1201(0)	3185(1)
741(38)	1259(1)	3179(20)	736(36)	1228(0)	3185(7)
780(1)	1262(0)	3182(31)	753(1)	1228(0)	3187(5)
786(1)	1270(1)	3182(18)	765(2)	1242(2)	3198(3)
839(3)	1271(1)	3189(10)	800(3)	1242(3)	3199(9)
850(7)	1291(1)	3196(16)	836(11)	1253(2)	3209(3)

Table S81 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) forthe**$(bcod)_2$Mn** structure **Mn-8X.**

M06-L			OPBE		
10(0)	858(3)	1292(2)	14(0)	844(2)	1254(2)
44(2)	869(1)	1308(6)	38(4)	850(5)	1284(5)
61(1)	877(12)	1317(2)	51(1)	867(22)	1290(5)
75(1)	879(10)	1320(3)	70(1)	869(8)	1292(1)
77(2)	894(14)	1321(7)	73(1)	872(7)	1296(4)
135(3)	895(2)	1358(6)	123(2)	875(12)	1325(11)
168(3)	901(7)	1359(11)	156(3)	884(4)	1327(16)
212(0)	905(3)	1405(1)	206(1)	887(2)	1382(1)
260(28)	945(0)	1431(1)	251(27)	940(9)	1410(2)
310(4)	947(10)	1471(6)	290(5)	941(1)	1437(7)
317(2)	961(7)	1472(5)	306(2)	955(6)	1440(5)
362(6)	967(12)	1529(38)	353(7)	965(11)	1508(19)
393(18)	986(17)	1554(18)	386(18)	975(14)	1516(22)
419(0)	987(9)	1556(24)	403(1)	975(14)	1536(17)
424(2)	1023(0)	1597(12)	407(2)	1010(5)	1551(14)
458(4)	1024(1)	3050(68)	443(3)	1016(2)	3060(30)
463(2)	1040(4)	3054(61)	455(0)	1017(3)	3063(27)
576(12)	1045(1)	3088(82)	549(9)	1018(1)	3096(36)
582(22)	1081(5)	3092(83)	556(13)	1054(4)	3099(36)
587(18)	1082(1)	3099(77)	575(22)	1058(2)	3108(32)
604(23)	1105(4)	3103(64)	593(16)	1089(4)	3111(29)
618(16)	1111(3)	3106(18)	618(11)	1096(1)	3122(5)
636(18)	1117(1)	3120(34)	624(4)	1099(1)	3131(4)
644(2)	1123(0)	3121(16)	629(10)	1103(1)	3133(12)
662(43)	1163(3)	3124(28)	652(57)	1135(2)	3137(9)
682(77)	1166(1)	3139(34)	671(122)	1139(1)	3138(9)
708(83)	1223(0)	3159(15)	679(53)	1199(0)	3171(4)
719(43)	1224(0)	3165(6)	695(29)	1201(0)	3185(1)
746(40)	1259(1)	3177(28)	736(36)	1228(0)	3185(7)
779(1)	1262(1)	3182(25)	753(1)	1228(0)	3187(5)
787(0)	1271(1)	3188(17)	765(2)	1242(2)	3198(3)
843(2)	1271(1)	3190(9)	800(3)	1242(3)	3199(9)
849(4)	1290(1)	3200(17)	836(11)	1253(2)	3209(3)

Table S82 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) forthe**$(bcod)_2$Mn** structure **Mn-9X.**

M06-L			OPBE		
33(0)	858(3)	1297(1)	14(0)	852(16)	1261(1)
41(0)	878(6)	1309(3)	27(1)	864(16)	1280(3)
49(0)	880(4)	1318(4)	39(0)	871(10)	1293(1)
73(2)	881(13)	1322(5)	54(1)	876(13)	1296(3)
104(1)	895(7)	1339(2)	96(1)	878(2)	1309(4)
144(0)	900(11)	1354(7)	126(0)	883(14)	1320(9)
164(6)	907(5)	1360(11)	153(3)	899(6)	1329(18)
215(1)	919(4)	1397(2)	215(1)	900(5)	1367(2)
254(17)	940(3)	1433(1)	239(17)	934(5)	1413(2)
311(6)	947(2)	1473(6)	288(7)	943(0)	1440(5)
324(1)	956(3)	1480(4)	313(1)	947(3)	1442(6)
367(5)	969(13)	1530(30)	353(3)	965(11)	1504(13)
399(28)	985(14)	1547(14)	391(12)	976(19)	1512(23)
419(1)	1001(2)	1556(19)	405(11)	990(2)	1572(13)
434(7)	1026(0)	1634(27)	409(16)	1014(14)	1608(23)
458(17)	1032(4)	3002(56)	444(22)	1017(9)	3033(31)
467(1)	1046(5)	3057(64)	458(0)	1019(1)	3044(14)
576(8)	1048(7)	3065(51)	549(7)	1031(2)	3066(26)
577(11)	1068(3)	3082(53)	555(9)	1052(4)	3067(33)
598(28)	1083(3)	3087(27)	584(18)	1057(4)	3089(31)
601(36)	1110(1)	3093(96)	602(44)	1089(2)	3104(41)
631(2)	1112(3)	3104(72)	610(4)	1099(0)	3113(29)
637(12)	1118(0)	3107(63)	625(0)	1101(1)	3115(29)
646(2)	1120(2)	3108(38)	650(10)	1103(2)	3118(10)
675(33)	1163(0)	3125(11)	674(80)	1137(2)	3139(8)
694(95)	1164(2)	3127(27)	684(76)	1146(1)	3143(2)
697(57)	1225(1)	3162(7)	689(39)	1202(0)	3171(0)
722(58)	1232(5)	3171(19)	709(62)	1210(3)	3174(4)
777(0)	1260(1)	3179(38)	751(0)	1228(0)	3177(19)
785(2)	1266(1)	3185(19)	764(3)	1236(1)	3192(2)
819(43)	1271(1)	3188(9)	797(1)	1243(4)	3193(3)
824(7)	1276(1)	3200(14)	833(27)	1246(3)	3199(7)
852(7)	1292(1)	3200(62)	850(5)	1254(2)	3202(23)

Table S83 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) forthe**$(bcod)_2$Mn** structure **Mn-10X.**

M06-L			OPBE		
23(0)	860(21)	1297(1)	13(0)	851(7)	1261(1)
33(0)	880(8)	1307(2)	29(1)	862(14)	1281(3)
48(0)	883(9)	1319(2)	43(0)	871(8)	1293(0)
64(1)	888(6)	1322(6)	63(1)	875(10)	1296(4)
86(1)	894(8)	1339(2)	95(1)	876(5)	1309(3)
120(1)	902(11)	1353(7)	120(1)	881(13)	1320(9)
156(3)	910(10)	1360(11)	153(2)	893(3)	1327(17)
227(2)	914(2)	1396(3)	224(0)	898(3)	1368(2)
244(17)	942(3)	1436(1)	241(15)	933(4)	1412(2)
302(7)	947(0)	1472(3)	291(6)	941(0)	1439(6)
318(0)	955(2)	1473(5)	311(1)	947(3)	1441(6)
359(6)	969(16)	1523(34)	354(4)	965(13)	1507(15)
397(25)	987(16)	1544(18)	391(16)	975(17)	1511(25)
419(0)	1001(2)	1578(18)	405(6)	991(2)	1561(11)
425(10)	1026(1)	1638(26)	408(19)	1013(15)	1606(26)
458(17)	1033(4)	3009(65)	444(21)	1017(5)	3027(34)
466(0)	1045(5)	3057(63)	456(0)	1019(1)	3058(10)
576(2)	1047(5)	3057(49)	552(5)	1030(1)	3065(26)
578(15)	1068(2)	3071(45)	554(9)	1053(5)	3071(32)
590(29)	1085(8)	3080(47)	581(18)	1056(5)	3089(28)
607(47)	1110(2)	3092(95)	599(47)	1089(2)	3103(42)
620(10)	1115(2)	3106(72)	610(2)	1097(1)	3112(30)
630(1)	1116(1)	3106(30)	626(0)	1100(1)	3115(26)
645(2)	1120(2)	3109(61)	643(10)	1103(2)	3116(10)
677(41)	1162(3)	3125(17)	673(63)	1135(2)	3132(3)
694(58)	1166(1)	3127(26)	686(76)	1144(0)	3139(8)
702(57)	1225(0)	3159(5)	690(42)	1202(0)	3174(4)
724(58)	1233(5)	3171(17)	708(68)	1209(3)	3177(18)
778(0)	1261(1)	3178(40)	752(0)	1229(0)	3179(1)
786(2)	1267(1)	3182(8)	763(3)	1235(2)	3192(2)
827(9)	1272(1)	3197(18)	807(2)	1243(3)	3196(1)
837(29)	1277(1)	3200(62)	829(35)	1245(3)	3201(6)
858(4)	1291(1)	3202(12)	846(10)	1254(2)	3202(22)

Table S84 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$(bcod)_2Mn$** structure **Mn-11X.**

M06-L			OPBE		
20(0)	866(1)	1306(1)	11(0)	853(2)	1269(3)
37(0)	869(1)	1319(2)	37(0)	858(1)	1293(1)
46(0)	875(8)	1322(0)	42(0)	870(15)	1296(3)
87(1)	878(11)	1322(7)	98(1)	872(10)	1297(2)
137(1)	896(9)	1325(2)	125(0)	875(14)	1303(1)
156(2)	901(5)	1360(9)	153(2)	891(5)	1327(16)
176(3)	918(3)	1375(6)	168(3)	894(1)	1343(10)
228(5)	926(0)	1376(1)	225(5)	900(0)	1353(1)
255(6)	943(12)	1433(1)	248(3)	937(8)	1411(2)
292(3)	946(0)	1466(7)	277(3)	941(0)	1436(10)
322(0)	962(7)	1471(5)	312(0)	949(14)	1441(6)
350(5)	968(14)	1491(0)	337(5)	965(10)	1475(1)
402(23)	987(21)	1500(1)	387(32)	976(23)	1487(0)
422(0)	989(2)	1523(40)	406(1)	981(5)	1508(16)
448(36)	1025(1)	1556(18)	426(43)	1016(5)	1511(25)
463(3)	1043(0)	2999(41)	455(1)	1018(1)	3028(22)
499(0)	1046(2)	3055(65)	485(0)	1019(1)	3064(27)
541(6)	1052(0)	3064(61)	520(1)	1033(0)	3086(31)
551(0)	1065(5)	3080(50)	527(6)	1055(1)	3089(21)
577(10)	1084(5)	3094(27)	549(7)	1055(10)	3102(12)
597(23)	1114(2)	3103(75)	585(21)	1097(0)	3112(29)
625(5)	1116(1)	3106(83)	620(18)	1100(1)	3114(33)
634(63)	1127(0)	3107(47)	627(2)	1109(0)	3119(12)
643(4)	1130(1)	3113(18)	631(45)	1117(1)	3121(10)
647(2)	1151(1)	3124(16)	646(12)	1128(1)	3131(3)
671(2)	1162(3)	3126(27)	663(9)	1135(2)	3138(8)
700(61)	1223(0)	3154(19)	682(116)	1193(0)	3156(11)
710(84)	1225(0)	3168(6)	688(33)	1202(0)	3179(16)
739(16)	1226(0)	3174(47)	724(15)	1204(0)	3182(0)
778(1)	1231(3)	3186(64)	753(1)	1213(3)	3190(21)
790(33)	1260(1)	3193(13)	783(35)	1228(0)	3192(2)
844(1)	1272(1)	3194(17)	801(2)	1243(3)	3196(2)
859(3)	1291(1)	3199(10)	850(5)	1254(2)	3205(4)

Table S85 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$(bcod)_2Fe$** structure **Fe-1S.**

M06-L			OPBE		
36(0)	866(2)	1294(1)	32(0)	860(1)	1259(1)
110(0)	875(7)	1321(4)	143(0)	863(12)	1297(1)
195(0)	875(1)	1322(0)	145(0)	869(7)	1299(0)
220(1)	886(1)	1328(1)	221(0)	873(8)	1299(0)
239(0)	894(9)	1329(0)	245(3)	876(1)	1300(1)
267(9)	904(5)	1364(7)	252(3)	891(1)	1331(12)
341(17)	945(4)	1367(2)	349(22)	914(0)	1332(7)
349(20)	949(2)	1443(1)	372(21)	923(1)	1416(8)
372(22)	952(0)	1444(3)	377(4)	944(1)	1417(0)
391(6)	955(1)	1464(5)	398(7)	945(0)	1435(1)
395(0)	970(1)	1465(19)	408(0)	962(5)	1436(13)
423(3)	978(1)	1487(5)	422(9)	962(4)	1459(1)
430(3)	982(3)	1487(3)	429(1)	975(2)	1463(3)
438(1)	991(11)	1521(6)	469(14)	977(1)	1497(1)
446(2)	1023(0)	1529(1)	474(16)	1010(5)	1506(0)
494(0)	1025(1)	3041(138)	483(1)	1014(2)	3047(65)
500(1)	1043(4)	3041(0)	484(0)	1018(0)	3047(0)
596(0)	1046(1)	3084(136)	574(1)	1019(1)	3091(42)
601(0)	1079(0)	3084(38)	586(0)	1047(0)	3091(31)
616(1)	1100(0)	3088(185)	589(0)	1049(0)	3093(93)
617(15)	1111(5)	3089(1)	599(9)	1092(1)	3093(1)
641(4)	1112(0)	3109(13)	628(3)	1099(0)	3118(12)
645(3)	1119(9)	3109(60)	639(4)	1104(0)	3118(16)
720(1)	1122(0)	3143(10)	724(3)	1106(6)	3150(1)
731(6)	1155(0)	3143(4)	733(4)	1125(0)	3155(1)
765(1)	1157(0)	3157(70)	736(0)	1130(0)	3160(15)
767(9)	1226(0)	3158(57)	767(11)	1203(0)	3163(22)
782(2)	1230(0)	3168(37)	790(7)	1203(0)	3174(28)
788(2)	1261(0)	3169(43)	802(4)	1231(0)	3177(21)
817(3)	1269(0)	3184(34)	835(0)	1233(1)	3199(10)
819(0)	1275(3)	3187(3)	842(0)	1242(4)	3202(3)
859(1)	1278(5)	3205(9)	851(14)	1242(7)	3218(7)
864(7)	1294(0)	3208(40)	859(0)	1258(1)	3222(11)

Table S86 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the**(bcod)$_2$Fe**structure **Fe-2S.**

M06-L			OPBE		
79(0)	862(0)	1294(1)	55(0)	857(0)	1259(2)
114(0)	864(9)	1322(4)	115(0)	859(3)	1298(1)
178(1)	878(15)	1322(0)	183(1)	875(20)	1298(0)
224(0)	883(0)	1330(0)	227(0)	878(0)	1301(0)
246(0)	900(0)	1331(1)	233(0)	880(16)	1302(0)
291(38)	902(11)	1365(9)	288(30)	881(0)	1335(16)
309(0)	943(10)	1370(0)	319(0)	923(9)	1342(0)
310(31)	952(0)	1435(4)	319(38)	932(0)	1412(6)
348(9)	956(0)	1438(0)	363(19)	950(0)	1415(0)
398(6)	962(1)	1466(17)	394(9)	959(1)	1432(16)
420(0)	974(2)	1468(0)	413(0)	967(0)	1436(0)
422(0)	979(0)	1496(10)	415(6)	970(14)	1457(3)
426(1)	981(0)	1496(0)	416(0)	973(1)	1459(0)
431(0)	981(15)	1520(0)	435(0)	982(0)	1506(3)
457(4)	1027(0)	1523(10)	466(8)	1010(7)	1508(0)
485(1)	1028(0)	3043(144)	471(0)	1017(0)	3049(69)
493(0)	1040(5)	3043(0)	487(0)	1020(0)	3049(0)
597(0)	1047(0)	3090(0)	578(0)	1022(0)	3100(0)
597(0)	1078(0)	3090(157)	578(0)	1061(0)	3100(65)
613(10)	1084(0)	3093(183)	596(8)	1066(1)	3101(82)
619(0)	1110(14)	3094(0)	600(0)	1098(0)	3102(0)
643(12)	1112(0)	3111(0)	624(10)	1101(7)	3119(0)
649(0)	1114(0)	3111(70)	631(0)	1101(0)	3119(27)
737(16)	1116(0)	3130(37)	725(0)	1103(0)	3148(9)
742(0)	1155(0)	3131(0)	740(1)	1126(0)	3149(0)
746(0)	1160(0)	3160(0)	746(8)	1134(0)	3168(0)
767(1)	1228(0)	3161(117)	753(0)	1205(0)	3168(37)
779(0)	1232(0)	3164(81)	780(30)	1211(1)	3173(30)
779(23)	1263(0)	3166(0)	784(0)	1235(0)	3174(0)
786(0)	1264(0)	3186(31)	793(0)	1237(1)	3194(0)
806(1)	1276(7)	3186(0)	813(0)	1246(11)	3194(13)
853(0)	1278(0)	3207(0)	854(0)	1248(0)	3212(16)
856(2)	1294(0)	3207(38)	854(17)	1258(0)	3212(0)

Table S87 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$(bcod)_2Fe$** structure **Fe-3T.**

M06-L			OPBE		
58(0)	857(0)	1294(3)	59(0)	851(0)	1259(5)
81(0)	857(0)	1308(9)	85(0)	855(0)	1282(3)
108(0)	882(5)	1309(0)	109(0)	857(16)	1283(0)
143(0)	896(11)	1310(0)	120(0)	862(1)	1286(0)
165(0)	897(0)	1316(7)	144(0)	866(9)	1293(9)
184(7)	904(0)	1358(13)	154(6)	876(0)	1328(21)
206(0)	921(3)	1362(0)	199(0)	903(2)	1332(0)
232(8)	931(0)	1417(7)	222(7)	913(0)	1395(10)
288(12)	947(0)	1418(0)	274(11)	944(0)	1397(0)
384(4)	949(6)	1468(8)	345(0)	948(2)	1438(10)
389(0)	950(1)	1469(0)	374(4)	950(5)	1438(0)
402(0)	954(0)	1498(10)	394(0)	955(0)	1484(5)
418(12)	990(23)	1499(0)	397(0)	979(20)	1485(0)
442(1)	991(0)	1619(11)	408(11)	981(0)	1578(8)
446(0)	1017(0)	1620(0)	422(3)	1013(0)	1580(0)
455(0)	1018(0)	3049(122)	446(0)	1013(0)	3056(53)
464(6)	1042(5)	3049(0)	457(9)	1016(9)	3056(0)
590(0)	1044(0)	3086(161)	533(0)	1016(0)	3092(0)
598(2)	1090(15)	3086(0)	569(3)	1072(6)	3092(69)
616(1)	1091(0)	3088(168)	600(1)	1072(0)	3094(76)
616(0)	1117(0)	3089(0)	602(0)	1094(0)	3094(0)
642(18)	1120(13)	3122(0)	623(17)	1102(0)	3133(0)
648(0)	1121(0)	3122(52)	631(0)	1106(12)	3133(24)
734(126)	1124(0)	3124(52)	697(0)	1107(0)	3141(9)
738(0)	1154(1)	3124(0)	719(126)	1126(0)	3141(0)
755(0)	1161(0)	3155(0)	724(0)	1130(1)	3162(0)
765(25)	1214(0)	3155(111)	748(0)	1196(0)	3162(40)
782(5)	1216(0)	3159(79)	758(35)	1198(0)	3167(31)
782(0)	1265(0)	3159(0)	760(3)	1232(0)	3167(0)
808(0)	1265(1)	3172(27)	770(0)	1233(0)	3192(0)
816(3)	1272(7)	3173(0)	810(2)	1244(10)	3193(4)
856(6)	1274(0)	3200(0)	847(11)	1246(0)	3219(0)
857(12)	1294(0)	3200(34)	848(0)	1258(0)	3219(9)

Table S88 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the**(bcod)$_2$Fe**tructure**Fe-4T.**

M06-L			OPBE		
52(0)	856(5)	1294(2)	41(1)	849(15)	1256(2)
74(0)	861(1)	1309(1)	69(1)	853(1)	1282(0)
117(1)	866(6)	1317(2)	123(1)	856(7)	1286(0)
135(0)	869(7)	1318(1)	143(2)	861(11)	1290(1)
165(1)	895(9)	1324(1)	164(1)	873(8)	1294(0)
177(2)	899(3)	1356(9)	178(3)	879(2)	1324(15)
222(4)	916(4)	1359(10)	209(5)	907(4)	1325(16)
259(5)	928(3)	1424(4)	249(4)	909(0)	1398(1)
291(1)	938(0)	1436(1)	265(4)	933(0)	1413(2)
340(1)	950(4)	1443(18)	334(2)	944(0)	1426(18)
367(0)	950(0)	1472(5)	357(1)	948(5)	1439(9)
388(9)	962(1)	1472(5)	387(6)	958(2)	1445(2)
407(2)	980(6)	1521(9)	406(2)	970(10)	1488(12)
433(2)	984(11)	1530(10)	422(3)	973(2)	1507(16)
436(1)	1019(0)	1549(16)	424(2)	1009(1)	1521(4)
461(0)	1020(0)	3040(79)	459(0)	1010(4)	3049(37)
494(1)	1036(6)	3050(64)	484(2)	1012(1)	3057(28)
579(10)	1044(3)	3085(81)	555(13)	1014(6)	3094(36)
592(7)	1070(4)	3089(100)	575(8)	1052(3)	3097(43)
599(10)	1083(1)	3093(76)	582(12)	1057(1)	3098(31)
608(13)	1101(4)	3097(70)	591(4)	1088(4)	3100(29)
631(2)	1111(7)	3109(37)	612(1)	1096(3)	3121(13)
635(8)	1116(0)	3120(31)	618(3)	1098(0)	3130(11)
643(29)	1119(1)	3131(10)	637(44)	1103(1)	3145(6)
686(17)	1157(1)	3136(11)	686(9)	1130(1)	3146(2)
707(19)	1161(0)	3153(34)	719(16)	1134(0)	3159(15)
731(9)	1214(1)	3155(41)	721(3)	1189(0)	3168(16)
738(5)	1220(0)	3171(42)	733(1)	1194(0)	3177(5)
752(1)	1249(2)	3176(31)	738(11)	1218(1)	3182(8)
773(1)	1263(0)	3176(29)	768(2)	1228(1)	3189(10)
781(0)	1267(5)	3181(15)	797(0)	1238(6)	3201(6)
835(2)	1270(3)	3206(9)	823(2)	1241(5)	3218(3)
849(3)	1291(1)	3233(9)	845(4)	1255(1)	3241(2)

Table S89 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$(bcod)_2Co$** structure **Co-1D.**

M06-L			OPBE		
70(0)	861(0)	1295(2)	58(2)	855(0)	1261(3)
86(0)	862(7)	1315(5)	66(0)	855(13)	1292(1)
89(0)	867(19)	1315(0)	91(0)	867(19)	1292(0)
135(0)	868(0)	1323(0)	158(0)	871(0)	1300(0)
141(0)	897(9)	1327(2)	168(0)	875(10)	1303(0)
190(0)	900(0)	1359(15)	184(0)	878(0)	1330(26)
203(0)	930(5)	1364(0)	205(0)	914(6)	1336(0)
237(10)	938(0)	1433(5)	219(7)	922(0)	1415(8)
289(1)	952(0)	1434(0)	279(1)	950(0)	1416(0)
363(0)	955(0)	1471(10)	317(0)	955(0)	1441(11)
380(3)	957(1)	1471(0)	365(1)	961(0)	1442(0)
409(0)	962(0)	1510(0)	404(0)	967(0)	1501(0)
426(2)	988(22)	1512(11)	416(1)	976(18)	1502(3)
441(0)	989(0)	1587(27)	419(0)	976(0)	1526(23)
442(0)	1020(0)	1588(0)	421(0)	1016(11)	1528(0)
449(3)	1020(0)	3049(125)	426(7)	1016(0)	3056(58)
458(3)	1044(6)	3049(0)	446(5)	1017(0)	3056(0)
579(0)	1047(0)	3087(0)	545(4)	1018(0)	3095(0)
584(3)	1090(7)	3087(166)	546(0)	1068(0)	3095(72)
613(0)	1090(0)	3090(179)	587(0)	1069(1)	3097(83)
615(5)	1117(0)	3091(0)	589(9)	1103(0)	3098(0)
638(13)	1119(0)	3119(0)	615(7)	1106(0)	3128(0)
646(0)	1119(12)	3119(67)	624(0)	1107(8)	3128(24)
718(94)	1119(0)	3137(26)	694(69)	1107(0)	3159(1)
718(0)	1156(0)	3137(0)	698(0)	1131(0)	3160(0)
753(0)	1157(0)	3164(0)	744(0)	1133(0)	3173(0)
761(25)	1218(0)	3164(101)	754(1)	1201(0)	3173(32)
773(0)	1221(0)	3169(77)	755(29)	1205(0)	3182(29)
779(5)	1265(0)	3170(0)	763(0)	1233(0)	3182(0)
789(0)	1266(0)	3187(0)	783(0)	1235(0)	3211(0)
806(3)	1272(2)	3187(24)	793(4)	1244(9)	3211(3)
852(0)	1274(0)	3213(0)	813(0)	1246(0)	3234(0)
858(2)	1295(0)	3214(30)	827(3)	1260(0)	3234(9)

Table S90 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$(bcod)_2Co$** structure **Co-2D.**

M06-L			OPBE		
37(1)	861(4)	1297(1)	56(0)	851(6)	1260(1)
80(0)	865(2)	1317(1)	94(0)	857(8)	1286(0)
112(2)	869(12)	1320(1)	151(1)	859(11)	1293(0)
129(0)	873(3)	1323(2)	171(1)	867(7)	1296(1)
145(0)	896(6)	1328(1)	192(0)	869(7)	1298(0)
175(0)	900(2)	1361(13)	211(2)	882(4)	1330(17)
210(1)	930(2)	1365(2)	258(5)	908(1)	1334(7)
241(6)	932(4)	1427(0)	277(4)	919(3)	1398(1)
272(4)	948(1)	1438(2)	304(8)	940(2)	1418(3)
355(2)	954(0)	1469(12)	342(6)	947(1)	1431(16)
381(2)	964(1)	1473(5)	365(3)	960(1)	1439(9)
409(2)	970(1)	1509(3)	393(3)	966(4)	1453(2)
417(0)	981(9)	1513(14)	412(2)	972(1)	1472(7)
428(1)	989(11)	1544(16)	422(2)	976(9)	1503(2)
439(1)	1023(0)	1569(22)	429(3)	1011(4)	1517(12)
447(2)	1024(0)	3045(77)	461(1)	1015(4)	3049(39)
474(1)	1043(4)	3048(57)	484(5)	1017(1)	3054(29)
574(2)	1047(2)	3087(82)	545(2)	1017(0)	3095(37)
581(3)	1082(2)	3090(133)	570(9)	1057(0)	3097(54)
595(19)	1094(2)	3090(63)	575(6)	1064(0)	3098(24)
608(3)	1106(6)	3094(65)	586(0)	1089(2)	3105(31)
633(2)	1117(2)	3115(33)	616(0)	1099(0)	3120(13)
641(2)	1120(3)	3118(34)	621(1)	1100(1)	3125(12)
687(25)	1122(4)	3138(15)	639(46)	1107(3)	3154(3)
693(24)	1157(0)	3147(5)	694(12)	1131(1)	3165(1)
708(43)	1162(1)	3160(66)	710(16)	1134(1)	3168(18)
756(1)	1223(0)	3162(31)	735(4)	1192(0)	3176(12)
764(4)	1224(0)	3173(40)	745(3)	1203(0)	3192(1)
773(2)	1260(1)	3183(25)	762(8)	1221(0)	3193(3)
789(2)	1268(0)	3194(17)	797(1)	1234(0)	3195(20)
800(2)	1273(2)	3196(9)	812(1)	1242(6)	3204(2)
833(4)	1275(3)	3219(18)	827(4)	1246(6)	3213(5)
835(7)	1294(1)	3220(10)	850(2)	1257(1)	3225(4)

Table S91 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$(bcod)_2Co$** structure **Co-3D.**

M06-L			OPBE		
54(0)	858(5)	1296(1)	55(0)	851(1)	1261(1)
104(0)	866(3)	1314(0)	109(0)	858(6)	1286(0)
124(0)	868(3)	1320(1)	134(0)	860(3)	1293(0)
158(0)	871(6)	1324(3)	183(0)	865(5)	1297(0)
189(1)	875(2)	1327(1)	204(1)	870(3)	1299(1)
216(2)	894(6)	1361(10)	227(4)	876(7)	1331(15)
246(5)	911(1)	1362(7)	266(5)	896(0)	1332(9)
260(5)	914(1)	1427(3)	292(12)	905(1)	1404(1)
295(4)	940(0)	1439(5)	310(5)	937(1)	1416(12)
361(6)	945(0)	1447(11)	352(8)	939(0)	1418(1)
381(2)	961(3)	1471(7)	373(2)	955(5)	1440(9)
392(7)	966(1)	1474(5)	378(2)	961(2)	1444(3)
419(1)	977(5)	1493(5)	408(3)	968(4)	1472(9)
433(1)	982(8)	1506(11)	431(2)	973(2)	1487(1)
440(2)	1022(0)	1541(13)	450(2)	1009(3)	1489(8)
467(0)	1025(0)	3040(84)	465(0)	1015(3)	3046(41)
498(3)	1036(4)	3047(59)	494(5)	1016(1)	3053(28)
574(13)	1045(3)	3086(79)	553(2)	1019(0)	3095(35)
584(11)	1071(2)	3089(118)	564(2)	1052(1)	3097(61)
596(3)	1081(1)	3090(70)	578(4)	1055(0)	3097(20)
600(13)	1102(4)	3096(69)	583(33)	1087(2)	3105(31)
611(28)	1114(0)	3109(36)	592(25)	1097(0)	3117(14)
635(4)	1114(0)	3117(32)	616(3)	1099(0)	3125(12)
642(1)	1118(7)	3139(13)	623(1)	1107(4)	3157(3)
697(36)	1155(0)	3146(1)	701(24)	1127(0)	3158(0)
721(5)	1156(1)	3157(60)	731(2)	1130(1)	3167(12)
749(2)	1217(1)	3161(39)	737(1)	1191(0)	3173(15)
768(4)	1227(0)	3169(58)	750(3)	1203(0)	3177(2)
769(3)	1251(1)	3170(4)	771(11)	1219(1)	3180(20)
785(1)	1264(0)	3180(36)	792(2)	1233(2)	3195(12)
812(1)	1269(3)	3191(15)	821(1)	1239(4)	3199(4)
838(4)	1271(4)	3206(10)	832(4)	1243(5)	3219(2)
854(3)	1293(1)	3230(11)	848(15)	1257(1)	3243(3)

Table S92 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$(bcod)_2Co$** structure **Co-4D.**

M06-L			OPBE		
44(0)	859(6)	1294(1)	-83(16)	851(2)	1259(1)
101(1)	863(0)	1318(3)	38(0)	859(1)	1291(1)
108(10)	870(9)	1319(0)	115(0)	861(9)	1293(0)
127(0)	872(8)	1322(0)	121(0)	866(13)	1295(0)
168(1)	893(7)	1323(3)	182(1)	870(5)	1295(1)
194(1)	895(2)	1360(12)	207(1)	874(2)	1329(18)
204(0)	912(3)	1361(8)	209(1)	896(1)	1331(11)
273(3)	916(6)	1422(3)	281(4)	904(5)	1403(0)
304(8)	943(0)	1422(1)	308(14)	938(2)	1403(0)
370(8)	943(1)	1466(29)	367(5)	938(0)	1435(28)
372(0)	960(3)	1466(2)	371(0)	958(6)	1435(0)
416(0)	964(2)	1498(7)	410(0)	961(2)	1468(3)
418(0)	979(9)	1499(14)	414(1)	968(6)	1470(9)
428(4)	983(3)	1540(56)	435(2)	972(1)	1511(35)
439(1)	1023(1)	1541(8)	436(3)	1011(5)	1513(5)
486(2)	1023(0)	3044(150)	476(3)	1012(5)	3051(70)
487(0)	1039(5)	3044(0)	479(0)	1018(0)	3051(0)
581(32)	1040(2)	3091(98)	557(24)	1018(1)	3099(42)
591(0)	1074(4)	3091(69)	569(1)	1050(0)	3099(31)
594(45)	1074(1)	3095(158)	574(26)	1051(3)	3103(68)
607(0)	1103(10)	3096(1)	588(0)	1092(6)	3103(2)
632(2)	1105(0)	3114(25)	614(3)	1095(0)	3123(9)
641(0)	1117(2)	3114(42)	623(0)	1100(2)	3123(14)
664(14)	1118(0)	3141(17)	667(13)	1100(0)	3152(6)
668(49)	1158(3)	3142(22)	667(56)	1130(2)	3154(7)
681(15)	1161(0)	3155(81)	692(20)	1135(0)	3165(1)
704(6)	1221(1)	3156(0)	718(6)	1198(0)	3168(27)
754(2)	1223(0)	3187(3)	731(2)	1199(0)	3191(16)
766(2)	1255(1)	3187(55)	743(2)	1225(1)	3191(1)
809(1)	1256(2)	3194(25)	811(1)	1226(1)	3209(3)
821(2)	1272(4)	3196(12)	822(4)	1242(8)	3213(6)
832(4)	1272(4)	3219(10)	828(4)	1242(3)	3232(2)
855(3)	1293(1)	3221(8)	850(14)	1257(1)	3233(3)

Table S93 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$(bcod)_2Co$structure Co-5D.**

M06-L			OPBE		
29(1)	860(4)	1298(0)	30(0)	852(13)	1261(0)
85(0)	868(0)	1314(6)	83(0)	857(1)	1285(4)
96(0)	872(10)	1318(1)	112(1)	857(4)	1288(5)
153(1)	883(6)	1318(1)	176(0)	866(5)	1293(0)
197(1)	895(5)	1323(2)	193(0)	870(9)	1296(0)
214(2)	907(6)	1357(9)	207(2)	889(7)	1323(15)
233(3)	928(3)	1361(6)	246(7)	901(2)	1331(10)
278(4)	937(1)	1425(1)	294(5)	916(1)	1396(1)
298(3)	939(1)	1427(1)	327(4)	925(0)	1414(3)
351(1)	945(0)	1467(11)	339(0)	940(0)	1433(13)
379(2)	962(1)	1482(8)	377(1)	958(2)	1436(11)
407(2)	965(7)	1491(4)	392(2)	961(10)	1457(4)
423(3)	978(8)	1503(11)	414(6)	968(5)	1468(1)
435(1)	995(4)	1527(14)	430(1)	983(2)	1488(1)
479(4)	1023(0)	1638(15)	461(5)	1011(6)	1603(6)
485(3)	1031(0)	3020(29)	473(3)	1015(3)	3036(21)
496(4)	1041(4)	3047(69)	489(3)	1017(0)	3055(30)
588(4)	1052(3)	3081(42)	561(2)	1023(0)	3092(26)
589(2)	1075(3)	3086(66)	569(1)	1052(1)	3096(38)
600(15)	1093(8)	3091(88)	575(5)	1073(2)	3097(18)
610(8)	1107(6)	3091(80)	592(3)	1096(1)	3101(58)
637(8)	1114(1)	3095(84)	620(4)	1098(1)	3101(21)
649(2)	1117(1)	3117(33)	628(6)	1100(3)	3127(12)
708(11)	1125(11)	3137(1)	712(28)	1110(10)	3145(1)
710(18)	1142(0)	3145(57)	715(43)	1115(1)	3155(20)
731(47)	1159(1)	3145(22)	724(3)	1129(0)	3159(4)
756(3)	1223(2)	3161(40)	760(3)	1200(0)	3167(12)
778(2)	1224(1)	3170(38)	767(3)	1203(2)	3173(18)
789(2)	1259(1)	3178(22)	793(4)	1228(2)	3180(7)
811(32)	1262(0)	3185(30)	806(32)	1229(1)	3185(11)
833(4)	1272(4)	3190(11)	825(1)	1240(5)	3195(4)
844(1)	1273(0)	3207(65)	842(4)	1240(1)	3207(23)
852(0)	1294(1)	3220(12)	844(1)	1258(2)	3218(3)

Table S94 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$(bcod)_2Ni$** structure **Ni-1S.**

M06-L			OPBE		
66(0)	865(4)	1301(0)	60(0)	853(13)	1266(0)
81(0)	869(0)	1312(0)	79(0)	856(1)	1282(0)
104(0)	873(10)	1314(4)	106(0)	860(0)	1288(4)
177(1)	878(14)	1324(1)	187(0)	870(12)	1296(0)
203(1)	893(5)	1325(0)	198(0)	870(7)	1297(0)
204(0)	903(4)	1355(12)	209(0)	889(5)	1322(19)
246(3)	920(3)	1364(6)	256(4)	902(5)	1332(10)
276(3)	930(7)	1421(0)	291(3)	913(4)	1397(1)
301(1)	932(3)	1446(2)	305(1)	921(1)	1420(4)
356(1)	951(0)	1457(1)	342(1)	945(0)	1430(9)
365(0)	962(6)	1471(7)	354(1)	956(6)	1442(0)
417(3)	964(1)	1474(8)	403(2)	959(3)	1443(9)
420(1)	985(13)	1510(2)	410(6)	972(10)	1485(14)
445(5)	989(4)	1527(18)	445(1)	978(4)	1495(0)
468(0)	1025(0)	1642(24)	463(1)	1009(2)	1613(20)
498(4)	1032(0)	3050(64)	486(2)	1017(5)	3058(28)
508(1)	1044(3)	3055(49)	489(2)	1017(0)	3060(32)
578(1)	1048(2)	3077(85)	560(1)	1025(0)	3088(40)
590(2)	1084(3)	3080(72)	569(2)	1062(2)	3090(29)
593(5)	1092(8)	3092(83)	574(5)	1074(1)	3100(35)
607(3)	1108(1)	3095(89)	588(2)	1094(1)	3102(39)
641(5)	1118(0)	3120(32)	621(4)	1101(0)	3130(11)
657(4)	1119(8)	3124(3)	644(5)	1105(4)	3138(1)
691(42)	1125(11)	3134(73)	688(34)	1114(10)	3148(24)
727(44)	1148(0)	3148(41)	711(57)	1125(0)	3160(13)
753(5)	1159(0)	3158(7)	736(0)	1132(0)	3165(5)
763(0)	1218(3)	3165(27)	748(6)	1199(2)	3170(17)
784(0)	1228(0)	3178(27)	767(2)	1203(0)	3181(6)
789(2)	1261(0)	3179(33)	787(1)	1230(0)	3182(11)
814(38)	1267(2)	3186(31)	805(39)	1236(0)	3190(10)
820(3)	1267(0)	3198(8)	812(3)	1236(5)	3208(24)
848(4)	1271(3)	3208(68)	843(6)	1239(5)	3211(1)
851(2)	1297(1)	3221(8)	845(1)	1260(1)	3231(2)

Table S95 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$(bcod)_2Ni$** structure **Ni-2S.**

M06-L			OPBE		
24(0)	863(4)	1301(0)	13(0)	852(15)	1265(0)
70(1)	863(10)	1316(5)	70(0)	858(2)	1285(0)
90(0)	870(4)	1317(0)	112(0)	859(1)	1290(3)
111(1)	882(14)	1318(0)	163(0)	863(5)	1294(0)
163(1)	891(3)	1323(2)	174(0)	865(8)	1297(0)
177(0)	905(6)	1357(10)	224(1)	889(7)	1322(15)
223(4)	928(3)	1358(6)	233(5)	904(2)	1327(14)
239(4)	934(2)	1426(0)	234(2)	916(3)	1399(4)
298(0)	938(3)	1436(2)	295(1)	921(0)	1415(3)
351(1)	949(0)	1471(10)	339(0)	941(0)	1423(10)
378(4)	957(2)	1473(8)	373(1)	957(1)	1441(9)
416(7)	967(9)	1488(4)	400(4)	960(8)	1462(1)
429(1)	989(15)	1497(2)	411(1)	972(12)	1482(1)
439(1)	992(2)	1601(16)	443(2)	978(4)	1517(19)
465(0)	1018(0)	1640(21)	445(3)	1009(5)	1612(19)
492(4)	1032(0)	3049(62)	476(3)	1013(0)	3058(26)
506(2)	1045(6)	3052(54)	484(2)	1017(6)	3058(35)
579(0)	1052(3)	3084(81)	548(1)	1023(0)	3091(40)
587(2)	1090(5)	3086(89)	566(1)	1061(1)	3093(32)
613(2)	1094(5)	3087(70)	588(3)	1074(1)	3094(36)
619(1)	1113(0)	3090(79)	593(1)	1096(0)	3097(40)
649(6)	1115(0)	3122(32)	626(5)	1100(0)	3131(11)
658(13)	1121(5)	3130(9)	645(15)	1105(3)	3143(1)
709(79)	1125(10)	3139(32)	684(42)	1115(11)	3154(22)
729(43)	1149(0)	3146(61)	710(55)	1123(0)	3165(15)
773(0)	1155(0)	3155(2)	747(0)	1131(0)	3166(14)
774(9)	1219(0)	3155(36)	761(12)	1199(0)	3171(1)
786(0)	1224(1)	3174(39)	766(2)	1202(1)	3180(7)
799(3)	1263(0)	3177(23)	799(2)	1231(0)	3181(10)
811(24)	1265(0)	3181(31)	802(37)	1232(0)	3193(10)
837(9)	1269(1)	3185(13)	809(6)	1237(3)	3205(1)
850(1)	1271(2)	3206(67)	836(4)	1238(8)	3208(24)
855(0)	1295(1)	3212(15)	845(1)	1259(2)	3228(3)

Table S96 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$(bcod)_2Ni$** structure **Ni-3S.**

M06-L			OPBE		
61(0)	859(2)	1291(1)	59(0)	852(1)	1261(2)
78(0)	864(5)	1298(1)	86(0)	854(6)	1261(1)
130(1)	873(5)	1314(1)	126(1)	868(7)	1284(1)
165(1)	896(7)	1322(0)	182(0)	873(7)	1293(0)
190(1)	896(4)	1325(1)	190(1)	889(6)	1298(0)
200(2)	909(3)	1346(6)	210(2)	894(2)	1316(9)
263(2)	919(1)	1364(10)	274(3)	909(1)	1332(15)
282(1)	931(3)	1393(6)	292(1)	918(1)	1366(4)
328(0)	942(5)	1422(8)	321(2)	928(5)	1400(8)
351(4)	948(1)	1447(1)	347(3)	942(0)	1420(3)
394(1)	956(2)	1475(8)	384(1)	950(2)	1443(10)
416(1)	967(3)	1475(4)	411(1)	962(4)	1444(3)
427(1)	985(12)	1518(4)	421(1)	972(9)	1502(2)
440(10)	994(1)	1554(12)	428(11)	982(1)	1507(10)
453(6)	1010(1)	1639(18)	450(1)	1001(3)	1614(11)
475(0)	1025(0)	3037(88)	470(0)	1009(3)	3045(45)
537(6)	1031(6)	3051(64)	527(5)	1017(4)	3057(28)
587(5)	1047(2)	3078(87)	564(5)	1018(0)	3085(39)
598(7)	1070(5)	3095(77)	580(6)	1055(1)	3102(33)
616(1)	1083(3)	3095(78)	598(3)	1056(3)	3103(42)
618(8)	1093(1)	3098(70)	601(4)	1082(1)	3104(25)
641(6)	1115(1)	3110(38)	623(5)	1096(1)	3121(16)
649(1)	1119(3)	3120(26)	632(1)	1101(0)	3130(10)
686(46)	1121(1)	3122(29)	676(54)	1105(3)	3136(8)
715(40)	1157(1)	3139(54)	701(28)	1129(1)	3152(19)
740(1)	1160(1)	3149(25)	735(2)	1133(1)	3164(5)
744(6)	1196(2)	3158(8)	741(10)	1171(1)	3170(4)
765(1)	1225(0)	3171(33)	747(2)	1201(0)	3184(3)
773(9)	1243(2)	3178(34)	772(4)	1212(2)	3186(17)
786(1)	1263(0)	3189(29)	781(4)	1231(0)	3191(12)
828(10)	1268(2)	3192(35)	820(9)	1238(4)	3193(9)
845(5)	1270(8)	3198(7)	825(10)	1243(8)	3220(0)
853(6)	1283(1)	3237(4)	844(8)	1252(1)	3254(1)

Table S97 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the**$(bcod)_2Ni$** structure **Ni-4S.**

M06-L			OPBE		
49(0)	861(3)	1292(2)	47(0)	855(2)	1260(1)
88(0)	864(1)	1297(1)	97(0)	855(4)	1263(3)
106(0)	875(6)	1312(1)	110(0)	868(8)	1284(1)
157(1)	893(8)	1324(1)	166(1)	870(11)	1294(0)
179(2)	903(1)	1325(1)	186(1)	891(1)	1298(0)
221(1)	907(4)	1345(7)	227(2)	897(5)	1315(10)
235(3)	918(1)	1363(10)	251(5)	900(1)	1332(15)
267(1)	921(1)	1391(7)	281(1)	915(0)	1365(4)
331(1)	934(4)	1431(6)	330(1)	924(3)	1410(7)
362(3)	946(0)	1442(1)	359(3)	940(0)	1418(3)
380(2)	956(2)	1472(10)	373(2)	951(2)	1441(11)
418(0)	966(3)	1474(5)	408(2)	961(5)	1443(5)
422(1)	984(8)	1517(5)	424(1)	971(4)	1490(9)
437(9)	993(2)	1539(13)	427(9)	983(2)	1503(4)
453(10)	1012(2)	1636(23)	444(4)	1002(5)	1614(15)
472(0)	1025(0)	3036(89)	470(0)	1010(3)	3045(45)
531(1)	1031(6)	3051(64)	522(1)	1016(7)	3057(29)
581(6)	1045(5)	3076(87)	560(6)	1018(0)	3082(39)
598(6)	1073(3)	3090(68)	582(4)	1053(3)	3101(32)
613(1)	1083(3)	3095(76)	598(2)	1059(1)	3103(31)
617(15)	1092(0)	3098(83)	601(8)	1083(0)	3106(37)
642(4)	1114(1)	3110(38)	624(4)	1097(1)	3121(16)
647(2)	1117(2)	3116(39)	631(2)	1101(0)	3129(10)
671(41)	1120(3)	3121(33)	665(51)	1105(2)	3136(11)
696(48)	1156(1)	3142(43)	697(29)	1129(1)	3155(18)
738(9)	1160(1)	3146(33)	735(10)	1134(1)	3163(9)
746(3)	1197(3)	3157(5)	739(8)	1172(1)	3174(1)
761(2)	1227(0)	3168(34)	746(8)	1202(0)	3182(9)
764(14)	1241(2)	3181(31)	764(4)	1211(2)	3190(10)
781(0)	1263(1)	3190(19)	778(2)	1230(1)	3194(11)
827(13)	1268(5)	3196(37)	820(13)	1241(7)	3205(6)
834(5)	1272(4)	3207(10)	827(8)	1241(6)	3215(2)
853(7)	1283(1)	3231(9)	845(8)	1251(1)	3237(1)

Table S98 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$(bcod)_2Cu$** structure **Cu-1D.**

M06-L			OPBE		
28(0)	862(5)	1296(2)	29(0)	850(2)	1261(3)
48(0)	866(6)	1313(4)	54(0)	851(3)	1285(1)
56(0)	873(11)	1318(2)	70(0)	864(7)	1290(0)
66(0)	876(7)	1322(4)	76(0)	869(12)	1294(7)
82(1)	890(8)	1323(2)	85(0)	871(6)	1295(1)
126(2)	896(7)	1360(20)	131(1)	880(4)	1328(27)
141(1)	899(3)	1360(2)	141(1)	882(3)	1329(7)
176(0)	919(8)	1423(2)	180(0)	898(5)	1396(1)
254(5)	943(4)	1436(2)	251(6)	935(3)	1414(0)
319(2)	952(0)	1473(13)	299(3)	944(0)	1441(8)
327(3)	958(1)	1474(2)	318(2)	955(1)	1442(12)
375(2)	961(2)	1486(54)	366(1)	959(2)	1466(53)
394(9)	990(12)	1503(20)	391(9)	975(12)	1491(13)
426(1)	991(10)	1598(30)	410(0)	980(6)	1537(33)
433(1)	1018(0)	1634(23)	416(3)	1008(1)	1611(23)
448(1)	1020(0)	3051(69)	440(1)	1012(15)	3060(29)
455(1)	1041(17)	3054(63)	444(1)	1014(1)	3063(28)
575(8)	1045(6)	3085(94)	548(8)	1016(7)	3089(43)
576(9)	1089(2)	3090(92)	556(7)	1063(2)	3093(40)
589(27)	1090(4)	3094(83)	577(14)	1071(1)	3104(34)
603(4)	1113(2)	3097(79)	589(24)	1099(1)	3106(37)
616(40)	1116(3)	3119(38)	611(17)	1101(2)	3131(16)
635(13)	1121(1)	3123(33)	622(17)	1103(1)	3132(2)
641(3)	1125(1)	3128(12)	624(16)	1112(2)	3136(11)
661(7)	1158(3)	3144(10)	674(7)	1132(2)	3152(11)
683(5)	1159(1)	3157(33)	678(17)	1134(1)	3166(2)
714(74)	1217(0)	3170(17)	689(57)	1191(0)	3185(4)
726(61)	1220(1)	3176(9)	714(67)	1199(0)	3187(11)
748(42)	1264(1)	3185(30)	758(18)	1230(0)	3194(0)
785(1)	1267(1)	3190(29)	761(2)	1233(0)	3196(6)
792(6)	1273(1)	3198(33)	777(23)	1241(4)	3202(5)
849(25)	1273(1)	3199(6)	819(8)	1245(3)	3215(6)
859(5)	1294(2)	3205(7)	830(43)	1257(2)	3219(2)

Table S99 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$(bcod)_2Cu$** structure **Cu-2D.**

M06-L			OPBE		
38(0)	860(4)	1296(2)	31(0)	851(3)	1261(3)
50(0)	865(7)	1314(3)	49(0)	852(5)	1284(0)
75(0)	875(7)	1318(2)	74(0)	865(14)	1291(1)
86(1)	879(19)	1321(1)	85(0)	866(4)	1292(0)
95(1)	894(4)	1322(3)	97(2)	874(8)	1294(6)
118(1)	900(3)	1361(21)	125(1)	881(1)	1328(33)
167(1)	901(6)	1363(2)	163(0)	888(5)	1329(2)
190(1)	919(5)	1425(2)	201(1)	904(5)	1398(1)
246(2)	944(2)	1440(1)	242(3)	934(2)	1416(1)
324(2)	948(0)	1473(2)	302(2)	942(0)	1441(7)
333(5)	963(0)	1474(11)	321(6)	959(0)	1442(15)
374(5)	966(2)	1484(74)	365(3)	961(2)	1466(66)
386(2)	984(17)	1512(6)	386(2)	971(14)	1494(14)
416(1)	992(7)	1544(28)	407(4)	980(7)	1501(15)
432(2)	1015(0)	1641(24)	417(4)	1007(1)	1616(25)
452(1)	1023(0)	3050(69)	441(1)	1012(14)	3060(29)
462(1)	1040(15)	3053(67)	455(1)	1014(3)	3062(29)
573(8)	1046(5)	3084(89)	548(5)	1017(5)	3088(43)
575(1)	1085(4)	3087(98)	556(10)	1059(2)	3092(42)
578(10)	1091(3)	3097(83)	562(0)	1072(1)	3105(34)
599(21)	1114(4)	3103(77)	584(28)	1098(1)	3110(34)
617(24)	1116(2)	3120(39)	611(10)	1100(2)	3132(16)
634(5)	1120(1)	3123(30)	621(4)	1102(1)	3134(2)
640(5)	1127(2)	3127(10)	625(19)	1113(2)	3135(10)
646(16)	1157(5)	3146(17)	653(19)	1132(4)	3156(2)
676(12)	1160(1)	3158(30)	662(47)	1134(1)	3157(12)
682(58)	1215(0)	3169(19)	685(9)	1190(0)	3184(5)
732(40)	1223(0)	3187(29)	716(65)	1200(0)	3188(11)
737(72)	1261(1)	3187(7)	747(34)	1228(0)	3194(5)
781(1)	1267(0)	3192(27)	753(1)	1234(0)	3203(5)
792(7)	1271(2)	3198(20)	772(14)	1242(5)	3204(1)
817(2)	1275(1)	3204(21)	793(2)	1245(2)	3214(7)
849(22)	1294(1)	3211(3)	834(46)	1256(2)	3227(1)

Table S100 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$(bcod)_2Cu$** structure **Cu-3D.**

M06-L			OPBE		
32(0)	861(2)	1296(1)	24(0)	851(5)	1267(4)
60(0)	861(0)	1306(1)	65(0)	854(1)	1273(0)
63(0)	868(12)	1314(2)	73(0)	856(4)	1289(0)
105(0)	871(4)	1320(6)	95(0)	868(13)	1296(3)
109(0)	894(5)	1328(3)	105(0)	873(9)	1300(6)
132(2)	899(6)	1359(9)	135(2)	875(1)	1327(15)
147(1)	918(4)	1370(9)	145(1)	903(6)	1341(14)
170(3)	929(2)	1432(1)	174(2)	911(2)	1411(2)
278(9)	938(5)	1435(54)	270(7)	925(4)	1417(51)
318(1)	950(0)	1449(0)	303(1)	944(0)	1440(1)
341(0)	956(2)	1468(2)	337(0)	956(3)	1441(9)
373(4)	961(0)	1472(7)	364(4)	964(0)	1447(0)
402(7)	990(13)	1496(0)	400(6)	976(12)	1473(0)
441(0)	992(4)	1508(22)	420(0)	982(3)	1497(15)
448(1)	1008(0)	1601(22)	441(1)	1001(0)	1542(25)
479(9)	1018(0)	3045(80)	461(0)	1014(0)	3054(36)
479(0)	1038(12)	3052(62)	472(6)	1014(7)	3061(27)
518(32)	1045(7)	3090(46)	502(33)	1018(11)	3094(33)
579(4)	1082(10)	3091(119)	552(4)	1060(2)	3096(33)
589(2)	1088(6)	3094(149)	567(2)	1067(15)	3101(38)
594(15)	1116(3)	3094(11)	587(16)	1100(0)	3103(37)
619(10)	1116(0)	3114(37)	613(19)	1102(2)	3126(16)
635(2)	1123(0)	3122(35)	620(4)	1108(0)	3134(11)
641(5)	1126(0)	3141(11)	626(4)	1117(0)	3158(5)
652(7)	1149(0)	3149(11)	661(4)	1127(0)	3169(1)
678(3)	1158(1)	3163(6)	666(19)	1135(1)	3170(1)
681(6)	1208(0)	3175(12)	689(2)	1186(0)	3188(9)
716(54)	1218(0)	3179(39)	701(58)	1199(0)	3189(9)
719(36)	1249(21)	3184(29)	705(24)	1222(12)	3194(1)
752(12)	1254(0)	3189(16)	733(12)	1222(0)	3197(8)
784(0)	1262(1)	3189(31)	761(0)	1229(0)	3197(8)
849(0)	1273(0)	3194(22)	818(3)	1244(3)	3202(7)
858(3)	1291(1)	3204(12)	850(3)	1256(2)	3219(2)

Table S101 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$(bcod)_2Cu$**tructure**Cu-4D.**

M06-L			OPBE		
37(0)	876(40)	1299(1)	29(0)	853(32)	1262(3)
38(0)	882(13)	1320(3)	37(0)	857(2)	1292(3)
53(0)	882(0)	1321(2)	46(0)	872(4)	1293(1)
61(0)	883(2)	1334(0)	55(0)	874(4)	1304(2)
67(0)	897(0)	1334(0)	78(0)	875(0)	1304(1)
156(0)	897(13)	1358(5)	141(0)	876(16)	1325(8)
174(3)	905(16)	1359(17)	157(2)	889(22)	1325(26)
205(0)	909(7)	1423(8)	197(0)	894(5)	1394(7)
256(4)	941(3)	1424(0)	246(3)	932(3)	1395(0)
309(14)	941(1)	1472(15)	292(17)	932(0)	1436(18)
314(1)	960(14)	1475(0)	297(1)	950(17)	1438(0)
388(0)	960(1)	1495(115)	386(0)	951(1)	1483(110)
420(13)	995(9)	1500(18)	407(6)	984(7)	1489(12)
441(2)	996(0)	1630(139)	408(0)	985(0)	1597(144)
443(0)	1031(0)	1633(1)	414(4)	1011(0)	1600(2)
458(1)	1032(4)	3005(57)	442(1)	1012(29)	3032(0)
464(17)	1049(24)	3006(0)	450(27)	1024(1)	3033(42)
576(6)	1051(0)	3085(1)	550(5)	1025(0)	3094(1)
576(5)	1082(0)	3086(67)	550(8)	1066(4)	3094(38)
583(2)	1084(1)	3090(6)	570(2)	1067(0)	3097(24)
591(0)	1112(1)	3090(92)	576(0)	1093(0)	3098(26)
632(1)	1113(2)	3098(219)	612(0)	1095(3)	3109(77)
635(1)	1122(0)	3099(2)	614(0)	1105(0)	3109(4)
652(86)	1122(1)	3126(19)	653(115)	1106(1)	3126(6)
657(8)	1152(3)	3126(4)	656(10)	1129(4)	3127(2)
719(139)	1154(0)	3157(36)	704(190)	1131(0)	3153(11)
721(0)	1230(4)	3157(20)	705(5)	1206(0)	3153(4)
743(133)	1231(6)	3178(5)	741(71)	1206(3)	3181(2)
777(12)	1264(1)	3178(32)	758(0)	1232(0)	3181(8)
787(5)	1264(1)	3187(9)	765(12)	1232(2)	3189(5)
796(48)	1270(25)	3187(45)	787(54)	1236(42)	3189(14)
853(6)	1271(1)	3206(149)	843(11)	1238(3)	3208(45)
854(0)	1299(0)	3207(0)	845(0)	1262(1)	3209(0)

Table S102 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for the **$(bcod)_2Cu$** structure **Cu-5D.**

M06-L			OPBE		
36(0)	881(34)	1299(0)	20(0)	853(39)	1263(3)
43(0)	883(6)	1320(6)	36(0)	860(8)	1293(7)
54(0)	886(9)	1321(0)	54(0)	873(11)	1294(0)
62(3)	887(1)	1333(1)	56(2)	876(13)	1304(1)
99(0)	897(9)	1335(0)	84(0)	876(0)	1305(1)
121(1)	897(0)	1357(26)	132(0)	876(2)	1325(37)
167(1)	902(45)	1359(0)	158(1)	888(37)	1326(1)
200(2)	914(1)	1425(4)	191(1)	895(0)	1398(6)
255(3)	941(1)	1427(0)	248(5)	932(0)	1399(1)
307(18)	944(4)	1464(12)	285(19)	933(4)	1434(3)
311(3)	960(8)	1473(5)	290(2)	951(9)	1441(9)
391(1)	961(8)	1492(208)	389(1)	952(13)	1470(216)
414(17)	995(6)	1520(0)	399(3)	983(4)	1498(0)
428(2)	997(2)	1633(145)	405(0)	985(2)	1598(161)
435(0)	1030(8)	1636(8)	413(10)	1010(24)	1601(5)
452(14)	1038(0)	3010(31)	441(27)	1015(2)	3048(14)
459(0)	1046(16)	3024(12)	445(0)	1024(0)	3052(21)
577(13)	1048(1)	3076(15)	549(20)	1026(1)	3091(36)
578(0)	1083(1)	3076(61)	551(2)	1066(3)	3091(4)
587(1)	1083(0)	3091(87)	570(2)	1067(0)	3099(37)
591(3)	1111(3)	3092(4)	572(2)	1093(3)	3099(25)
631(2)	1112(0)	3099(58)	609(0)	1094(0)	3116(36)
631(1)	1123(1)	3102(122)	612(1)	1106(0)	3118(23)
653(2)	1124(0)	3126(10)	650(114)	1106(0)	3120(10)
654(92)	1156(8)	3127(22)	650(3)	1133(0)	3120(3)
718(84)	1163(0)	3153(24)	704(85)	1133(11)	3143(6)
720(59)	1228(19)	3153(33)	706(104)	1206(6)	3144(11)
750(151)	1230(0)	3177(36)	746(87)	1207(0)	3181(9)
766(17)	1264(4)	3177(0)	756(7)	1232(0)	3181(1)
788(0)	1267(0)	3190(36)	770(67)	1232(1)	3190(14)
789(30)	1270(34)	3190(22)	772(0)	1237(63)	3190(4)
852(3)	1274(0)	3206(157)	844(8)	1240(0)	3208(49)
854(1)	1298(2)	3207(0)	847(1)	1263(0)	3208(1)

Table S103 Total energies (E in hartree), total free energies (G, in hartree), relative energies (ΔE and ΔG in kcal mol^{-1}), and the staggered angles χ for the **(bcod)$_2$Ti** structures optimized at the M06-L/DZP level. The temperature is 298.150 Kelvin and the pressure is 1.00000 Atm from Table S103 to Table S110.

Structure		E+1469	ΔE	G+1469	ΔG	χ
Ti-1S	C_2	-0.91265	0.0	-0.65942	0.0	118.0°
Ti-2S	C_1	-0.90860	2.5	-0.65657	1.8	25.3°
Ti-3S	C_1	-0.90597	4.2	-0.65498	2.8	143.9°
TI-4T	C_2	-0.89728	9.6	-0.64795	7.2	174.3°
TI-5T	C_1	-0.89722	9.7	-0.64870	6.7	40.6°
TI-6T	C_1	-0.89722	9.7	-0.64870	6.7	40.9°

Table S104 Total energies (E in hartree), total free energies (G, in hartree), relative energies (ΔE and ΔG in kcal mol^{-1}), and the χ angles for the **(bcod)$_2$V** structures optimized at the M06-L/DZP level.

Structure		E+1564	ΔE	G+1564	ΔG	χ
V-1Q	C_{2h}	-0.44728	0.0	-0.19540	0.0	180.0°
V-2Q	C_2	-0.44642	0.5	-0.19592	-0.3	51.0°
V-3D	C_1	-0.43296	9.0	-0.18139	8.8	98.7°
V-4D	C_1	-0.43075	10.4	-0.17870	10.5	51.8°
V-5D	C_1	-0.42680	12.9	-0.17577	12.3	153.1°
V-6Q	C_s	-0.42594	13.4	-0.17541	12.5	
V-7D	C_1	-0.41283	21.6	-0.16095	21.6	

Table S105 Total energies (E in hartree), total free energies (G in hartree), relative energies (ΔE and ΔG in kcal mol^{-1}), and the χ angles for the **(bcod)$_2$Cr** structures optimized at the M06-L/DZP level.

Structure		E+1664	ΔE	G+1664	ΔG	χ
Cr-1T	C_2	-0.90702	0.0	-0.65474	0.0	77.7°
Cr-2T	C_{2h}	-0.90695	0.0	-0.65395	0.5	180.0°
Cr-3P	C_{2h}	-0.89412	8.1	-0.64672	5.0	180.0°
Cr-4P	C_2	-0.89268	9.0	-0.64450	6.4	18.9°
Cr-5P	C_s	-0.89016	10.6	-0.64056	8.9	
Cr-6P	C_2	-0.88910	11.2	-0.64075	8.8	89.1°
Cr-7T	C_1	-0.88861	11.6	-0.63634	11.5	
Cr-8S	C_1	-0.87139	22.4	-0.61634	24.1	100.3°
Cr-9S	C_2	-0.86886	23.9	-0.61248	26.5	146.4°

Table S106 Total energies (E in hartree), total free energies (G in hartree), relative energies (ΔE and ΔG in kcal mol^{-1}), and the χ angles for the **(bcod)$_2$Mn** structures optimized at the M06-L/DZP level.

Structure		E+1771	ΔE	G+1771	ΔG	χ
Mn-1D	C_{2h}	-0.41947	0.0	-0.16419	0.0	180.0°
Mn-2D	C_2	-0.41716	1.5	-0.16256	1.0	56.3°
Mn-3Q	C_1	-0.41714	1.5	-0.16721	-1.9	33.4°
Mn-4Q	C_1	-0.41532	2.6	-0.16540	-0.8	124.2°
Mn-5X	C_2	-0.41313	4.0	-0.16560	-0.9	179.8°
Mn-6Q	C_1	-0.41312	4.0	-0.16300	0.7	
Mn-7X	C_1	-0.41286	4.1	-0.16629	-1.3	46.0°
Mn-8X	C_1	-0.41265	4.3	-0.16752	-2.1	102.6°
Mn-9X	C_1	-0.40751	7.5	-0.16102	2.0	
Mn-10X	C_1	-0.40727	7.7	-0.16191	1.4	
Mn-11X	C_1	-0.40334	10.1	-0.15795	3.9	

Table S107 Total energies (E in hartree), total free energies (G in hartree), relative energies (ΔE and ΔG in kcal mol^{-1}), and the χ angles for the **(bcod)$_2$Fe** structures optimized at the M06-L/DZP level.

Structure		E+1884	ΔE	G+1883	ΔG	χ
Fe-1S	C_2	-0.15549	0.0	-0.89714	0.0	51.4°
Fe-2S	C_{2h}	-0.15296	1.6	-0.89422	1.8	180.0°
Fe-3T	C_{2h}	-0.12461	19.4	-0.87094	16.4	180.0°
Fe-4T	C_1	-0.11742	23.9	-0.86622	19.4	115.2°

Table S108 Total energies (E in hartree), total free energies (G in hartree), relative energies (ΔE and ΔG in kcal mol^{-1}), and the χ angles for the **(bcod)$_2$Co** structures optimized at the M06-L/DZP level.

Structure		E+2003	ΔE	G+2002	ΔG	χ
Co-1D	C_{2h}	-0.20066	0.0	-0.94668	0.0	180.0°
Co-2D	C_1	-0.19409	4.1	-0.94188	3.0	41.3°
Co-3D	C_1	-0.19036	6.5	-0.93730	5.9	110.6°
Co-4D	C_2	-0.18986	6.8	-0.93677	6.2	85.0°
Co-5D	C_1	-0.18902	7.3	-0.93570	6.9	

Table S109 Total energies (E in hartree), total free energies (G in hartree), relative energies (ΔE and ΔG in kcal mol^{-1}), and the χ angles for the **(bcod)$_2$Ni** structures optimized at the M06-L/DZP level.

Structure		E+2128	ΔE	G+2128	ΔG	χ
Ni-1S	C_1	-0.73953	0.0	-0.48424	0.0	
Ni-2S	C_s	-0.73614	2.1	-0.48277	0.9	
Ni-3S	C_1	-0.73611	2.1	-0.48121	1.9	139.9°
Ni-4S	C_1	-0.73176	4.9	-0.47765	4.1	75.8°

Table S110. Total energies (E in hartree), total free energies (G, in hartree), relative energies (ΔE and ΔG in kcal mol^{-1}), and the χangles for the **$(bcod)_2Cu$**structures optimized at the M06-L/DZP level..

Structure		E+2260	ΔE	G+2260	ΔG	χ
Cu-1D	C_1	-0.87877	0.0	-0.63164	0.0	163.9°
Cu-2D	C_1	-0.87670	1.3	-0.62871	1.8	6.2°
Cu-3D	C_s	-0.87480	2.5	-0.62701	2.9	0.0°
Cu-4D	C_2	-0.87457	2.6	-0.62638	3.3	
Cu-5D	C_2	-0.87029	5.3	-0.62196	6.1	

Table S111. Energy gaps between the lowest unoccupied and the highest occupied molecular orbitals (in eV) and the spin values $\langle S^2 \rangle$for the $(bcod)_2M$ structures optimized at the M06-L/DZP level.

Structure	HOMO(α)	LUMO(α)	Gap/eV	$\langle S^2 \rangle$
Ti-1S	-0.13522	-0.06284	2.0	0.00
Ti-2S	-0.13682	-0.06488	2.0	0.00
Ti-3S	-0.13464	-0.06774	1.8	0.00
TI-4T	-0.11040	-0.08233	0.8	2.02
TI-5T	-0.11320	-0.08274	0.8	2.02
TI-6T	-0.11320	-0.08274	0.8	2.02
V-1Q	-0.12749	-0.01772	2.8	3.79
V-2Q	-0.12749	-0.01772	3.0	3.80
V-3D	-0.12710	-0.07320	1.5	0.79
V-4D	-0.12765	-0.07837	1.3	0.80
V-5D	-0.12710	-0.08793	1.1	0.82
V-6Q	-0.13544	-0.04364	2.5	3.79
V-7D	-0.13048	-0.08102	1.3	0.78
Cr-1T	-0.15532	-0.03819	3.2	2.14
Cr-2T	-0.15830	-0.03441	3.4	2.12
Cr-3P	-0.10444	-0.03899	1.8	6.11
Cr-4P	-0.11094	-0.04338	1.8	6.12
Cr-5P	-0.13671	-0.04771	2.4	6.12
Cr-6P	-0.10477	-0.05127	1.5	6.09
Cr-7T	-0.15867	-0.06094	2.7	2.14
Cr-8S	-0.10875	-0.07090	1.0	0.00
Cr-9S	-0.12606	-0.09674	0.8	0.00
Mn-1D	-0.15206	-0.02765	3.4	0.79
Mn-2D	-0.15916	-0.03614	3.3	0.87
Mn-3Q	-0.13582	-0.06156	2.0	4.01
Mn-4Q	-0.13663	-0.06743	1.9	4.02
Mn-5X	-0.12016	-0.02115	2.7	8.80
Mn-6Q	-0.14803	-0.06501	2.3	3.98

Mn-7X	-0.12628	-0.02255	2.8	8.79
Mn-8X	-0.13141	-0.01829	3.1	8.79
Mn-9X	-0.13340	-0.02994	2.8	8.80
Mn-10X	-0.13451	-0.02969	2.9	8.79
Mn-11X	-0.13660	-0.03229	2.8	8.90
Fe-1S	-0.14611	-0.02359	3.3	0.00
Fe-2S	-0.14019	-0.03274	2.9	0.00
Fe-3T	-0.14438	-0.04016	2.8	2.10
Fe-4T	-0.12386	-0.05276	1.9	2.12
Co-1D	-0.12794	-0.04709	2.2	0.81
Co-2D	-0.11350	-0.05306	1.6	0.81
Co-3D	-0.11287	-0.04831	1.8	0.80
Co-4D	-0.11091	-0.05335	1.6	0.79
Co-5D	-0.13459	-0.05561	2.2	0.79
Ni-1S	-0.15343	-0.05995	2.5	0.00
Ni-2S	-0.13557	-0.05577	2.2	0.00
Ni-3S	-0.15010	-0.05870	2.5	0.00
Ni-4S	-0.14049	-0.06015	2.2	0.00
Cu-1D	-0.12445	-0.01421	3.0	0.77
Cu-2D	-0.12702	-0.01846	3.0	0.77
Cu-3D	-0.13406	-0.03660	2.7	0.77
Cu-4D	-0.13485	-0.02442	3.0	0.77
Cu-5D	-0.14162	-0.01993	3.3	0.77

Table S112. Optimized coordinates for the **(bcod)Ti** structure **Ti-D.**

	M06-L/DZP		
	x	y	z
C	0.670050	-0.718653	1.176041
C	0.670050	-0.718653	-1.176041
C	1.536583	-1.190479	0.000000
H	1.599900	-2.283768	0.000000
H	2.547426	-0.765639	0.000000
C	-0.747193	-1.152357	0.755573
C	-0.747193	-1.152357	-0.755573
H	0.975490	-1.112867	2.151122
H	0.975490	-1.112867	-2.151122
C	0.904128	1.504346	0.000000
C	0.670050	0.820773	-1.205218
C	0.670050	0.820773	1.205218
H	-1.273000	-1.935984	1.303113
H	-1.273000	-1.935984	-1.303113
H	0.761432	1.341820	2.156873
H	1.036848	2.588295	0.000000
H	0.761432	1.341820	-2.156873
Ti	-1.266871	0.663401	0.000000

Table S113. Optimized coordinates for the **(bcod)V** structure **V-T.**

	M06-L/DZP		
	x	y	z
C	0.656100	-0.757256	1.180194
C	0.656100	-0.757256	-1.180194
C	1.520464	-1.228968	0.000000
H	1.587312	-2.322070	0.000000
H	2.530197	-0.802314	0.000000
C	-0.757103	-1.158862	0.733590
C	-0.757103	-1.158862	-0.733590
H	0.954964	-1.170223	2.149529
H	0.954964	-1.170223	-2.149529
C	0.900005	1.457143	0.000000
C	0.656100	0.781183	-1.217057
C	0.656100	0.781183	1.217057
H	-1.398653	-1.799257	1.340119
H	-1.398653	-1.799257	-1.340119
H	0.779658	1.303078	2.164148
H	1.032640	2.541757	0.000000
H	0.779658	1.303078	-2.164148
V	-1.174176	0.702852	0.000000

Table S114. Optimized coordinates for the **(bcod)Cr** structure **Cr-X.**

	M06-L/DZP		
	x	y	z
C	0.707036	-0.839281	1.179427
C	0.707036	-0.839281	-1.179427
C	1.576125	-1.305096	0.000000
H	1.664032	-2.397153	0.000000
H	2.573645	-0.855528	0.000000
C	-0.676197	-1.276629	0.690066
C	-0.676197	-1.276629	-0.690066
H	0.985208	-1.276438	2.142543
H	0.985208	-1.276438	-2.142543
C	0.919554	1.361789	0.000000
C	0.707036	0.690516	-1.229885
C	0.707036	0.690516	1.229885
H	-1.507730	-1.537827	1.342442
H	-1.507730	-1.537827	-1.342442
H	0.896929	1.197097	2.171932
H	1.091229	2.439833	0.000000
H	0.896929	1.197097	-2.171932
Cr	-1.246096	0.867157	0.000000

Table S115. Optimized coordinates for the **(bcod)Mn** structure **Mn-P.**

	M06-L/DZP		
	x	y	z
C	0.698400	-0.746674	1.179436
C	0.698400	-0.746674	-1.179436
C	1.565154	-1.215053	0.000000
H	1.640388	-2.307678	0.000000
H	2.570378	-0.780076	0.000000
C	-0.709608	-1.182312	0.731479
C	-0.709608	-1.182312	-0.731479
H	0.994744	-1.160142	2.147942
H	0.994744	-1.160142	-2.147942
C	0.899879	1.475205	0.000000
C	0.698400	0.793553	-1.222246
C	0.698400	0.793553	1.222246
H	-1.362223	-1.793028	1.350662
H	-1.362223	-1.793028	-1.350662
H	0.829335	1.308935	2.169635
H	1.019748	2.559334	0.000000
H	0.829335	1.308935	-2.169635
Mn	-1.167630	0.635247	0.000000

Table S116. Optimized coordinates for the **(bcod)Fe** structure **Fe-Q.**

	M06-L/DZP		
	x	y	z
C	0.697790	-0.789244	1.182345
C	0.697790	-0.789244	-1.182345
C	1.551881	-1.268168	0.000000
H	1.612319	-2.361844	0.000000
H	2.563531	-0.848601	0.000000
C	-0.718948	-1.162277	0.718531
C	-0.718948	-1.162277	-0.718531
H	0.988970	-1.220190	2.145794
H	0.988970	-1.220190	-2.145794
C	0.895337	1.439328	0.000000
C	0.697790	0.743959	-1.218200
C	0.697790	0.743959	1.218200
H	-1.455808	-1.660529	1.346132
H	-1.455808	-1.660529	-1.346132
H	0.780623	1.268993	2.167120
H	1.022734	2.522293	0.000000
H	0.780623	1.268993	-2.167120
Fe	-1.101117	0.668284	0.000000

Table S117. Optimized coordinates for the **(bcod)Co** structure **Co-T.**

	M06-L/DZP		
	x	y	z
C	0.672914	-0.835597	1.185896
C	0.672914	-0.835597	-1.185896
C	1.520942	-1.319596	0.000000
H	1.579075	-2.413600	0.000000
H	2.533643	-0.903873	0.000000
C	-0.744798	-1.166735	0.705997
C	-0.744798	-1.166735	-0.705997
H	0.947604	-1.288394	2.143555
H	0.947604	-1.288394	-2.143555
C	0.885615	1.380138	0.000000
C	0.672914	0.694866	-1.234682
C	0.672914	0.694866	1.234682
H	-1.549370	-1.510979	1.352509
H	-1.549370	-1.510979	-1.352509
H	0.812514	1.214220	2.179533
H	1.023178	2.462734	0.000000
H	0.812514	1.214220	-2.179533
Co	-1.007744	0.716718	0.000000

Table S118. Optimized coordinates for the **(bcod)Ni** structure **Ni-D.**

	M06-L/DZP		
	x	y	z
C	0.670907	-0.829917	1.179827
C	0.670907	-0.829917	-1.179827
C	1.523953	-1.312363	0.000000
H	1.583693	-2.406258	0.000000
H	2.535336	-0.893157	0.000000
C	-0.746311	-1.201574	0.702776
C	-0.746311	-1.201574	-0.702776
H	0.953382	-1.268466	2.142475
H	0.953382	-1.268466	-2.142475
C	0.897183	1.414697	0.000000
C	0.670907	0.701529	-1.217163
C	0.670907	0.701529	1.217163
H	-1.533996	-1.574004	1.352094
H	-1.533996	-1.574004	-1.352094
H	0.739488	1.216007	2.173596
H	1.073225	2.488433	0.000000
H	0.739488	1.216007	-2.173596
Ni	-0.970816	0.693195	0.000000

Table S119. Optimized coordinates for the **(bcod)Cu** structure **Cu-S**

	M06-L/DZP		
	x	y	z
C	0.723860	-0.846127	1.182191
C	0.723860	-0.846127	-1.182191
C	1.581674	-1.321896	0.000000
H	1.654751	-2.414844	0.000000
H	2.586916	-0.889886	0.000000
C	-0.681835	-1.226471	0.699984
C	-0.681835	-1.226471	-0.699984
H	0.998158	-1.293693	2.141404
H	0.998158	-1.293693	-2.141404
C	0.892020	1.371060	0.000000
C	0.723860	0.682995	-1.237128
C	0.723860	0.682995	1.237128
H	-1.501421	-1.512879	1.352958
H	-1.501421	-1.512879	-1.352958
H	0.869320	1.197915	2.181498
H	1.021044	2.453038	0.000000
H	0.869320	1.197915	-2.181498
Cu	-1.035435	0.705147	0.000000

Table S120. Optimized coordinates for thestructure **bcod.**

	M06-L/DZP		
	x	y	z
C	-0.214692	0.472930	1.177167
C	-0.214692	0.472930	-1.177167
C	-1.099808	0.920965	0.000000
H	-1.217133	2.009735	0.000000
H	-2.086991	0.447124	0.000000
C	1.152345	0.925543	0.670679
C	1.152345	0.925543	-0.670679
H	-0.499588	0.904530	2.141404
H	-0.499588	0.904530	-2.141404
C	-0.213090	-1.727760	0.000000
C	-0.214692	-1.036100	-1.211403
C	-0.214692	-1.036100	1.211403
H	2.010349	1.088625	1.316377
H	2.010349	1.088625	-1.316377
H	-0.167872	-1.567455	2.159634
H	-0.179802	-2.815967	0.000000
H	-0.167872	-1.567455	-2.159634

Table S121. The single point energies (kcal/mol), relative energies (∆E in kcal mol^{-1}), and the spin values $\langle S^2 \rangle$ for the**(bcod)$_2$Ti** structures at the M06-L/cc-pVTZ level.

	Ti-1S(C_2)	**Ti-2S**(C_1)	**Ti-3S**(C_1)	**Ti-4T**(C_2)
E	-1470.03635	-1470.03295	-1470.03016	-1470.02224
ΔE	0.0	2.1	3.9	8.8
$\langle S^2 \rangle$	0.00	0.00	0.00	2.02
	Ti-5T(C_1)	**Ti-6T**(C_1)		
E	-1470.02165	-1470.02165		
ΔE	9.2	9.2		
$\langle S^2 \rangle$	2.02	2.02		

Table S122. The single point energies (kcal/mol), relative energies (∆E in kcal mol^{-1}), and the spin values $\langle S^2 \rangle$ for the**(bcod)$_2$V** structures at the M06-L/cc-pVTZlevel.

	V-1Q (C_{2h})	**V-2Q** (C_2)	**V-3D** (C_1)	**V-4D** (C_1)
E	-1564.57741	-1564.57626	-1564.56278	-1564.56083
ΔE	0.0	0.7	9.2	10.4
$\langle S^2 \rangle$	3.79	3.80	0.79	0.80
	V-5D (C_1)	**V-6Q** (C_s)	**V-7D** (C_1)	
E	-1564.55538	-1564.55615	-1564.54253	
ΔE	13.8	13.3	21.9	
$\langle S^2 \rangle$	0.83	3.79	0.78	

Table S123. The single point energies (kcal/mol), relative energies (ΔE in kcal mol^{-1}), and the spin values $\langle S^2 \rangle$ for the **(bcod)$_2$Cr** structures at the M06-L/cc-pVTZlevel.

	Cr-1T (C_2)	**Cr-2T** (C_{2h})	**Cr-3P** (C_{2h})	**Cr-4P** (C_2)
E	-1665.04029	-1665.04107	-1665.02760	-1665.02584
ΔE	0.0	-0.5	8.0	9.1
$\langle S^2 \rangle$	2.13	2.11	6.11	6.11
	Cr-5P (C_s)	**Cr-6P** (C_2)	**Cr-7T** (C_1)	**Cr-8S** (C_1)
E	-1665.02378	-1665.02194	-1665.02226	-1665.00642
ΔE	10.4	11.5	11.3	21.2
$\langle S^2 \rangle$	6.11	6.09	2.13	0.00
	Cr-9S (C_2)			
E	-1665.00217			
ΔE	23.9			
$\langle S^2 \rangle$	0.00			

Table S124. The single point energies (kcal/mol), relative energies (ΔE in kcal mol^{-1}), and the spin values $\langle S^2 \rangle$ for the **(bcod)$_2$Mn** structures at the M06-L/cc-pVTZlevel.

	Mn-1D (C_{2h})	**Mn-2D** (C_2)	**Mn-3Q** (C_1)	**Mn-4Q**(C_1)
E	-1771.55916	-1771.55619	-1771.55443	-1771.55252
ΔE	0.0	1.9	3.0	4.2
$\langle S^2 \rangle$	0.79	0.86	3.99	4.01
	Mn-5X (C_2)	**Mn-6Q** (C_1)	**Mn-7X** (C_1)	**Mn-8X** (C_1)
E	-1771.55017	-1771.55095	-1771.54982	-1771.54964
ΔE	5.6	5.2	5.9	6.0
$\langle S^2 \rangle$	8.80	3.97	8.79	8.79
	Mn-9X (C_1)	**Mn-10X** (C_1)	**Mn-11X** (C_1)	
E	-1771.54491	-1771.54483	-1771.54054	
ΔE	8.9	9.0	11.7	
$\langle S^2 \rangle$	8.80	8.79	8.90	

Table S125. The single point energies (kcal/mol), relative energies (ΔE in kcal mol^{-1}), and the spin values $\langle S^2 \rangle$ for the **(bcod)$_2$Fe** structures at the M06-L/cc-pVTZlevel.

	Fe-1S (C_2)	**Fe-2S** (C_{2h})	**Fe-3T** (C_{2h})	**Fe-4T** (C_1)
E	-1884.29934	-1884.29765	-1884.26915	-1884.26146
ΔE	0.0	1.1	18.9	23.8
$\langle S^2 \rangle$	0.00	0.00	2.10	2.12

Table S126. The single point energies (kcal/mol), relative energies (ΔE in kcal mol^{-1}), and the spin values $\langle S^2 \rangle$ for the **(bcod)$_2$Co** structures at the M06-L/cc-pVTZlevel.

	Co-1D (C_{2h})	**Co-2D** (C_1)	**Co-3D** (C_1)	**Co-4D** (C_2)
E	-2003.35360	-2003.34622	-2003.34192	-2003.34139
ΔE	0.0	4.6	7.3	7.7
$\langle S^2 \rangle$	0.81	0.81	0.80	0.79
	Co-5D (C_1)			
E	-2003.34175			
ΔE	7.4			
$\langle S^2 \rangle$	0.79			

Table S127. The single point energies (kcal/mol), relative energies (ΔE in kcal mol^{-1}), and the spin values $\langle S^2 \rangle$ for the **(bcod)$_2$Ni** structures at theM06-L/cc-pVTZlevel.

	Ni-1S (C_s)	**Ni-2S** (C_s)	**Ni-3S** (C_1)	**Ni-4S** (C_1)
E	-2128.89928	-2128.89676	-2128.89528	-2128.89115
ΔE	0.0	1.6	2.5	5.1
$\langle S^2 \rangle$	0.00	0.00	0.00	0.00

Table S128. The single point energies (kcal/mol), relative energies (ΔE in kcal mol^{-1}), and the spin values $\langle S^2 \rangle$ for the **(bcod)$_2$Cu** structures at the M06-L/cc-pVTZlevel.

	Cu-1D (C_1)	**Cu-2D** (C_1)	**Cu-3D**(C_s)	**Cu-4D** (C_2)
E	-2261.04755	-2261.04526	-2261.04325	-2261.04391
ΔE	0.0	1.4	2.7	2.3
$\langle S^2 \rangle$	0.77	0.77	0.78	0.77
	Cu-5D (C_2)			
E	-2261.03968			
ΔE	4.9			
$\langle S^2 \rangle$	0.77			

Table S129. Optimized coordinates for thestructure **(bcod)Cr(C_5H_6).**

	M06-L/cc-pVTZ		
	x	y	z
C	2.298784	-0.206709	-1.140325
C	2.298773	-0.206681	1.140338
C	2.872553	-1.022607	0.000019
H	3.980181	-1.071006	0.000025
H	2.524417	-2.058260	0.000031
C	2.189178	1.144279	-0.704249
C	2.189171	1.144296	0.704226
H	2.390380	-0.487171	-2.179358
H	2.390361	-0.487116	2.179379
H	2.032284	2.007380	-1.334668
H	2.032271	2.007413	1.334622
C	-2.190775	0.137915	1.173969
C	-2.190779	0.137929	-1.173963
C	-3.145562	-0.093736	0.000003
H	-3.933579	0.659348	0.000009
H	-3.591315	-1.086914	-0.000002
C	-1.425657	1.354036	0.676910
C	-1.425660	1.354044	-0.676892
H	-2.682890	0.276829	2.134181
H	-2.682897	0.276853	-2.134172
C	-0.888771	-1.638727	-0.000009
C	-1.157227	-0.977353	-1.209651
C	-1.157224	-0.977369	1.209641
H	-0.903525	2.049083	1.320968
H	-0.903530	2.049099	-1.320943
H	-0.897032	-1.435965	2.152688
H	-0.283573	-2.539520	-0.000015
H	-0.897040	-1.435940	-2.152704
Cr	0.492695	0.015832	-0.000006

Table S130.Optimized coordinates for thestructure **(bcod)Cr(C_6H_7).**

	M06-L/cc-pVTZ		
	x	y	z
C	-2.069336	-1.134248	-0.561183
C	-1.898499	0.252655	1.386707
C	-2.581582	-0.988705	0.853305
H	-2.285616	-1.857416	1.442694
H	-3.680612	-0.929665	0.915455
H	-2.052684	-2.113399	-1.020753
H	-1.746222	0.361546	2.451921
C	-2.003300	1.291153	-0.829954
C	-1.895340	1.408475	0.579683
C	-2.072163	0.004216	-1.405761
H	-1.982923	-0.100772	-2.478820
H	-1.901625	2.165698	-1.457254
H	-1.652248	2.374997	1.003931
C	2.303745	0.317219	-1.058505
C	2.139005	-0.083471	1.251133
C	3.171717	-0.123348	0.121777
H	3.960297	0.607253	0.305084
H	3.614645	-1.108148	-0.017481
C	1.494775	1.433665	-0.419259
C	1.394798	1.196628	0.914738
H	2.862010	0.611845	-1.944501
H	2.563654	-0.110636	2.252407
C	0.913224	-1.621194	-0.292531
C	1.095044	-1.166302	1.027548
C	1.255574	-0.745084	-1.349801
H	1.030438	2.242991	-0.966420
H	0.842946	1.784864	1.634137
H	1.066286	-1.034974	-2.373950
H	0.361788	-2.530335	-0.489598
H	0.767283	-1.770666	1.861823
Cr	-0.385558	0.048203	-0.101086

Table S131. Optimized coordinates for thestructure**(bcod)Fe(C_5H_6).**

	M06-L/cc-pVTZ		
	x	y	z
C	-2.096472	0.171422	-1.141429
C	-2.096472	0.171435	1.141426
C	-2.668555	0.980283	-0.000007
H	-3.773782	1.015635	-0.000007
H	-2.335606	2.020864	-0.000013
C	-1.902282	-1.157652	-0.714139
C	-1.902282	-1.157644	0.714152
H	-2.161197	0.470815	-2.177226
H	-2.161197	0.470842	2.177219
H	-1.730211	-2.015208	-1.345963
H	-1.730212	-2.015193	1.345986
C	2.012602	-0.163085	1.174345
C	2.012598	-0.163079	-1.174348
C	2.977291	0.005401	-0.000003
H	3.710757	-0.801071	-0.000006
H	3.494113	0.965019	-0.000002
C	1.140287	-1.311912	0.690589
C	1.140285	-1.311909	-0.690594
H	2.498916	-0.328716	2.134349
H	2.498908	-0.328706	-2.134354
C	0.807232	1.687011	0.000005
C	1.042742	1.002442	-1.204519
C	1.042745	1.002434	1.204524
H	0.734726	-2.075177	1.336756
H	0.734723	-2.075172	-1.336763
H	0.767516	1.453365	2.148507
H	0.231518	2.607030	0.000009
H	0.767513	1.453380	-2.148499
Fe	-0.407877	0.025054	0.000000

Table S132. Optimized coordinates for thestructure **(bcod)Fe(C_6H_7).**

	M06-L/cc-pVTZ		
	x	y	z
C	-1.832994	-0.717792	-1.170762
C	-1.832994	-0.717792	1.170762
C	-2.396305	-1.469065	0.000000
H	-2.006597	-2.489082	0.000000
H	-3.495035	-1.564547	0.000000
H	-1.651407	-1.244518	-2.099906
H	-1.651406	-1.244518	2.099906
C	-1.927497	1.413986	0.000000
C	-1.876742	0.678514	1.211931
C	-1.876742	0.678514	-1.211931
H	-1.709212	1.206332	-2.142995
H	-1.904780	2.494808	0.000000
H	-1.709212	1.206332	2.142995
C	2.060617	-0.346315	1.176238
C	2.060617	-0.346315	-1.176238
C	3.035724	-0.303694	0.000000
H	3.665551	-1.194245	0.000000
H	3.668064	0.584105	0.000000
C	1.031155	-1.352828	0.690106
C	1.031155	-1.352828	-0.690107
H	2.522803	-0.580252	2.133900
H	2.522803	-0.580251	-2.133900
C	1.069308	1.637101	0.000000
C	1.222590	0.914610	-1.203151
C	1.222590	0.914610	1.203151
H	0.523550	-2.058998	1.328443
H	0.523551	-2.058997	-1.328444
H	1.004729	1.391740	2.150600
H	0.670892	2.644850	0.000000
H	1.004729	1.391740	-2.150599
Fe	-0.304689	0.165818	0.000000

Table S133. Optimized coordinates for thetructure**C_2H_2-Singlet.**

	M06-L/cc-pVTZ		
	x	y	z
C	0.000000	0.000000	0.598652
C	0.000000	0.000000	-0.598652
H	0.000000	0.000000	1.659130
H	0.000000	0.000000	-1.659130

Table S134. Optimized coordinates for thestructure **C_3H_3-Quartet.**

	M06-L/cc-pVTZ		
	x	y	z
C	0.000000	0.328357	0.000001
C	-1.210503	-0.292934	-0.000006
C	1.210503	-0.292924	0.000004
H	2.227461	0.058423	-0.000010
H	-0.000013	1.428133	-0.000004
H	-2.227452	0.058446	0.000024

Table S135. Total energies (E in hartree), and the spin values $\langle S^2 \rangle$ forthe**(bcod)Fe(C_5H_6)**, **(bcod)Fe(C_6H_7)**, **(bcod)Cr(C_5H_6), (bcod)Cr(C_6H_7)**,**C_3H_3-Quartet**, **C_2H_2-Singlet** structures optimized at the M06-L/cc-pVTZ level.

	(bcod)Fe(C_5H_6)	(bcod)Fe(C_6H_7)	(bcod)Cr(C_5H_6)	(bcod)Cr(C_6H_7)
E	-1548.91462	-1587.64389	-1768.16394	-1806.90076
$\langle S^2 \rangle$	3.93	2.12	0.79	0.00
	C_2H_2(singlet)	C_3H_3(quartet)		
E	-77.34384	-115.91437		
$\langle S^2 \rangle$	0.00	3.81		

Complete Gaussian 09 reference (Reference 15)

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Gaussian 09, Revision A.02, Gaussian, Inc., Wallingford CT, 2009.