

Revealing well-defined cluster-supported bi-atom catalysts for enhanced CO₂ Electroreduction: A theoretical investigation

Huong T. D. Bui,^{†,‡,#} Viet Q. Bui,^{†,‡,#} Seong-Gon Kim,[¶] Yoshiyuki Kawazoe,[‡] Hyoyoung Lee^{†,‡,¶,Δ}*

[†]Center for Integrated Nanostructure Physics (CINAP), Institute for Basic Science (IBS), Sungkyunkwan University, Suwon 16419, Korea

[‡]Department of Chemistry, Sungkyunkwan University (SKKU), Suwon, 16419, Republic of Korea

[¶]Department of Physics & Astronomy and Center for Computational Sciences, Mississippi State University, Mississippi State, MS 39762, USA

[‡]New Industry Creation Hatchery Center, Tohoku University, Sendai, 980-8579, Japan

[¶]Creative Research Institute, Sungkyunkwan University (SKKU), Suwon, 16419, Republic of Korea

^ΔDepartment of Biophysics, Sungkyunkwan University (SKKU), Suwon, 16419, Republic of Korea

*To whom correspondence should be addressed. Email: hyoyoung@skku.edu

[#]These authors contributed equally to this work

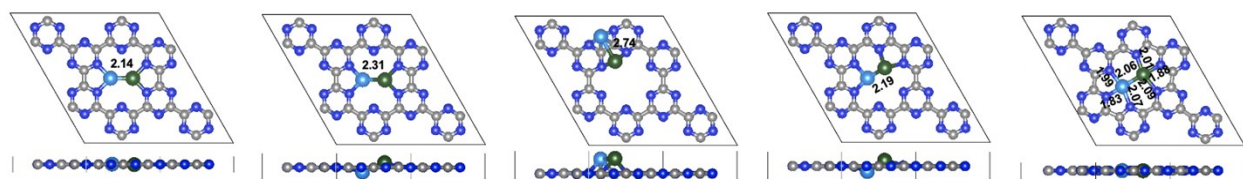


Fig. S1. Possible optimized geometries of MN@g-CN (taking CoNi@g-CN for example) from top and side views. Color code: Co-light blue, Ni-green, C-gray and N-dark blue.

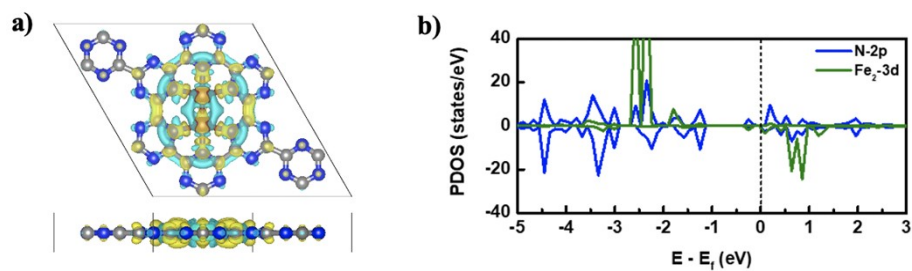


Fig. S2. (a) The charge density difference of Fe₂@g-CN. Color code: yellow – charge accumulation, cyan – charge depletion. (b) Partial density of states (PDOS) of N-2p and Fe-3d orbitals of Fe₂@g-CN.

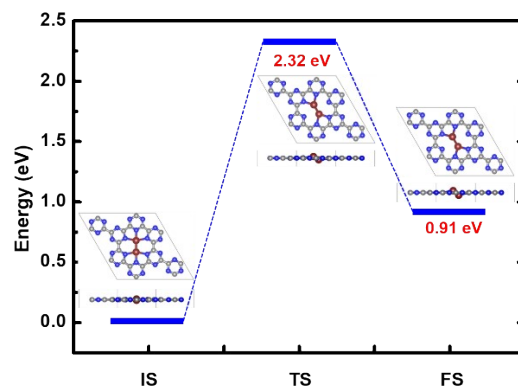


Fig. S3. Kinetic barrier and atomic structures (top and side views) diagram including initial state (IS), transition state (TS), and final state (FS) for the degradation process of Fe₂@g-CN.

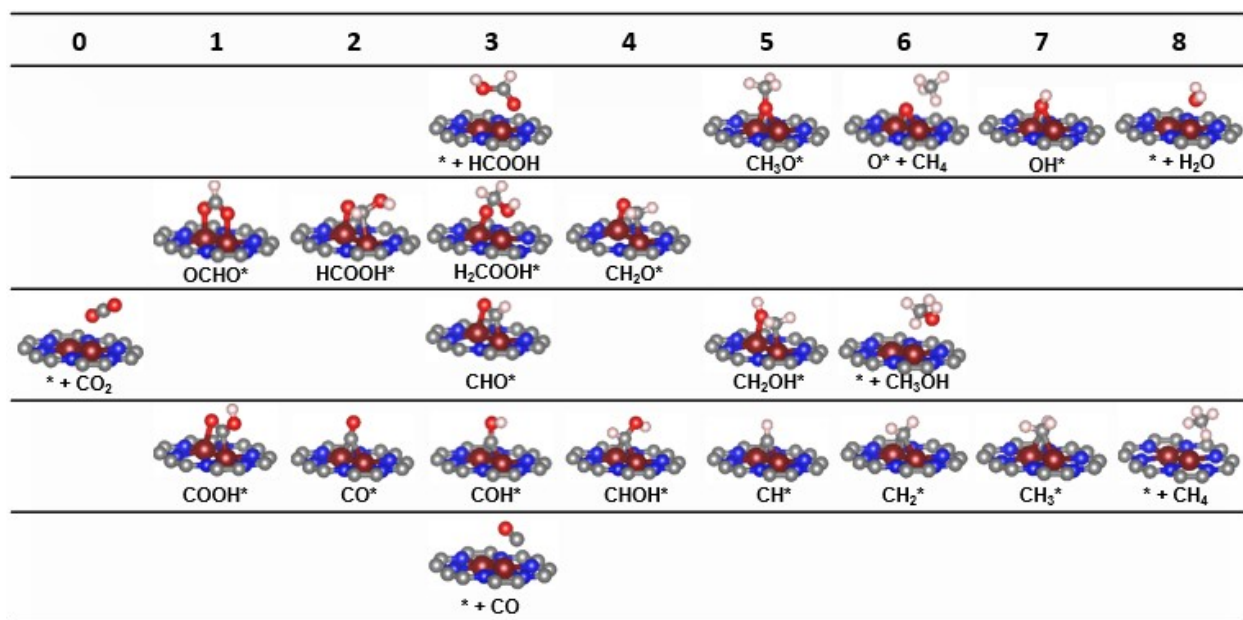


Fig. S4. Optimized intermediate structures along all possible CO₂RR pathways towards various C₁ products on Fe₂@g-CN.

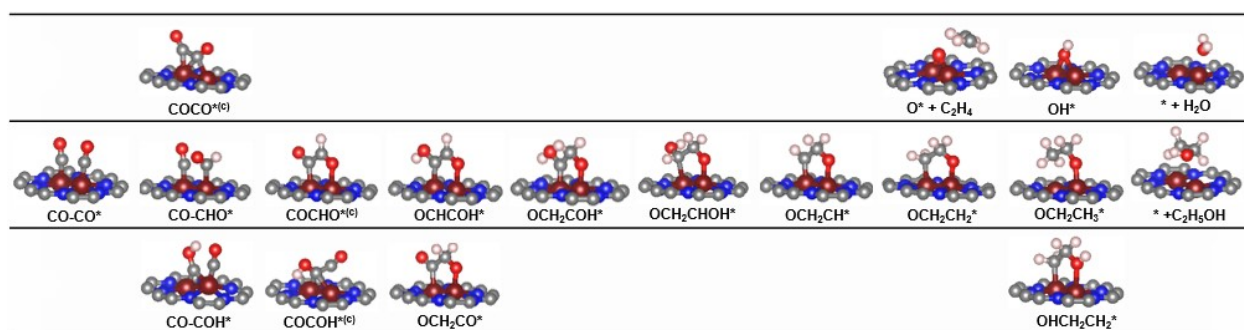


Fig. S5. Optimized intermediate structures along all possible CO₂RR pathways towards various C₂ products on Fe₂@g-CN.

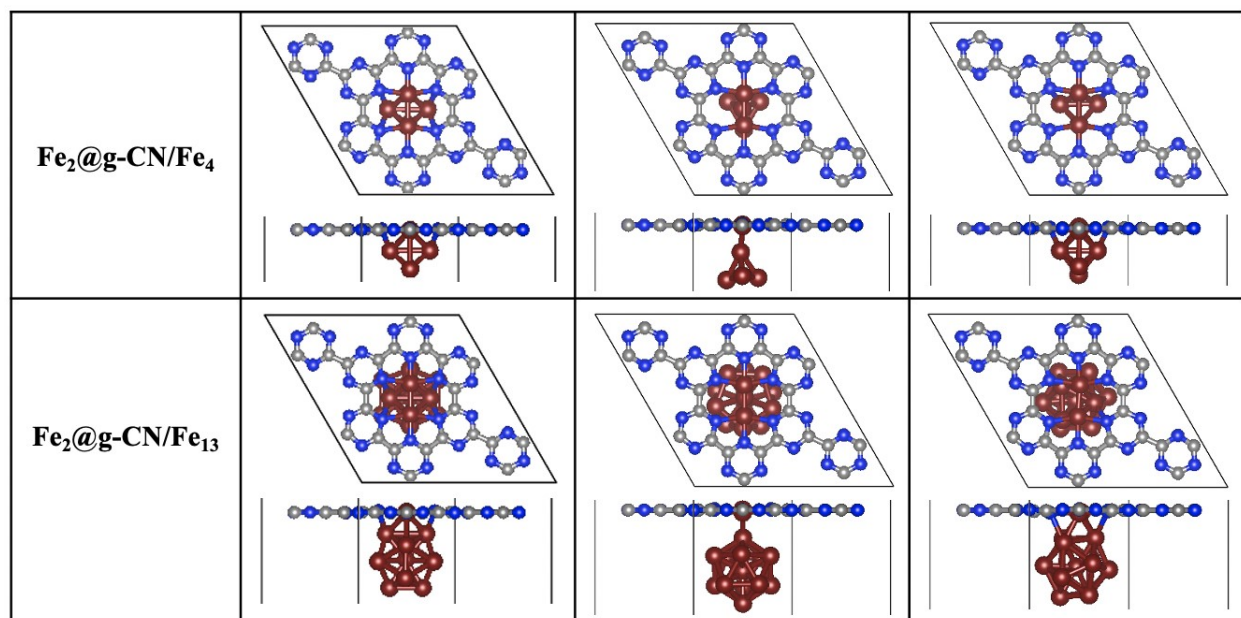


Fig. S6. Possible optimized geometries of $\text{Fe}_2@\text{g-CN}/\text{Fe}_4$ and $\text{Fe}_2@\text{g-CN}/\text{Fe}_{13}$ from top and side views.

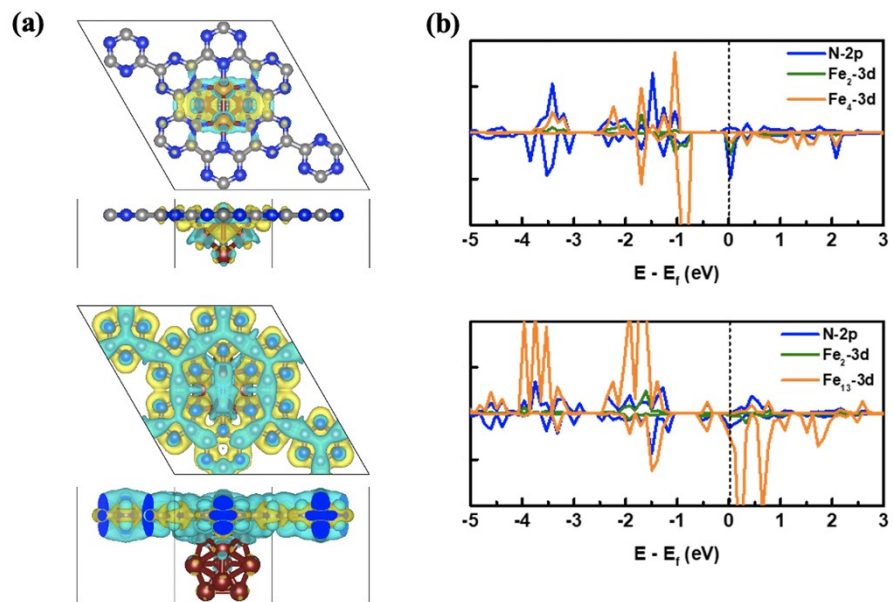


Fig. S7. (a) The charge density difference and (b) partial density of states (PDOS) of N-2p and Fe-3d orbitals (in atomic Fe_2 dimer and in $\text{Fe}_{4(13)}$ clusters support of $\text{Fe}_2@\text{g-CN}/\text{Fe}_4$ and $\text{Fe}_2@\text{g-CN}/\text{Fe}_{13}$. Color code: yellow – charge accumulation, cyan – charge depletion. Isosurface: 0.0025, 0.001 $\text{e}/\text{\AA}^3$.

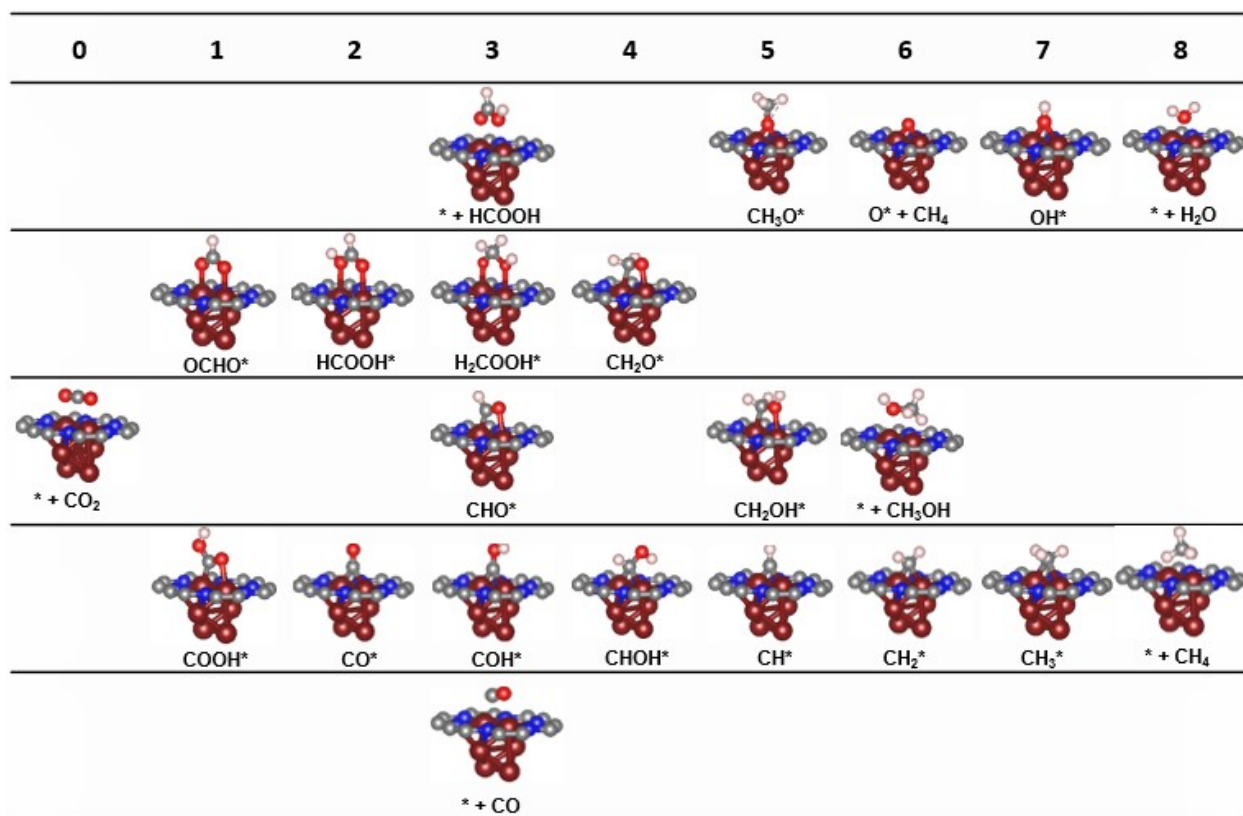


Fig. S8. Optimized intermediate structures along all possible CO₂RR pathways towards various C₁ products on Fe₂@g-CN/Fe₄.

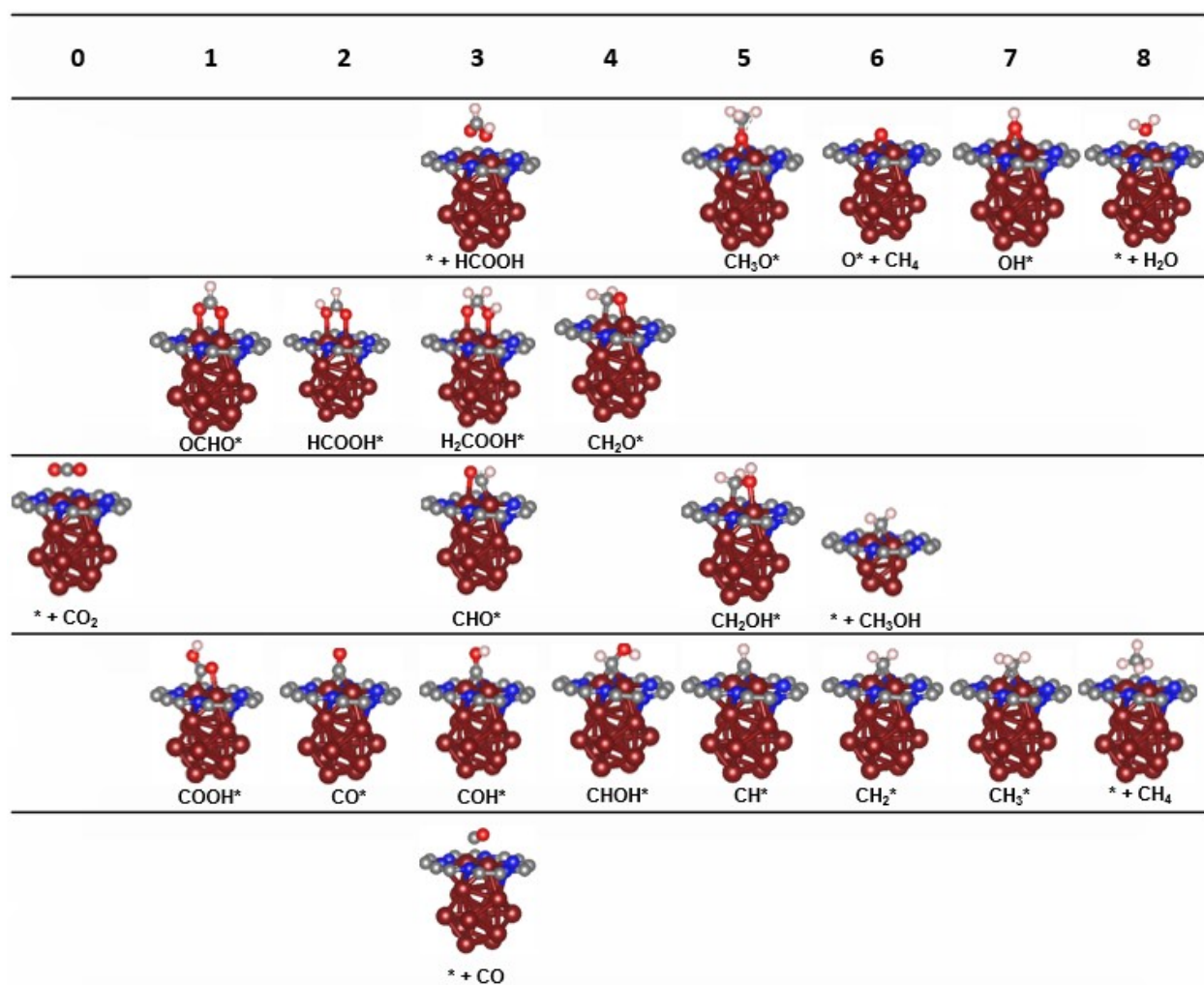


Fig. S9. Optimized intermediate structures along all possible CO₂RR pathways towards various C₁ products on Fe₂@g-CN/Fe₁₃.

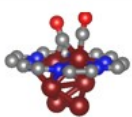
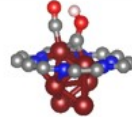
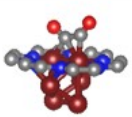
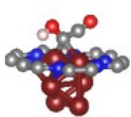
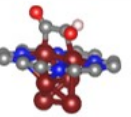
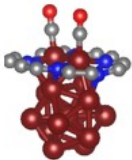
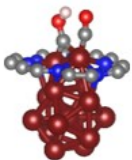
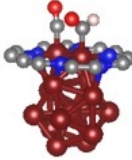
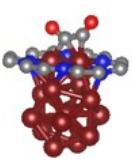
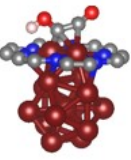
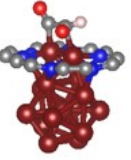
	CO-CO*	CO-COH*	CO-CHO*	COCO*(c)	COCOH*(c)	COCHO*(c)
$\text{Fe}_2@\text{g-CN}/\text{Fe}_4$						
$\text{Fe}_2@\text{g-CN}/\text{Fe}_{13}$						

Fig. S10. Optimized intermediate structures along the C-C coupling process of C_2 paths on $\text{Fe}_2@\text{g-CN}/\text{Fe}_4$ and $\text{Fe}_2@\text{g-CN}/\text{Fe}_{13}$

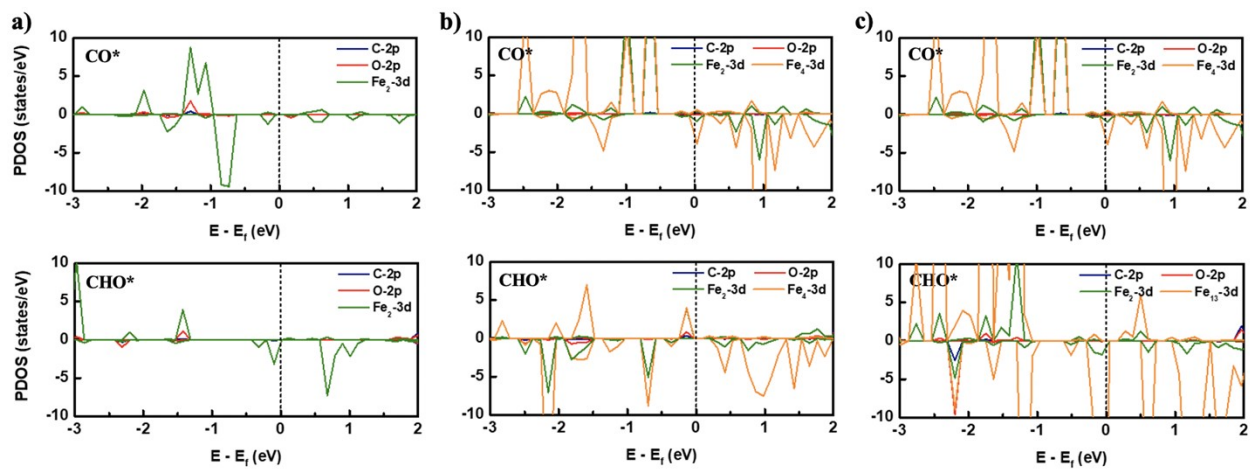


Fig. S11. Partial density of states (PDOS) of C-2p, O-2p and Fe-3d orbitals (Fe_2 dimer and $\text{Fe}_{4(13)}$ clusters) in CO^* and CHO^* intermediates of (a) $\text{Fe}_2@\text{g-CN}$, (b) $\text{Fe}_4/\text{Fe}_2@\text{g-CN}$ and (c) $\text{Fe}_{13}/\text{Fe}_2@\text{g-CN}$.

Table S1 Bimetal bond length ($\text{\AA}$), formation energy (E_f) and total Bader charge (e) of bimetallic

MN@g-CN	$d_{\text{M-N}}$	E_f	Total Bader charge [MN]	MN@g-CN	$d_{\text{M-N}}$	E_f	Total Bader charge [MN]
Fe ₂	2.04	0.42	1.53	Pd ₂	2.48	0.34	1.19
FeCo	2.44	0.41	1.16	Cr ₂	1.48	0.15	1.54
FeNi	2.42	0.31	1.33	CrCo	2.10	0.37	1.51
FeCu	2.27	0.56	1.39	CrCu	2.40	0.28	1.71
FePd	2.21	0.36	1.33	CrFe	1.92	0.44	1.41
Co ₂	1.96	0.56	1.26	CrMn	1.47	-0.15	1.68
CoNi	2.06	0.34	1.10	CrNi	2.28	0.13	1.12
CoCu	2.50	0.48	1.20	CrPd	2.32	0.23	1.31
CoPd	2.21	0.42	1.11	Mn ₂	1.50	-0.28	1.54
Ni ₂	2.51	0.08	1.18	MnCo	2.20	-0.07	1.20
NiCu	2.17	0.32	1.14	MnCu	2.32	0.01	1.45
NiPd	2.53	0.15	1.17	MnFe	1.92	0.21	1.34
Cu ₂	2.71	0.43	1.07	MnNi	2.28	-0.31	1.26
CuPd	2.68	0.45	1.15	MnPd	2.31	-0.18	1.09

dimer [MN] in 28 BACs.

Table S2 Calculated Gibbs free energy change (eV) of the first hydrogenation steps in the HER and CO₂RR on 28 BACs.

MN@g-CN	ΔG_{*H}	ΔG_{*COOH}	ΔG_{*OCHO}	MN@g-CN	ΔG_{*H}	ΔG_{*COOH}	ΔG_{*OCHO}
Fe ₂	-0.36	-0.23	-0.52	Pd ₂	0.30	1.71	1.62
FeCo	-0.46	0.39	-0.27	Cr ₂	0.19	-0.32	-1.07
FeNi	-0.27	0.38	0.22	CrCo	-0.46	-0.37	-0.67
FeCu	-0.36	-0.01	-0.21	CrCu	-0.31	0.26	-0.26
FePd	0.20	1.18	0.92	CrFe	-0.63	-1.07	-1.46
Co ₂	-0.68	-0.17	-0.25	CrMn	-0.46	-0.12	-0.88
CoNi	-0.58	0.52	0.12	CrNi	-0.32	0.12	-0.18
CoCu	-0.42	0.23	0.09	CrPd	-0.20	0.51	0.21
CoPd	-0.32	0.50	0.89	Mn ₂	-0.12	-0.45	-0.69
Ni ₂	-0.06	0.95	0.68	MnCo	-0.52	-0.37	-0.36
NiCu	-0.05	1.08	0.30	MnCu	-0.33	0.32	-0.27
NiPd	0.05	1.47	1.36	MnFe	-0.07	-0.57	-0.61
Cu ₂	-0.25	1.13	0.27	MnNi	-0.21	0.28	-0.05
CuPd	-0.05	1.14	1.00	MnPd	0.03	0.82	0.34

Table S3 Calculated adsorption energies (eV) of the H adsorption (HER) and initial CO₂ adsorption (CO₂RR) on seven BACs.

MN@g-CN	Cr ₂	CrMn	CrFe	CrCo	Mn ₂	MnFe	Fe ₂
$E_{\text{ads}}(\text{H}^*)$	-0.02	-0.71	-0.51	-0.72	-0.36	-0.32	-0.62
$E_{\text{ads}}(\text{CO}_2^*)$	-0.18	0.05	-1.07	-0.38	-1.04	-0.89	-0.57

Table S4 Adsorption energies and energy difference (E_{diff}) of intermediates along the CO₂RR

Fe ₂ @g-CN	*OCHO	*COOH	*CO	*CHO	*CH ₂ O	*CH ₃ O	*O+CH ₄	*OH
D3	-1.273	-0.907	-1.461	-0.984	-1.373	-1.771	-2.461	-2.820
optPBE	-1.071	-0.417	-1.376	-0.396	-1.252	-1.657	-2.395	-2.650
E_{diff}	-0.202	-0.489	-0.084	-0.588	-0.121	-0.114	-0.067	-0.171

pathways into CH₄ on Fe₂@g-CN via two different functionals D3 and optPBE.

Our calculation results indicate that the difference in adsorption energies (E_{diff}) for adsorbed species via D3 and optPBE ranges from -0.067 to -0.588 eV. The adsorption energy difference of adsorbed species between D3 and optPBE corrections are generally not significant, and not all adsorption energies calculated by the D3 correction are much more negative than optPBE, such as the cases of CO*, CH₂O*, CH₃O*, O* and OH* (-0.084, -0.121, -0.114, -0.067 and -0.171 eV), respectively.

Cartesian Coordination

Cr2@CN

1.0

14.2519006729	0.0000000000	0.0000000000
-7.1261024411	12.3424147100	0.0000000000
0.0000000000	0.0000000000	19.9325370789

C N Cr

24 24 2

Cartesian

3.563037395	0.747320473	2.989874125
-0.021560907	6.909087658	2.989687920
10.687394142	0.752414048	2.989787102
7.186231613	6.918272495	2.991042852
2.409864426	2.698232651	2.989688873
-1.134351730	8.883301735	2.989876032
9.558437347	2.707985878	2.989787817
6.021777630	8.935505867	2.991056204
4.693448067	2.723582506	2.989611387
1.142346859	8.874294281	2.989606619
11.819873810	2.710002899	2.989798784
8.279681206	8.894439697	2.989910126
-1.147232056	3.451782465	2.989893198
-4.691666126	9.633744240	2.989987373
5.984086037	3.469694853	2.989516020
2.433558941	9.618529320	2.989507675
1.115167737	3.418683767	2.990306854
-2.432148695	9.634227753	2.989911795
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4.719684124	9.646784782	2.989812374

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3.562609673	11.596142769	2.989784479
-1.208348751	4.804027081	2.990081787
-4.756470680	10.978626251	2.989904165
5.917272091	4.842041492	2.987214088
2.375589371	10.950700760	2.990236282
1.164106131	4.786464214	2.989204884
-2.363990068	10.977679253	2.989768505
8.319031715	4.801822186	2.990450859
4.755046368	10.974569321	2.990444422
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-3.559349537	8.905231476	2.989901781
7.108752251	2.753007650	2.990214825
3.589265823	8.873814583	2.987163305
3.540427208	3.468059063	2.989260197
0.016892910	9.590306282	2.989885330
10.686194420	3.437583923	2.989856243
7.143026829	9.632082939	2.989330530
2.370835781	1.369660616	2.990090132
-1.191483974	7.539543152	2.990089178
9.489719391	1.364758611	2.989855051
5.982469559	7.567952633	2.994308710
4.751037121	1.390926242	2.989881039
1.210490227	7.503373623	2.989248991
11.883093834	1.364504576	2.989855766
8.350148201	7.540976524	2.989317417
2.931411743	5.809938908	2.965250969
4.208826065	6.555550575	2.950767517

CrFe@CN

1.0

14.2519006729	0.0000000000	0.0000000000
-7.1261024411	12.3424147100	0.0000000000
0.0000000000	0.0000000000	19.9325370789

C N Cr Fe

24 24 1 1

Cartesian

3.577732801	0.798135757	2.990510702
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10.632824898	0.705615222	2.989847898
7.236803532	6.953902245	2.994296789
2.339607239	2.701323986	2.989462137
-1.079610825	8.874936104	2.990576267
9.500355721	2.676661253	2.989821196
6.094799995	8.960008621	2.992720366
4.639078617	2.831839561	2.986070633
1.203615665	8.770192146	2.987082958
11.756900787	2.672752619	2.989973068
8.346939087	8.925239563	2.991834879
-1.214016438	3.414254427	2.989673138
-4.624137878	9.670530319	2.989789724
5.931249619	3.570852995	2.983980417
2.486867905	9.502701759	2.984470606
1.042186141	3.376387119	2.990877151
-2.368001461	9.668037415	2.990023851
8.211405754	3.470043659	2.990461826
4.788259029	9.636808395	2.986097813
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3.546975136	11.542154312	2.990316629
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-4.694325924	11.012859344	2.989825726
5.906790733	4.940517426	2.976937532
2.407638073	10.834352493	2.991747379
1.103604555	4.751411915	2.993128300
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8.314947128	4.812717915	2.992203474
4.765932083	10.947365761	2.992486238
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7.037400246	2.817079306	2.991871595
3.674954891	8.777682304	2.974602699
3.452489614	3.551172733	2.987140894
0.093165874	9.523190498	2.988932371
10.628125191	3.405221224	2.990096331
7.208654404	9.655603409	2.992105961
2.362583876	1.383962750	2.991236687
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9.433575630	1.331349850	2.989070177
6.033634663	7.592688560	2.993247986
4.726231575	1.505858541	2.988775492
1.221276283	7.393112183	2.985697985
11.824580193	1.329250574	2.990109444
8.402462959	7.576653957	2.992444038
2.881647110	5.556797981	2.998097897
4.249773502	6.909532070	2.949319363

Mn2@CN

1.0

14.2519006729	0.0000000000	0.0000000000
-7.1261024411	12.3424147100	0.0000000000
0.0000000000	0.0000000000	19.9325370789

C N Mn

24 24 2

Cartesian

3.578431129	0.799777627	3.001677752
-0.027235508	6.850646019	2.941004276
10.612942696	0.711379766	2.986914635
7.204393387	6.951957226	2.999135256
2.369143724	2.713330984	2.948096275
-1.077735901	8.864157677	3.000078201
9.478728294	2.671247005	2.986256123
6.055191994	8.932037354	2.996618509
4.637042999	2.816891432	2.958027601
1.211384296	8.771915436	2.956201792
11.750572205	2.670271873	3.007478476
8.327701569	8.920912743	2.956688404
-1.201966524	3.420463800	3.030768156
-4.625102043	9.670510292	2.974307775
5.912754059	3.570647717	3.009568453
2.488018990	9.523053169	3.009046078
1.071031213	3.410446644	2.977243423
-2.353514433	9.669528961	2.994302273
8.202175140	3.477169275	2.982506514
4.756718636	9.627893448	3.023415804
-0.079633236	5.389875889	2.974336147
-3.488115311	11.629409790	2.993555307

7.150523186	5.490529537	3.028938293
3.546185970	11.541157722	2.981387854
-1.247270823	4.769433498	3.013761759
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5.866102695	4.948968410	3.079326391
2.395146370	10.853810310	2.976253748
1.146757603	4.775694370	2.961245298
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-0.048803568	2.708405256	3.017730474
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3.471288919	3.523523092	2.887640476
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4.729615211	1.486459851	3.002754927
1.256761074	7.393774033	2.877697945
11.809732437	1.327449203	2.989190817
8.372699738	7.571757317	2.971362829
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4.263341904	6.404107094	3.066689730

MnFe@CN

1.0

14.2519006729	0.0000000000	0.0000000000
-7.1261024411	12.3424147100	0.0000000000
0.0000000000	0.0000000000	19.9325370789

C N Mn Fe

24 24 1 1

Cartesian

3.579388380	0.834827065	2.989678621
-0.015991449	6.849133968	2.990104675
10.569836617	0.703706264	2.989942074
7.217807293	6.985260963	2.989750385
2.312720776	2.721383095	2.990288496
-1.037451744	8.883243561	2.989692926
9.440211296	2.681103468	2.989850760
6.098399639	8.996889114	2.989389181
4.597486496	2.895572662	2.990183115
1.242656231	8.735015869	2.990371704
11.702226639	2.676676035	2.989689112
8.358453751	8.950698853	2.990350246
-1.249255657	3.413192511	2.989474058
-4.592940331	9.689229012	2.990066051
5.880509377	3.622965574	2.989874840
2.504969597	9.468338013	2.990027189
1.009131432	3.369634390	2.990214825
-2.326297045	9.692598343	2.989750624
8.157902718	3.487015009	2.989968538
4.788492680	9.652285576	2.989392042
-0.115816832	5.380041599	2.990012169
-3.470259190	11.665186882	2.989755392
7.134184837	5.517019272	2.989790201

3.504551411	11.534697533	2.990086317
-1.281187177	4.771800995	2.989288807
-4.659877300	11.033497810	2.989810467
5.860778809	4.996710777	2.989421844
2.387087345	10.799840927	2.990543127
1.088956118	4.743319511	2.990599394
-2.266955376	11.044447899	2.989915133
8.269957542	4.832558155	2.990058661
4.733583927	10.961591721	2.989825726
-0.115099192	2.681944370	2.989664793
-3.459126472	8.965462685	2.989812851
6.976490974	2.853050470	2.990059137
3.700832844	8.761006355	2.989038229
3.404914618	3.608186007	2.990729332
0.142761230	9.506153107	2.989940643
10.573560715	3.409413815	2.989823103
7.219663620	9.684762001	2.990107536
2.357917309	1.409346104	2.989713192
-1.147734404	7.536896229	2.989526272
9.371893883	1.333633661	2.989740372
6.016215324	7.625185013	2.988676310
4.704784393	1.574114919	2.989665031
1.263294220	7.356638432	2.990665913
11.761219025	1.334136248	2.989900589
8.387725830	7.599724293	2.990705729
2.851080656	5.571032047	2.989939451
4.256011963	6.876322746	2.988786697

Fe2_CN

1.0

14.2519006729	0.0000000000	0.0000000000
-7.1261024411	12.3424147100	0.0000000000
0.0000000000	0.0000000000	19.9325370789

C N Fe

24 24 2

Cartesian

3.566383839	0.517319500	2.991408587
0.346191645	6.908316612	3.005449533
10.692778587	0.982768893	2.988856554
6.778076172	6.908256531	3.005790710
2.408879757	2.450097561	3.005819798
-1.033022881	8.763574600	2.989482880
9.549235344	2.944424391	2.988171339
5.900535107	9.026106834	3.000408888
4.715530396	2.455593824	3.005993605
1.222278595	9.033785820	3.000572681
11.831884384	2.944947720	2.988319159
8.159617424	8.762766838	2.989475727
-1.033774257	3.579668045	2.990419149
-4.702409744	9.399881363	2.991039038
5.900317192	3.318446875	2.982472658
2.409921646	9.891215324	2.971088171
1.222382426	3.310647488	2.982504845
-2.420149326	9.399157524	2.990853310
8.159975052	3.580660105	2.990388870
4.714851379	9.885822296	2.970854044
0.345616579	5.435444832	2.984423637
-3.559039593	11.360516548	2.990084171
6.778551102	5.435873508	2.983682156
3.566045761	11.826889038	2.985820532

-0.887507081	4.904110909	3.001626968
-4.750358582	10.744628906	2.990958929
5.601335526	4.696757793	2.948349476
2.360103607	11.212573051	2.989555120
1.521598816	4.692101479	2.951043606
-2.369187117	10.743771553	2.990936041
8.013312340	4.904591560	3.002160072
4.770479202	11.207202911	2.990525007
0.039382577	2.740396738	2.997100592
-3.561349869	8.657687187	2.991552353
7.085065842	2.744248629	2.997978210
3.561050892	9.176758766	2.944925547
3.560779095	3.166997671	3.028207064
0.039993763	9.603268623	2.979824781
10.690551758	3.687275648	2.987467051
7.085297585	9.599662781	2.978860617
2.359067440	1.132862210	2.988759518
-0.886183500	7.440217495	2.982588053
9.500988007	1.601008654	2.988508940
5.601202488	7.648200989	3.043250084
4.771533489	1.138455987	2.987873316
1.522269726	7.652390480	3.040857553
11.883218765	1.601665378	2.988522768
8.012666702	7.439832687	2.981793404
3.540031433	5.103596687	2.856089830
3.538738728	7.241124630	3.132417440

COOH@Fe2_CN

1.0

14.2519006729	0.0000000000	0.0000000000
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-7.1261024411	12.3424147100	0.0000000000
0.0000000000	0.0000000000	19.9325370789

C N Fe O H

25 24 2 2 1

Cartesian

3.562240601	0.505120635	2.987983942
0.346388340	6.917936325	2.949709892
10.687762260	0.989139974	2.995340824
6.777407169	6.918319702	2.955517292
2.406472683	2.444936275	2.976077080
-1.039035797	8.760867119	2.999002695
9.547291756	2.946048021	2.994386673
5.904762268	9.042789459	2.943902016
4.716734409	2.445626736	2.978103399
1.219401836	9.043111801	2.939393759
11.827862740	2.945986748	2.994865179
8.163488388	8.760835648	2.998991489
-1.046087384	3.589407444	2.992271185
-4.705110550	9.398489952	2.999884129
5.912122250	3.308994293	2.960450888
2.406543732	9.904367447	2.921047688
1.210756898	3.307943821	2.955444813
-2.422001839	9.398578644	3.000230074
8.169427872	3.589835644	2.991753340
4.717527866	9.904370308	2.922769547
0.334225893	5.430136681	2.952939749
-3.563469887	11.356069565	2.997427940
6.789183617	5.431038857	2.958814383
3.561906815	11.843109131	2.996847868
3.523962498	6.933411121	4.757790089

-0.902232647	4.915066719	2.989819288
-4.753718853	10.741084099	2.999082804
5.627573013	4.685625076	2.931681395
2.358290195	11.223046303	2.997354031
1.494694948	4.684103489	2.919794321
-2.373268127	10.741228104	2.998960257
8.025630951	4.915436268	2.989798069
4.765811920	11.223131180	2.998345613
0.019126892	2.747567654	2.989693165
-3.563519478	8.659219742	2.996153593
7.103673458	2.748471022	2.988912106
3.562173843	9.185987473	2.834153891
3.561398029	3.157793760	3.001977444
0.024744034	9.599876404	2.994199276
10.687638283	3.684780359	2.999624968
7.099406242	9.599899292	2.993885279
2.355576992	1.121952176	2.973598957
-0.887714863	7.437664032	2.994780540
9.496520042	1.603898168	2.989569902
5.604382515	7.663978100	2.902238369
4.768504143	1.122680187	2.974832535
1.518905640	7.664157867	2.891542435
11.878864288	1.603890777	2.989261150
8.012049675	7.437791824	2.995656252
3.560087919	5.127106190	3.138649225
3.558800697	7.282571793	2.945572376
3.509130001	8.063975334	5.507371426
3.505826235	5.797872543	5.273797989
3.493622303	7.860152721	6.455849648

OCHO@Fe2_CN

1.0

14.2519006729	0.0000000000	0.0000000000
-7.1261024411	12.3424147100	0.0000000000
0.0000000000	0.0000000000	19.9325370789

C N Fe O H

25 24 2 2 1

Cartesian

3.563120842	0.502300024	3.014544487
0.332961082	6.917881012	2.950873375
10.688745499	0.996927857	2.988150597
6.791357040	6.917808533	2.953464985
2.407551765	2.434471369	2.929730654
-1.044400215	8.755586624	3.001693726
9.546521187	2.951617002	2.991347551
5.911397457	9.036649704	2.949687719
4.716392517	2.435699224	2.930105209
1.212870121	9.037806511	2.947296858
11.829946518	2.951833725	2.991695404
8.169077873	8.755760193	3.000683308
-1.037751079	3.590335131	3.005626202
-4.704331398	9.397104263	2.991296530
5.909123421	3.311615229	2.930411100
2.407447815	9.906491280	2.930552483
1.213977695	3.309405327	2.928345203
-2.422417879	9.396872520	2.991797686
8.161811829	3.590386391	3.005027294
4.717007637	9.906274796	2.931600332
0.330714941	5.430923462	2.935055733
-3.562910795	11.354057312	2.998514891

6.792954445	5.431532860	2.937824011
3.562875748	11.843418121	2.999080420
3.556593895	6.152673721	5.526119232
-0.900887609	4.910748005	3.012498856
-4.753555298	10.739617348	2.989168644
5.639871120	4.681935787	2.826464653
2.358005524	11.228178024	3.008885384
1.482717514	4.680075169	2.819139242
-2.372304916	10.739523888	2.988721609
8.025386810	4.910695553	3.011707067
4.767094135	11.227442741	3.009397745
0.025189281	2.743469000	3.018701553
-3.563344002	8.659281731	2.993900776
7.098490715	2.744570017	3.017864227
3.562072277	9.205281258	2.828900814
3.561526299	3.132212639	2.808066607
0.021241665	9.600478172	3.004315853
10.688238144	3.690009356	2.991465092
7.103518486	9.600270271	3.003586531
2.353752851	1.113971233	3.024008036
-0.903908491	7.431657791	3.002857924
9.497207642	1.609385967	2.983993769
5.631275654	7.663863182	2.885109901
4.771765709	1.115350962	3.023392916
1.492918015	7.664508343	2.878977060
11.879973412	1.609515786	2.983598232
8.029376030	7.432035446	3.001822233
3.556298256	5.116792679	2.888009548
3.558990002	7.278561115	2.996573925
3.550810814	7.307273388	4.984267235

3.547408104	5.057657719	4.892616272
3.572438478	6.046111584	6.632143497

HCOOH@Fe2_CN

1.0

14.2519006729	0.0000000000	0.0000000000
-7.1261024411	12.3424147100	0.0000000000
0.0000000000	0.0000000000	19.9325370789

C N Fe O H

25 24 2 2 2

Cartesian

3.561954498	0.509467363	3.004513264
0.320993423	6.921607971	2.879200697
10.686538696	0.989369273	2.985274792
6.799570560	6.916018486	2.940120697
2.408171654	2.448650599	2.971258879
-1.053742886	8.764516830	3.002773523
9.549433708	2.943929911	2.987740993
5.916096210	9.041454315	2.941812754
4.718185425	2.446701050	2.969673634
1.197654247	9.038639069	2.875773430
11.828392982	2.943453074	2.990348101
8.173281670	8.763516426	2.997810841
-1.051366329	3.586185217	3.009806633
-4.706408978	9.400509834	2.986572504
5.922542572	3.309691429	2.943816423
2.399390697	9.903213501	2.932207108
1.200793862	3.315099239	2.945268393
-2.427751780	9.401012421	2.992991686
8.175689697	3.585195780	3.004195452

4.717798233	9.904770851	2.958460569
0.313827991	5.430664539	2.919289112
-3.565372944	11.358188629	2.990309954
6.806718826	5.430236816	2.940937996
3.560608387	11.841428757	2.997935295
3.495765924	6.763912201	4.787672043
-0.923591852	4.911065578	3.015516043
-4.757654190	10.744986534	2.989103079
5.656263351	4.677576542	2.835120678
2.357089520	11.224113464	3.001258612
1.461442471	4.678633213	2.830019951
-2.376665354	10.744037628	2.984039307
8.044546127	4.910616875	3.018708467
4.764237404	11.223167419	3.002593756
0.016790628	2.743335724	3.020346165
-3.566914558	8.662849426	2.984779119
7.108683109	2.743867397	3.020902395
3.560762405	9.187879562	2.882276535
3.562166214	3.153395891	2.939415455
0.015348434	9.598127365	3.015441179
10.688276291	3.682477951	2.984199047
7.108387470	9.600954056	3.012095451
2.355021000	1.128203392	3.007253170
-0.907840967	7.433522701	3.016726971
9.497010231	1.603679061	2.984595537
5.628145218	7.668889999	2.832184553
4.767772675	1.122941375	3.004960060
1.488450527	7.673061371	2.705927849
11.879049301	1.602220774	2.984467506
8.032314301	7.434974194	3.018517733

3.574201822	5.115621090	3.077099085
3.555751324	7.287408829	2.766062498
2.418598652	7.316278458	5.465787411
3.528460979	5.444703579	4.884084225
4.447038174	7.279153824	5.007869244
2.523203373	8.283248901	5.447740078

CHO@Fe2_CN

1.0

14.2519006729	0.0000000000	0.0000000000
-7.1261024411	12.3424147100	0.0000000000
0.0000000000	0.0000000000	19.9325370789

C N Fe O H

25 24 2 1 1

Cartesian

3.562127590	0.503678441	2.983850241
0.344557524	6.917130947	2.948560238
10.687709808	0.990936041	2.996681690
6.779087543	6.917444229	2.954571009
2.407901049	2.446144104	2.974593163
-1.038070679	8.760141373	2.995371103
9.547196388	2.946686506	2.995357513
5.906574249	9.040015221	2.940030336
4.715212822	2.446774721	2.976694584
1.217433929	9.040539742	2.935306549
11.827944756	2.946648359	2.995757580
8.162338257	8.760158539	2.995788097
-1.046555161	3.589049578	2.988660812
-4.704861641	9.398758888	3.001101732
5.909831047	3.312158108	2.963343382

2.405110359	9.901966095	2.918874025
1.213062167	3.311052084	2.958403349
-2.422411203	9.398829460	3.001347303
8.169807434	3.589463711	2.988555670
4.718790054	9.901838303	2.920644522
0.333185911	5.429838657	2.955290794
-3.563594341	11.354632378	2.997568130
6.790011406	5.430706501	2.961221457
3.561790943	11.844695091	2.991879225
3.523978233	6.925551891	4.766069412
-0.903628230	4.914513111	2.984781265
-4.754665852	10.740760803	3.000340462
5.624898434	4.686820507	2.947457552
2.360721588	11.222680092	2.994118929
1.497403383	4.685481071	2.936222315
-2.372612476	10.740926743	3.000335217
8.026874542	4.914852142	2.985259056
4.763207436	11.222620964	2.995305777
0.022111535	2.750261307	2.984916210
-3.563679695	8.661059380	2.998164415
7.100543499	2.751000166	2.984583139
3.561992168	9.186722755	2.846379519
3.561370611	3.158185959	3.006690502
0.026385784	9.598953247	2.991203547
10.687585831	3.685616970	3.000250816
7.097347260	9.598901749	2.991212130
2.359051466	1.124060035	2.969860554
-0.888006449	7.437775135	2.993423462
9.495990753	1.605670691	2.991987467
5.612875462	7.667584419	2.896560431

4.764984131	1.124720812	2.971375227
1.510036945	7.667881012	2.885997057
11.879205704	1.605660081	2.991807222
8.012094498	7.437799931	2.994717598
3.559148312	5.110247612	3.178352833
3.558683872	7.297415257	2.979813337
3.509833813	5.750077724	5.207785130
3.504281044	7.800575733	5.487717152

CH2O@Fe2_CN

1.0

14.2519006729	0.0000000000	0.0000000000
-7.1261024411	12.3424147100	0.0000000000
0.0000000000	0.0000000000	19.9325370789

C N Fe O H

25 24 2 1 2

Cartesian

3.562085152	0.509541392	2.977320671
0.343795776	6.915621281	2.937409163
10.687663078	0.991636217	2.997466326
6.780704021	6.917047501	2.941666842
2.411275148	2.457416534	2.974415064
-1.042499065	8.758950233	2.990614891
9.548913002	2.947255135	2.994630814
5.905238152	9.039531708	2.924481392
4.711597443	2.458206892	2.976845741
1.218708515	9.040480614	2.921139717
11.825916290	2.947349787	2.994717360
8.167231560	8.759328842	2.991792917
-1.045703769	3.589860201	2.985873222

-4.705268860	9.399157524	3.001378298
5.912765503	3.318602085	2.964412212
2.404079914	9.902103424	2.920400858
1.209516168	3.317019463	2.958986759
-2.422033072	9.398735046	3.001319408
8.168592453	3.589865446	2.986532688
4.719821930	9.900940895	2.922216415
0.326684237	5.431746483	2.956103802
-3.563825607	11.356406212	2.997433662
6.796535015	5.432695866	2.961928129
3.561759949	11.844253540	2.989265442
3.540243626	7.010674477	4.825334072
-0.917065144	4.912728310	2.982710600
-4.754191875	10.743335724	3.000849009
5.647052765	4.686525822	2.944969177
2.360827923	11.216808319	2.988195658
1.474569082	4.684482574	2.932818890
-2.373135805	10.743065834	3.001117706
8.039748192	4.912915707	2.983583212
4.762408257	11.216249466	2.989631414
0.018105984	2.746454239	2.983786821
-3.563707113	8.661502838	2.999325752
7.104027748	2.747578859	2.983948708
3.561652660	9.176290512	2.839310408
3.561151505	3.171574593	3.022739172
0.024127007	9.596563339	2.988718271
10.687471390	3.685983181	2.998119354
7.100723743	9.597065926	2.990005016
2.359040737	1.132414818	2.959037066
-0.890293837	7.437764645	2.997235060

9.496848106	1.605660915	2.994433641
5.608785629	7.662233829	2.846272707
4.764692783	1.133172274	2.961028576
1.516359329	7.662220478	2.840402603
11.878288269	1.605839491	2.994439125
8.016195297	7.438068390	2.999742746
3.554696798	5.145129681	3.348099709
3.548056126	7.291095257	2.859052181
3.513093948	5.667790413	5.096004009
2.635205746	7.540981770	5.138241291
4.477102280	7.495253563	5.080982685

CH3O@Fe2_CN

1.0

14.2519006729	0.0000000000	0.0000000000
-7.1261024411	12.3424147100	0.0000000000
0.0000000000	0.0000000000	19.9325370789

C N Fe O H

25 24 2 1 3

Cartesian

3.563714504	0.497841448	2.997375011
0.356179953	6.913892269	3.000162601
10.689557076	0.981306434	2.984759092
6.769827843	6.913489342	3.001900911
2.401752949	2.435604572	2.992145538
-1.040961266	8.756430626	2.992785931
9.552192688	2.939471006	2.984947920
5.911242962	9.044687271	2.990491152
4.722402096	2.436705112	2.992838383
1.211833954	9.049208641	2.987302303

11.823780060	2.939565659	2.984443665
8.166069031	8.756176949	2.992207766
-1.056391954	3.583923578	2.996204376
-4.705792427	9.398554802	2.990355968
5.929938316	3.293465614	2.949417114
2.394593239	9.909126282	2.950339317
1.191763639	3.290768623	2.944550514
-2.420491934	9.397901535	2.990335941
8.180090904	3.584766865	2.995709181
4.729151726	9.905855179	2.950772285
0.325507879	5.418546200	2.956548691
-3.562185287	11.351799965	2.993360758
6.798942566	5.421243191	2.959778786
3.563502789	11.838928223	2.980670691
3.521059513	5.994779587	5.868782520
-0.916768789	4.912868023	3.031531572
-4.754767895	10.742726326	2.991270781
5.658251762	4.659165382	2.828248978
2.358171940	11.221304893	2.996480465
1.461686373	4.654494286	2.813542604
-2.370600700	10.742559433	2.990893602
8.040452957	4.913281441	3.028122425
4.768391609	11.218461990	2.996777058
0.000462770	2.730374098	3.029596090
-3.563494682	8.663824081	2.989838123
7.121732235	2.733210325	3.026374340
3.561339855	9.175957680	2.873225927
3.562046528	3.152399063	3.003577948
0.013914585	9.601140976	2.987025976
10.688112259	3.678909302	2.983203650

7.108749866	9.598649979	2.985085249
2.356525421	1.112476468	2.991530657
-0.878313065	7.429409027	2.993552446
9.499665260	1.596445322	2.984910965
5.595566273	7.670808792	3.022387743
4.770455837	1.113524675	2.991378546
1.528487682	7.674688816	3.012758255
11.878405571	1.596593022	2.984517336
8.005106926	7.429593086	2.991211414
3.566920757	5.096762657	2.854881287
3.553763390	7.375614166	3.198137283
3.506018162	6.031586170	4.478322506
2.618258953	5.467381954	6.221762657
3.521582603	7.028859138	6.241466045
4.427791595	5.467329979	6.208575249

O@Fe2_CN

1.0

14.2519006729	0.0000000000	0.0000000000
-7.1261024411	12.3424147100	0.0000000000
0.0000000000	0.0000000000	19.9325370789

C N Fe O

24 24 2 1

Cartesian

3.564907312	0.504861295	2.996617556
0.356909752	6.916965485	3.006858826
10.690851212	0.984516621	2.987552881
6.769838333	6.917132378	3.007268429
2.397018909	2.440948963	2.985018253
-1.041146278	8.755774498	2.989778519

9.548721313	2.942340374	2.987596989
5.910861492	9.043317795	2.990014076
4.727075100	2.445032835	2.984165192
1.213561058	9.048377991	2.988493204
11.829963684	2.943190813	2.987449646
8.166740417	8.756088257	2.989496946
-1.041426897	3.587442160	2.990961313
-4.703340530	9.400770187	2.989881516
5.910999775	3.299919844	2.967061996
2.400527477	9.905205727	2.966024876
1.212752461	3.293861389	2.966184616
-2.421358824	9.399929047	2.989888191
8.166412354	3.587604761	2.991330147
4.723642826	9.901355743	2.966265917
0.356734753	5.425758362	2.979136944
-3.560956717	11.361042976	2.991091728
6.769396782	5.426115513	2.979673624
3.564795971	11.842516899	2.983454466
-0.883904696	4.910471439	3.009493113
-4.753477097	10.743838310	2.989610672
5.613877296	4.664809704	2.906522989
2.359881878	11.218851089	2.987130404
1.509658337	4.659705639	2.901555777
-2.369826078	10.743342400	2.989361286
8.010212898	4.911320686	3.008441925
4.767663956	11.215357780	2.987654924
0.012365103	2.739092588	3.009113789
-3.562872410	8.662966728	2.991052389
7.110110283	2.742414951	3.008674383
3.560902596	9.176793098	2.932632923

3.560863018	3.157886505	2.949263573
0.016643524	9.603492737	2.985035658
10.688800812	3.680597544	2.986464024
7.106377125	9.600706100	2.984064579
2.361701488	1.123782158	3.003517389
-0.882308245	7.431346893	2.990785599
9.497761726	1.600315094	2.987224102
5.607404709	7.672734261	3.018122911
4.766171932	1.127364993	3.003377199
1.517506123	7.676784515	3.013550520
11.882439613	1.600826383	2.987232208
8.009056091	7.430723667	2.989465714
3.547250271	4.996462345	2.968537569
3.548590183	7.346193790	3.163718939
3.527638674	6.063023090	4.332498074

OH@Fe2_CN

1.0

14.2519006729	0.0000000000	0.0000000000
-7.1261024411	12.3424147100	0.0000000000
0.0000000000	0.0000000000	19.9325370789

C N Fe O H

24 24 2 1 1

Cartesian

3.563464165	0.491104513	2.999895573
0.359691143	6.909780979	2.992696762
10.689310074	0.990244806	2.983733654
6.767106056	6.909414291	2.993577957
2.401844978	2.433515310	2.987006187
-1.034450054	8.756625175	2.995243549

9.552925110	2.941614628	2.985302448
5.909023762	9.047485352	2.982146025
4.722743988	2.434460640	2.986965179
1.214493752	9.050059319	2.980627775
11.823358536	2.941939831	2.985024929
8.159727097	8.757230759	2.994693041
-1.052117944	3.586416245	3.000920296
-4.704064846	9.397799492	2.990139484
5.925779819	3.290309191	2.938291550
2.402525425	9.909764290	2.935124636
1.198040605	3.289174795	2.936028242
-2.422818661	9.397332191	2.990218878
8.177142143	3.586176157	3.000497103
4.721207142	9.907251358	2.935284376
0.335129738	5.420142651	2.947332859
-3.562481403	11.347205162	2.994156837
6.791113853	5.421815395	2.949138165
3.563160896	11.850963593	2.984944820
-0.905258060	4.909303188	3.035207033
-4.755510330	10.737422943	2.991065741
5.646047592	4.662459373	2.812246084
2.359390259	11.223611832	3.003757715
1.477134943	4.660263538	2.805818081
-2.370678186	10.736878395	2.990764856
8.030635834	4.909563065	3.033177853
4.766124725	11.222215652	3.003741026
0.006279349	2.738589764	3.030999660
-3.563650131	8.658391953	2.989064693
7.117136002	2.739324808	3.029378414
3.561402798	9.174280167	2.847053289

3.562128305	3.149268866	2.993952274
0.018473625	9.599986076	2.989296198
10.688020706	3.681491852	2.981709242
7.104549408	9.598631859	2.988064766
2.355386019	1.108979464	2.993073702
-0.879850626	7.433174133	2.998345613
9.498466492	1.600294590	2.982508183
5.598082066	7.667247295	3.001375675
4.770855427	1.109476805	2.992855310
1.526336670	7.669373512	2.995735168
11.879114151	1.600741029	2.982243538
8.005294800	7.432887077	2.996758461
3.567363501	5.104773998	2.863856554
3.557081699	7.343873978	3.167150974
3.522663832	6.086540699	4.581335068
3.569927216	6.572904110	5.411076546

2CO@Fe2_CN

1.0

14.2519006729	0.0000000000	0.0000000000
-7.1261024411	12.3424147100	0.0000000000
0.0000000000	0.0000000000	19.9325370789

C N Fe O

26 24 2 2

Cartesian

3.563721180	0.490701646	3.022016525
0.348198652	6.913446426	2.944736004
10.689347267	0.987409711	2.984021664
6.777901649	6.911704540	2.956541300
2.400905609	2.430341482	2.922385216

-1.037392616	8.756287575	3.009043932
9.551371574	2.943154335	2.989312172
5.909680367	9.034511566	2.947162390
4.726767063	2.429649830	2.922643900
1.215679169	9.034739494	2.936441898
11.826935768	2.943516731	2.989393950
8.162947655	8.756396294	3.006879807
-1.041788697	3.584284306	3.013866425
-4.703524590	9.396618843	2.987430096
5.912692547	3.291566372	2.921341896
2.396943092	9.901214600	2.936646461
1.214024901	3.290843964	2.916669607
-2.423480034	9.396579742	2.987936735
8.168300629	3.584780455	3.012656212
4.729164124	9.901126862	2.938784599
0.350711823	5.418768406	2.925386906
-3.562938213	11.349904060	2.992480755
6.775089264	5.419138908	2.933356047
3.563974380	11.842678070	2.987398863
3.435316086	7.482484341	4.849790573
3.488443851	5.092345715	4.579699039
-0.884614706	4.906388283	3.026191235
-4.752401352	10.736693382	2.983413696
5.628109932	4.658255577	2.810348749
2.359615803	11.227888107	2.988819361
1.495764732	4.656754017	2.793527842
-2.373793125	10.736596107	2.981995106
8.011170387	4.906106472	3.024119139
4.766829491	11.227878571	2.988182545
0.015199304	2.742314816	3.027181864

-3.563526154	8.658591270	2.986249924
7.110706329	2.742696047	3.025529385
3.563427925	9.192171097	2.894911528
3.564503670	3.135175705	2.798627615
0.018766880	9.594181061	3.007440329
10.688891411	3.682733297	2.980788469
7.105828285	9.593725204	3.003790617
2.362148523	1.107064605	3.031768560
-0.888261557	7.430092335	3.021522045
9.500975609	1.601532936	2.984194756
5.620101452	7.663697720	2.897326708
4.765330315	1.106399894	3.031106234
1.501587391	7.665921211	2.867264271
11.877035141	1.601956487	2.983761311
8.014236450	7.429826736	3.017644167
3.561797380	5.021033764	2.866458178
3.564710617	7.314841747	3.135063410
3.279500961	7.616089344	6.005236626
3.409483910	4.781479359	5.699966431

COCHO_decoupled/Fe2_CN

1.0

14.2519006729	0.0000000000	0.0000000000
-7.1261024411	12.3424147100	0.0000000000
0.0000000000	0.0000000000	19.9325370789

C N Fe O H

26 24 2 2 1

Cartesian

3.563917160	0.496731669	3.004255056
0.352827549	6.909700394	2.984521866

10.689639091	0.988435626	2.985770226
6.772114754	6.913708687	2.973239660
2.401749611	2.426703215	2.943008900
-1.040446758	8.752169609	2.993265867
9.548713684	2.943374395	2.987128258
5.909779549	9.032832146	2.963295460
4.722177505	2.429654360	2.943975687
1.214443684	9.039109230	2.973079205
11.827404976	2.943512917	2.986681700
8.164201736	8.752497673	2.994270802
-1.044291019	3.586710453	3.000459194
-4.703492165	9.398925781	2.988490105
5.912924290	3.296835661	2.947577000
2.405014515	9.901561737	2.963362694
1.207336783	3.291757822	2.941720009
-2.421668768	9.397502899	2.988600254
8.166854858	3.588561058	3.001454592
4.718935013	9.895632744	2.964594603
0.348041058	5.422796726	2.955853462
-3.561928034	11.350731850	2.991586208
6.772428036	5.426246166	2.960325241
3.564163208	11.839555740	2.981842518
3.515106916	5.037274837	4.713401794
3.640733242	7.431807995	5.006961823
-0.886901617	4.910544395	3.025792837
-4.753575802	10.740278244	2.985799551
5.612240791	4.670088768	2.850917339
2.361054897	11.223731041	2.983157158
1.508373976	4.665270805	2.834060907
-2.370867491	10.739578247	2.987357855

8.008359909	4.913177967	3.023710251
4.766973972	11.219022751	2.984743834
0.019056082	2.744103193	3.022313833
-3.563426495	8.662653923	2.989187717
7.103808880	2.747952223	3.020085573
3.561498165	9.180673599	2.941501141
3.560818195	3.143875837	2.837244987
0.026021004	9.592797279	2.991025925
10.688028336	3.680547714	2.982195616
7.098737240	9.591642380	2.998211384
2.358553648	1.113956571	3.022254705
-0.884733438	7.428106785	3.005777121
9.498892784	1.601607084	2.986047029
5.607048035	7.661206722	2.918840408
4.768181801	1.116243482	3.021683931
1.524155140	7.658902168	2.958064079
11.879679680	1.601932406	2.985403538
8.010269165	7.429212570	3.009044647
3.558066130	5.033829212	2.999612093
3.543443680	7.284199715	3.146754980
3.467836380	4.740658760	5.839356899
4.642148495	7.424169064	5.672341824
2.600282669	7.414471626	5.456350803

COCHO/Fe2_CN

1.0

14.2519006729	0.0000000000	0.0000000000
-7.1261024411	12.3424147100	0.0000000000
0.0000000000	0.0000000000	19.9325370789

C N Fe O H

26 24 2 2 1

Cartesian

3.563959599	0.504237831	3.007678270
0.328301430	6.916003704	2.971852064
10.689500809	0.991967738	2.983605623
6.796865940	6.916099548	2.973522425
2.411231041	2.438162565	2.879264355
-1.047908306	8.756358147	2.998242140
9.547026634	2.943920612	2.989974737
5.915406704	9.036363602	2.969610929
4.714070797	2.439551592	2.879737139
1.209565163	9.037412643	2.968067646
11.830470085	2.944231987	2.990036726
8.173309326	8.756575584	2.997372866
-1.039991856	3.587409735	3.005184889
-4.701387882	9.400395393	2.987342119
5.900861740	3.310478926	2.933301449
2.406427860	9.909148216	2.953505993
1.223365784	3.308171988	2.930729866
-2.424751043	9.400105476	2.987623453
8.164990425	3.587695360	3.004920244
4.718508244	9.908049583	2.954212427
0.341811895	5.429947853	2.948928833
-3.562141895	11.356404305	2.993669987
6.782364845	5.430368423	2.952204466
3.563435078	11.846992493	2.986772776
3.530556917	4.848836422	4.785912991
3.521330595	6.099474907	5.566164017
-0.891827464	4.908863544	3.012995720
-4.752040386	10.741297722	2.984798908

5.615877151	4.682529926	2.863391399
2.355429649	11.230611801	2.999894142
1.506497145	4.680490971	2.855401754
-2.373073578	10.740841866	2.984501362
8.016760826	4.909551620	3.011911869
4.770965576	11.229359627	2.999933004
0.029654264	2.751245975	3.017495394
-3.563256264	8.661166191	2.989594936
7.094119549	2.752497911	3.016804457
3.562051773	9.203345299	2.885622025
3.562168598	3.122741222	2.684005260
0.017437458	9.598075867	3.002576113
10.688571930	3.681016207	2.985077620
7.106901169	9.597333908	3.001604795
2.367620945	1.125616193	3.033058167
-0.909569025	7.434853554	3.005606890
9.498164177	1.602216959	2.984701395
5.644288063	7.665771484	2.929282665
4.759601593	1.127420187	3.034676552
1.480123043	7.666418552	2.925951958
11.880214691	1.602434754	2.984412670
8.034748077	7.434742451	3.004966259
3.554463387	5.059213638	2.924949884
3.561753273	7.230955124	3.078993559
3.508373022	3.759473801	5.373276711
3.552639484	7.231721878	5.007865906
3.483778000	5.992941856	6.656377792

COHCHO@Fe2_CN

1.0

14.2519006729	0.0000000000	0.0000000000
-7.1261024411	12.3424147100	0.0000000000
0.0000000000	0.0000000000	19.9325370789

C N Fe O H

26 24 2 2 2

Cartesian

3.563043118	0.497171491	3.001611471
0.328551054	6.916513443	2.971999884
10.688983917	0.993770659	2.983111858
6.796393394	6.916199207	2.974605560
2.399087429	2.435256720	2.897261858
-1.048994541	8.755029678	3.001068354
9.547204971	2.947061300	2.990374327
5.916884899	9.039638519	2.966775179
4.725705147	2.436250925	2.897748470
1.207333565	9.040466309	2.963661194
11.830161095	2.947464466	2.990122795
8.173595428	8.755396843	3.000108004
-1.040510774	3.585722923	3.006489992
-4.701361656	9.399292946	2.988072157
5.906167984	3.305274487	2.938761711
2.406151295	9.909478188	2.942523956
1.218476892	3.303205729	2.936936855
-2.425633669	9.398941040	2.988276720
8.165723801	3.585896254	3.006572485
4.718471050	9.908815384	2.943482399
0.343165874	5.430418968	2.961787462
-3.562895298	11.355079651	2.994418859
6.781692505	5.430324554	2.963178396
3.563006401	11.847924232	2.990523100

3.537883997	6.241561413	5.663054466
3.543141127	5.080805302	4.883465290
-0.889531851	4.909958839	3.004544735
-4.752903461	10.739896774	2.986261129
5.609416962	4.683563232	2.897290707
2.356461525	11.230243683	3.004718542
1.514816046	4.682535172	2.892917395
-2.373272896	10.739618301	2.985669851
8.014966965	4.909896374	3.003736019
4.769017696	11.229716301	3.004887104
0.023329973	2.748613119	3.012190580
-3.563567638	8.659377098	2.987654924
7.100946426	2.749575615	3.011906147
3.562122822	9.204606056	2.861160517
3.562428474	3.158690929	2.803833961
0.014955997	9.600260735	3.002864599
10.688537598	3.685112476	2.986256123
7.109113216	9.599803925	3.001316547
2.358698368	1.119667768	3.007355928
-0.911173344	7.432739258	3.008321047
9.498220444	1.605391383	2.983615398
5.644818306	7.667575359	2.938016415
4.767680645	1.121078491	3.007162571
1.479062080	7.668644428	2.930335522
11.879360199	1.605735779	2.983671904
8.035858154	7.432810307	3.006706476
3.556908369	5.059469223	3.042376757
3.561073303	7.248604774	3.115903854
3.545573711	7.383983135	5.060317516
3.530371666	3.934774399	5.602211952

3.534054518	6.205656528	6.752769947
3.517588377	3.200448751	4.952230930

OCH2COH@Fe2_CN

1.0

14.2519006729	0.0000000000	0.0000000000
-7.1261024411	12.3424147100	0.0000000000
0.0000000000	0.0000000000	19.9325370789

C N Fe O H

26 24 2 2 3

Cartesian

3.562942743	0.502654135	3.008829355
0.312469006	6.918825626	2.961844444
10.688348770	0.989060760	2.984987259
6.810624123	6.918133736	2.969789743
2.404850245	2.438972950	2.906857729
-1.055257320	8.758956909	3.001451969
9.544901848	2.945590734	2.990754843
5.922547340	9.036270142	2.963148117
4.718500137	2.440569401	2.908291578
1.200714588	9.035533905	2.955785036
11.830890656	2.945706606	2.991057158
8.179180145	8.758857727	2.999395370
-1.041625857	3.583743334	3.003810644
-4.701387882	9.403783798	2.987882614
5.900567055	3.307690382	2.957502365
2.406822205	9.897327423	2.942890167
1.221605420	3.305125952	2.952572346
-2.426763535	9.403955460	2.988415003
8.164579391	3.584226847	3.002931356

4.717814922	9.897534370	2.945117950
0.338033676	5.432167053	2.965193033
-3.563370466	11.360002518	2.994586229
6.783981323	5.432175159	2.971360683
3.562630653	11.839791298	2.989926338
3.466255426	6.073004723	5.760799885
3.510740995	4.873614788	4.849720955
-0.892099261	4.909054279	3.002236843
-4.753507137	10.744922638	2.985980272
5.607584953	4.687425137	2.924494028
2.356118202	11.219875336	2.998578072
1.512737989	4.686001301	2.911421061
-2.373248577	10.744808197	2.984868765
8.015038490	4.909316540	3.000823021
4.768668652	11.220411301	2.998502254
0.026423693	2.748876095	3.003849030
-3.563804626	8.663559914	2.989111423
7.096302986	2.750049829	3.002986193
3.562245369	9.190399170	2.878665924
3.561410427	3.150415897	2.762669086
0.009507656	9.602694511	3.008421421
10.687771797	3.683263063	2.989073277
7.114379883	9.602444649	3.004764318
2.359681845	1.124095798	3.023841619
-0.928400517	7.432604313	3.008223295
9.496597290	1.602227211	2.985296249
5.663236141	7.668149471	2.921514988
4.765589237	1.125386357	3.024295807
1.457579613	7.669067383	2.900944948
11.879794121	1.602354169	2.984935999

8.051174164	7.432077885	3.005140066
3.552799702	5.033318996	3.068948746
3.566461563	7.238111973	3.260197401
3.500729561	7.283803463	5.099264622
3.513347387	3.671831131	5.445586681
4.345247269	6.006681442	6.437562466
2.537268162	6.009190083	6.369901180
3.496856213	3.746867895	6.443455696

HOCH2COH@Fe2_CN

1.0

14.2519006729	0.0000000000	0.0000000000
-7.1261024411	12.3424147100	0.0000000000
0.0000000000	0.0000000000	19.9325370789

C N Fe O H

26 24 2 2 4

Cartesian

3.568186283	0.524523139	2.992611170
0.307187319	6.917797089	2.949372292
10.690190315	0.981365860	2.996079206
6.822655678	6.916431904	2.935134649
2.406508446	2.455833197	2.874410391
-1.050445557	8.765766144	2.993142843
9.547437668	2.936266422	3.009461641
5.919823170	9.019442558	2.938798428
4.716246605	2.465814829	2.844485998
1.201484680	9.026765823	2.926803827
11.830882072	2.938651562	3.004990816
8.175659180	8.765501976	2.999864101
-1.045184255	3.582071543	2.990861177

-4.700513363	9.419877052	3.007122278
5.911912918	3.324434519	2.849629879
2.410984993	9.883019447	2.912439823
1.218162656	3.311964512	2.937108517
-2.426661491	9.416813850	3.003015518
8.169287682	3.579740047	2.995638132
4.710820675	9.876106262	2.919069290
0.329743385	5.436673164	2.967575550
-3.560124874	11.374260902	3.010442019
6.805637836	5.431525230	2.892020464
3.563959122	11.822797775	2.978067636
3.449133635	6.042477608	5.894914150
3.818258047	4.811758518	5.051357746
-0.897683024	4.908627987	2.975808382
-4.751574516	10.758462906	3.006722450
5.631638527	4.699813366	2.767302275
2.358878136	11.205186844	2.967300892
1.516296387	4.698069572	2.970919371
-2.370366096	10.755982399	3.003986597
8.033997536	4.909269810	2.994390011
4.766089916	11.199556351	2.973303556
0.028559923	2.754083395	2.958937883
-3.564067841	8.677069664	3.004661798
7.092231274	2.754092216	2.966821671
3.558540821	9.168873787	2.864310026
3.557615280	3.174649715	2.741763115
0.017314911	9.603398323	2.981846094
10.689077377	3.673315763	3.009915352
7.103598118	9.599514961	2.978543758
2.364355564	1.139884472	2.982538462

-0.930587292	7.439063072	2.994995117
9.501097679	1.591766119	2.992390871
5.668708801	7.654467583	2.905474424
4.766819954	1.150730014	2.976345062
1.454501152	7.659860134	2.886105061
11.882637978	1.592036247	3.004390001
8.058566093	7.439804077	2.990761280
3.490565300	5.058180809	3.004631281
3.542551041	7.200301647	3.307391644
3.483148098	7.222729206	5.120388508
3.327186108	3.593864918	5.527204514
4.178238869	6.154844284	6.737078667
2.444901228	5.930980206	6.362248421
2.378606081	3.679437399	5.695640564
4.898015976	4.698605061	4.981440544

OCH₂CH@Fe₂_CN

1.0

14.2519006729	0.0000000000	0.0000000000
-7.1261024411	12.3424147100	0.0000000000
0.0000000000	0.0000000000	19.9325370789

C N Fe O H

26 24 2 1 3

Cartesian

3.562261105	0.505186737	3.004286051
0.333725214	6.915488720	2.969115973
10.687902451	0.983931839	2.991429329
6.788550377	6.914518356	2.977730036
2.407824039	2.446072817	2.903743744
-1.047209740	8.757639885	2.998635769

9.547696114	2.943558455	2.992631912
5.906133175	9.031019211	2.968201637
4.715363979	2.446770430	2.905587196
1.217052937	9.029788017	2.960632086
11.827685356	2.943612337	2.993342161
8.171244621	8.757459641	2.997135162
-1.042363763	3.581876516	2.999773264
-4.705408573	9.402053833	2.992781878
5.904706955	3.309463739	2.946324587
2.408070564	9.888293266	2.948852777
1.217384696	3.306856871	2.940684795
-2.422986031	9.402482033	2.993629456
8.164596558	3.582275867	2.999168396
4.715598106	9.888875961	2.951218128
0.330526829	5.433228016	2.961409807
-3.563662767	11.358855247	2.998679876
6.790987015	5.433633804	2.968467236
3.561659336	11.833837509	2.987409830
3.471923351	6.064510345	5.738267422
3.515651464	4.889522552	4.898333549
-0.903573990	4.908360958	3.005815029
-4.753987312	10.744936943	2.990923166
5.629716396	4.686045647	2.903925419
2.361760139	11.207039833	2.979131222
1.490625858	4.684854031	2.890614271
-2.373398781	10.745028496	2.989892483
8.026002884	4.908349514	3.005802393
4.761825085	11.207431793	2.979823589
0.023474216	2.744017363	2.997859716
-3.563794136	8.665316582	2.993999481

7.098578453	2.744888783	2.997756004
3.561844349	9.166071892	2.929272890
3.562108994	3.155618429	2.787597179
0.023306847	9.591032982	2.991994858
10.687467575	3.683342457	2.994580030
7.099589825	9.590438843	2.989335299
2.360873699	1.126330018	3.013481617
-0.901952744	7.433741570	2.997686386
9.497756004	1.602477312	2.988533735
5.614037037	7.654207230	2.960685492
4.763909340	1.127032161	3.014393330
1.504334450	7.655279636	2.939016581
11.877631187	1.602282643	2.988329172
8.023273468	7.433423519	2.995670557
3.550809622	5.081440449	3.122976780
3.572035313	7.253921986	3.201567411
3.502618313	7.282726765	5.063234806
4.326165199	5.986280441	6.455503941
2.559364557	5.988537788	6.382583618
3.514829874	3.892659664	5.370876789

OCH2CH2@Fe2_CN

1.0

14.2519006729	0.0000000000	0.0000000000
-7.1261024411	12.3424147100	0.0000000000
0.0000000000	0.0000000000	19.9325370789

C N Fe O H

26 24 2 1 4

Cartesian

3.562704086	0.504038513	3.007117033
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0.315079212	6.920172215	2.962791443
10.688407898	0.991498709	2.985963345
6.808442116	6.919509411	2.970782995
2.403686285	2.447831392	2.909892559
-1.052581787	8.758400917	3.001658678
9.544837952	2.945643902	2.992398500
5.920200348	9.034132957	2.961677551
4.719291687	2.448889732	2.911075592
1.204308510	9.033265114	2.954474688
11.831068993	2.945651293	2.992927313
8.176725388	8.758691788	2.999546766
-1.039996743	3.585047483	3.002217293
-4.700701714	9.404681206	2.988592148
5.898805618	3.310544729	2.958972454
2.408329010	9.896183968	2.940696478
1.224419475	3.308634520	2.954100609
-2.426908493	9.404809952	2.989349604
8.163163185	3.585287333	3.001514912
4.716433048	9.896644592	2.943084240
0.340873480	5.430735588	2.965314627
-3.563181400	11.360917091	2.996190786
6.781903267	5.430965424	2.972194672
3.562547684	11.837232590	2.990906000
3.470330715	6.055180073	5.792503357
3.506734610	4.797487736	4.960438251
-0.894274235	4.907072544	2.999525785
-4.754333496	10.743905067	2.987057447
5.600035667	4.692836761	2.928011894
2.356406689	11.217653275	2.997333050
1.520580530	4.692369938	2.911283970

-2.372994184	10.743981361	2.985925913
8.016827583	4.907560825	2.998245239
4.767935753	11.218387604	2.997421980
0.025172114	2.748965025	2.998993874
-3.564024925	8.663819313	2.990280867
7.096394539	2.750077724	2.998461723
3.561956406	9.190496445	2.872435570
3.561326027	3.157088041	2.771371603
0.008737087	9.603832245	3.006850719
10.687574387	3.682929277	2.991106272
7.113968849	9.603326797	3.003574133
2.360955238	1.122411013	3.020189285
-0.928336620	7.434198856	3.006392717
9.497457504	1.601163149	2.985839367
5.664052010	7.666075706	2.919319630
4.764005661	1.123481989	3.020781279
1.456693172	7.666824341	2.899046898
11.878378868	1.601054907	2.985455990
8.050783157	7.433301449	3.003720760
3.554937840	5.047935486	2.971885204
3.565608025	7.222245216	3.282850504
3.502174854	7.290352345	5.077779770
4.343495369	6.031000614	6.452601433
2.542120457	6.032451153	6.378365517
4.375577927	4.180016518	5.223184586
2.603960037	4.207042217	5.148400307

OCH2CH3@Fe2_CN

1.0

14.2519006729	0.0000000000	0.0000000000
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-7.1261024411	12.3424147100	0.0000000000
0.0000000000	0.0000000000	19.9325370789

C N Fe O H

26 24 2 1 5

Cartesian

3.559994221	0.519053876	3.006164074
0.310343742	6.917593002	2.931012392
10.685804367	0.985048592	2.989643574
6.810108185	6.917165279	2.943997145
2.404520988	2.453997135	2.843081713
-1.049676418	8.759670258	3.000009537
9.542737007	2.938727856	3.003071785
5.915573597	9.028697968	2.942258358
4.716385841	2.454408884	2.851956844
1.206961632	9.026905060	2.935950756
11.828950882	2.939162493	3.004573345
8.172672272	8.759695053	2.999535561
-1.044326782	3.584890604	3.000438690
-4.703110218	9.408110619	2.999618769
5.908603668	3.316703081	2.879245043
2.407721996	9.885856628	2.921874285
1.210373402	3.315959215	2.860890150
-2.425828934	9.408889771	3.000576496
8.165166855	3.585092068	3.001184225
4.715753078	9.887455940	2.924865007
0.326964617	5.436467648	2.897917032
-3.565275431	11.365429878	3.007277250
6.792834282	5.437361240	2.915556192
3.560694218	11.830203056	2.980389118
3.468092680	6.021694660	5.977313519

3.481343031	4.640505791	5.362817764
-0.904212236	4.906886578	3.005120039
-4.755482674	10.752437592	2.998478651
5.622677326	4.694436550	2.785058975
2.357255459	11.209551811	2.977717876
1.493863583	4.693409920	2.750699759
-2.374110222	10.753107071	2.998797417
8.024274826	4.906800270	3.008024693
4.764708042	11.211285591	2.979865551
0.026070237	2.750027418	2.979588509
-3.564002752	8.672069550	3.002030611
7.094343185	2.750414133	2.984468699
3.561796665	9.180794716	2.865139008
3.561114311	3.151995182	2.673181772
0.016220570	9.603577614	2.987637997
10.685931206	3.673838377	3.002482891
7.107011795	9.604309082	2.987779617
2.359592676	1.140358806	3.006428480
-0.928029537	7.437814236	2.993893147
9.493350029	1.593677282	2.994134665
5.660845757	7.663156986	2.898804903
4.760914803	1.140190601	3.010437965
1.459729671	7.662256718	2.882848740
11.878578186	1.594264269	2.993798018
8.049337387	7.437866211	2.996535778
3.563868284	5.071237564	2.747354746
3.564760685	7.220070362	3.241846561
3.528990746	7.023814678	5.003001690
4.342400074	6.140824318	6.658028126
2.544096708	6.153306961	6.581442356

4.423250198	4.465214729	4.797483444
2.601489067	4.517609119	4.698006630
3.413784504	3.856296539	6.131909370

OHCH2CH2@Fe2_CN

1.0

14.2519006729	0.0000000000	0.0000000000
-7.1261024411	12.3424147100	0.0000000000
0.0000000000	0.0000000000	19.9325370789

C N Fe O H

26 24 2 1 5

Cartesian

3.562223911	0.508710444	3.000146866
0.321453333	6.913433552	2.965843678
10.687594414	0.986824572	2.991273403
6.802480698	6.912625790	2.974241495
2.403274536	2.441410303	2.906984568
-1.047861576	8.759381294	2.996849298
9.544480324	2.944162607	2.994073391
5.914109707	9.035290718	2.958848000
4.718632698	2.443891048	2.909237862
1.208993912	9.035619736	2.950399637
11.830899239	2.944531202	2.994685650
8.171775818	8.758973122	2.995385647
-1.040989280	3.583055735	2.995789766
-4.704165459	9.402920723	2.993607283
5.898404598	3.316659212	2.951813698
2.404520035	9.896470070	2.941694021
1.222406745	3.311995029	2.944038630
-2.424334288	9.403067589	2.994733095

8.162917137	3.583541393	2.995568514
4.717882633	9.896548271	2.945107937
0.339513540	5.432541847	2.961800098
-3.563963890	11.360956192	2.999053240
6.782314301	5.431285858	2.970093012
3.561279297	11.838945389	2.986942053
3.476561785	6.018538475	5.911140919
3.488498211	4.801217556	5.003090858
-0.891147614	4.907480717	3.000153303
-4.753987312	10.746467590	2.992317677
5.599443436	4.695879459	2.909370184
2.355427265	11.223713875	2.982815504
1.522419453	4.694590092	2.888040543
-2.373574018	10.746366501	2.991488695
8.015586853	4.907342911	2.998879433
4.768047810	11.222752571	2.983445168
0.029412031	2.751227140	2.996979475
-3.563697338	8.664260864	2.996119022
7.092976570	2.751729250	2.996473551
3.560977936	9.189079285	2.903822660
3.560801983	3.154425859	2.771297693
0.017717361	9.600002289	2.992786884
10.687463760	3.682796240	2.997588873
7.105302334	9.599724770	2.990957260
2.359074354	1.134230137	3.012918234
-0.914970398	7.433788300	2.995739460
9.496330261	1.601548910	2.990046501
5.641973495	7.659212589	2.940985918
4.764584541	1.136050940	3.013164997
1.481418610	7.660030365	2.923587084

11.878849983	1.601512671	2.989699602
8.038585663	7.433848858	2.994593382
3.527456045	5.038786888	3.008142948
3.568774700	7.213594437	3.048051596
3.513201714	7.289412022	5.171800137
4.374625683	6.022017956	6.554990292
2.524886847	6.032102585	6.466617107
4.386759281	4.185222149	5.193305969
2.590518951	4.187724590	5.204235077
3.362435341	8.031232834	5.780136585

Fe2_CN@Fe_4

1.0

14.2519006729	0.0000000000	0.0000000000
-7.1261024411	12.3424147100	0.0000000000
0.0000000000	0.0000000000	22.9325370789

C N Fe

24 24 6

Cartesian

3.563361168	0.491359651	5.996420383
0.298616409	6.903033257	6.024798393
10.689237595	0.986875534	5.987977982
6.828226089	6.903295994	6.024757385
2.393685818	2.421455145	6.008666992
-1.056937695	8.759256363	5.987243176
9.549764633	2.937554359	5.989353657
5.917384624	9.057224274	5.994972229
4.732103825	2.421065807	6.007392883
1.207893848	9.056122780	5.993286133
11.827315331	2.937647104	5.988916397

8.182248116	8.760143280	5.986828327
-1.056980729	3.583415508	5.988951206
-4.702403069	9.406869888	5.990589142
5.917487621	3.283671618	5.977500439
2.395696640	9.916937828	5.998907566
1.207786560	3.284714937	5.978946686
-2.423911095	9.406811714	5.990716457
8.182464600	3.583398581	5.989188194
4.729778290	9.917161942	5.999450684
0.302737474	5.435513973	6.009625912
-3.562606812	11.357747078	5.992558956
6.824954987	5.436570644	6.008930683
3.563469887	11.849495888	5.979834557
-0.929181814	4.901648521	5.997901440
-4.755031109	10.745455742	5.991054535
5.625308037	4.679935455	5.978234768
2.353013992	11.242281914	5.964249134
1.501745224	4.679574966	5.977680206
-2.370288134	10.745497704	5.990807056
8.055906296	4.902220249	5.995477200
4.773757458	11.242351532	5.964684010
0.012362480	2.741999388	5.989556789
-3.563356161	8.668203354	5.992203712
7.113206863	2.742777824	5.989981651
3.562889576	9.212934494	6.056586742
3.563052654	3.126892090	6.043388844
0.013341904	9.600057602	5.974730015
10.688524246	3.675674915	5.987200260
7.112038136	9.599776268	5.973714828
2.349319220	1.095961809	5.988510132

-0.932363749	7.440104008	5.980539322
9.496722221	1.598162532	5.989211559
5.628751278	7.662251472	6.050879955
4.777105331	1.095649123	5.988222599
1.499021053	7.661443710	6.044693470
11.881528854	1.598381042	5.989244938
8.058265686	7.440590382	5.978818417
3.570203543	5.004282951	5.911150455
3.576103687	7.334832668	5.964603901
3.589156151	7.397555351	3.098693609
5.017358303	6.236322403	4.455069065
3.575491905	5.103655815	3.096055031
2.115411520	6.254848957	4.428236961

COOH@Fe2_CN@Fe_4

1.0

14.2519006729	0.0000000000	0.0000000000
-7.1261024411	12.3424147100	0.0000000000
0.0000000000	0.0000000000	22.9325370789

C N Fe O H

25 24 6 2 1

Cartesian

3.563056707	0.499208838	5.994349003
0.289586782	6.905702114	6.007438183
10.688864708	0.989159107	5.983803272
6.836120605	6.905940056	6.010143280
2.392975569	2.429769039	6.007244587
-1.056609154	8.761807442	5.983901978
9.549542427	2.941119432	5.987186432
5.928936958	9.063324928	5.993378162

4.733894348	2.429040670	6.006556034
1.197896004	9.063116074	5.988766670
11.828553200	2.941337585	5.987189293
8.182822227	8.762138367	5.983284473
-1.050988913	3.579361200	5.987521172
-4.699724674	9.403209686	5.987539768
5.919867516	3.275560141	5.976094723
2.394805431	9.917516708	6.006707668
1.207405210	3.277123928	5.976938725
-2.425845861	9.402740479	5.987550735
8.177990913	3.579347372	5.986801147
4.732131481	9.918676376	6.007689476
0.312663555	5.432482719	6.007859230
-3.562917948	11.357599258	5.993570328
6.814806938	5.433127880	6.007939339
3.562651157	11.846199036	5.972214222
3.545124292	5.637182713	7.669279575
-0.918164611	4.898316383	6.010545254
-4.752731800	10.742953300	5.990844727
5.621894836	4.661081791	5.930720329
2.353966713	11.238548279	5.967452526
1.504423857	4.661538601	5.930100441
-2.373238564	10.742654800	5.990421772
8.045793533	4.897774696	6.008495331
4.772364616	11.239576340	5.967766285
0.007755637	2.730643749	5.996092319
-3.563042879	8.662398338	5.989457607
7.118909359	2.729909897	5.996611595
3.563737392	9.222610474	6.038929939
3.563635349	3.138042927	6.019831181

0.003469467	9.616650581	5.988727093
10.689049721	3.678932905	5.984974861
7.122907162	9.617486954	5.986208916
2.358838081	1.112704158	5.990286350
-0.946175098	7.442364693	5.993627071
9.498579025	1.599442959	5.988372326
5.664341450	7.682155132	5.985378742
4.767511845	1.112134695	5.989385128
1.461077690	7.681090355	5.967906475
11.879217148	1.599612355	5.988221645
8.072583199	7.443279266	5.990629673
3.564162254	4.962108135	5.937228203
3.564624786	7.357280254	5.930505753
3.585991859	7.402728558	3.103930235
5.034130096	6.223112106	4.464018345
3.573143005	5.113627911	3.095842123
2.114155054	6.241129398	4.451727867
3.502455473	6.855920315	7.992655754
3.572282553	4.677103996	8.647129059
3.520134926	5.130142212	9.534896851

CO@Fe2_CN@Fe_4

1.0

14.2519006729	0.0000000000	0.0000000000
-7.1261024411	12.3424147100	0.0000000000
0.0000000000	0.0000000000	22.9325370789

C N Fe O

25 24 6 1

Cartesian

3.563089609	0.491605639	5.996273994
-------------	-------------	-------------

0.305165529	6.908115387	6.023298740
10.689083099	0.986612618	5.986464024
6.821656227	6.908225060	6.024188519
2.391277790	2.425880909	6.007246017
-1.055229187	8.762698174	5.985448360
9.550703049	2.937872648	5.988910198
5.918498993	9.059157372	5.994830608
4.734807014	2.425348997	6.006113052
1.208099365	9.058279037	5.992906570
11.826755524	2.938130379	5.988621712
8.181162834	8.763138771	5.984902382
-1.053508282	3.578709364	5.988291740
-4.701414108	9.405425072	5.989527225
5.917425156	3.283224821	5.978561878
2.392021656	9.914958954	6.001112938
1.208919406	3.283985853	5.979754448
-2.424702644	9.405090332	5.989674091
8.179815292	3.579085112	5.988154888
4.734199047	9.915922165	6.001627445
0.307984114	5.430636883	6.011147022
-3.562739611	11.355882645	5.993351936
6.819437504	5.431800842	6.010928631
3.563022137	11.849376678	5.976968765
3.546159029	6.126842499	7.364546776
-0.925291657	4.902123451	6.001551628
-4.754728317	10.744008064	5.991061687
5.625954628	4.666905880	5.967096806
2.355979919	11.234016418	5.965939045
1.500409842	4.666928291	5.965784550
-2.370962381	10.743793488	5.990785599

8.052806854	4.901925087	5.999091148
4.770725250	11.234511375	5.966263294
0.009996891	2.739207745	5.989639282
-3.563179970	8.666094780	5.991516590
7.115755558	2.739135265	5.990014553
3.563674450	9.209647179	6.049298286
3.563333988	3.136646271	6.036122799
0.011477947	9.602468491	5.976900101
10.688743591	3.677785158	5.986621857
7.114551544	9.603432655	5.975913048
2.355733395	1.106433511	5.988566399
-0.927426100	7.439435482	5.986670971
9.497613907	1.599231958	5.989194393
5.626219273	7.674129009	6.030800343
4.770756721	1.106173635	5.988009453
1.500959396	7.672558784	6.023269653
11.880323410	1.599471211	5.989113808
8.054412842	7.440464020	5.984736443
3.564571857	4.950158596	5.919770718
3.570237637	7.395172596	5.983385563
3.587588310	7.397843838	3.100128174
5.021057606	6.231608391	4.452230930
3.574250221	5.103384495	3.094086885
2.118985653	6.250148773	4.430505276
3.514937878	6.128014088	8.545319557

CHO/Fe2_CN@Fe_4

1.0

14.2519006729	0.0000000000	0.0000000000
-7.1261024411	12.3424147100	0.0000000000

0.0000000000	0.0000000000	22.9325370789
C N Fe O H		
25 24 6 1 1		
Cartesian		
3.563267946	0.497761905	5.993878841
0.312855721	6.908858776	6.008714199
10.688922882	0.982043326	5.981884956
6.814297676	6.909971237	6.011281967
2.398945808	2.428403139	6.002879620
-1.054942131	8.763496399	5.983308315
9.554265022	2.937853336	5.987191200
5.923205853	9.076216698	5.978618622
4.727508545	2.429051638	6.002113342
1.204817772	9.075323105	5.975963593
11.824438095	2.937990189	5.987572670
8.181648254	8.764149666	5.982329369
-1.057276368	3.577366829	5.989830494
-4.701488495	9.399150848	5.985505104
5.929358482	3.281438828	5.975656509
2.388417244	9.922262192	6.007780552
1.197861791	3.281574011	5.977978230
-2.423338413	9.398594856	5.986021042
8.184357643	3.577651262	5.988751411
4.738608360	9.922825813	6.008698463
0.293243647	5.432919025	5.998585701
-3.562762976	11.350546837	5.993290424
6.834646702	5.433373451	5.998269558
3.562968254	11.846096039	5.971751690
3.582088947	6.631783009	7.704958439
-0.946958065	4.896867752	6.005433559

-4.752799511	10.742329597	5.989978790
5.670978546	4.660808563	5.924950123
2.354300499	11.239050865	5.965144634
1.457094669	4.661062717	5.931204319
-2.372999430	10.741921425	5.989615440
8.075659752	4.896563530	6.003602505
4.771950245	11.239684105	5.965593815
0.002620459	2.721560478	5.998802662
-3.562817574	8.661700249	5.987084389
7.124563217	2.720847607	6.001106739
3.563683987	9.207577705	6.065169811
3.563077927	3.127997875	6.001388550
0.004432678	9.616601944	5.990753174
10.689234734	3.681667566	5.983477116
7.123911858	9.618676186	5.990521431
2.355412483	1.104062080	5.992702961
-0.914829016	7.443978310	6.007213116
9.500172615	1.599373221	5.987886429
5.619845390	7.685056210	5.947947025
4.770814896	1.104501009	5.991493225
1.509034157	7.682708740	5.941802979
11.877590179	1.599412560	5.987735748
8.042839050	7.445050240	6.005709171
3.554966688	4.999298096	5.890770912
3.560853004	7.375706196	6.034395218
3.584862709	7.372063160	3.120528698
5.035283089	6.210427284	4.478413105
3.572686434	5.093352318	3.088788509
2.114630461	6.228164673	4.464236736
3.595503092	5.395629406	7.969323635

3.574447632 7.376763344 8.527669907

CHOH@Fe2_CN@Fe_4

1.0

14.2519006729	0.0000000000	0.0000000000
-7.1261024411	12.3424147100	0.0000000000
0.0000000000	0.0000000000	22.9325370789

C N Fe O H

25 24 6 1 2

Cartesian

3.560074568	0.483566165	6.002748966
0.302358866	6.909434319	5.957581043
10.686525345	1.002860308	5.977516174
6.800515175	6.917884350	5.997648716
2.396760464	2.419769287	5.988719463
-1.056509495	8.766279221	5.987779617
9.548372269	2.950029135	5.985645771
5.926307678	9.100802422	5.968319416
4.739493847	2.403548479	5.985428333
1.205878735	9.073348045	5.945013046
11.829071999	2.945860386	5.986762524
8.177673340	8.769075394	5.993643761
-1.049444556	3.572792768	5.996520996
-4.703929901	9.393905640	5.985511303
5.923542976	3.251975060	5.947587013
2.397757053	9.928603172	5.983604908
1.209304810	3.275391102	5.958939075
-2.426357508	9.398723602	5.987355709
8.176368713	3.571786165	5.997783661
4.742428303	9.949254990	5.992202282

0.308721781	5.430541992	5.973060131
-3.567173481	11.345624924	5.990320683
6.798482895	5.422841072	5.988709927
3.561407566	11.867918015	5.985713005
3.753172159	6.117973328	7.335640907
-0.920705795	4.893898964	6.019133091
-4.755728245	10.736254692	5.986484528
5.617698193	4.641409874	5.874517918
2.361804485	11.242809296	5.992112160
1.502076626	4.658500671	5.899295807
-2.374336720	10.739602089	5.987607956
8.026481628	4.895214081	6.029429436
4.766921997	11.262892723	5.991989613
0.010839343	2.723214388	5.996968269
-3.564609766	8.657963753	5.982355118
7.122668743	2.716773510	6.003310680
3.575687885	9.233967781	5.980700016
3.572457314	3.124140501	5.967532158
0.010227203	9.615932465	5.997594357
10.689561844	3.685355186	5.981379986
7.127723694	9.627566338	5.997131348
2.360123634	1.109045863	6.009823322
-0.927980423	7.446251392	5.994192123
9.495943069	1.609829664	5.978941441
5.622519016	7.708773613	5.919170380
4.765541077	1.093901277	6.006844997
1.497209072	7.687099934	5.878032207
11.880269051	1.607314587	5.981901169
8.028516769	7.444749355	6.015964031
3.612576485	4.944295883	5.877011776

3.654672623	7.408767223	5.887190342
3.574668407	7.397192001	3.110986233
5.077937126	6.205461502	4.346191406
3.563042641	5.103950024	3.062417984
2.115690231	6.229549885	4.429709435
2.731727123	6.286313057	8.256998062
4.699473381	6.078638077	7.892681599
1.917756081	6.384350300	7.691942215

CH@Fe2_CN@Fe_4

1.0

14.2519006729	0.0000000000	0.0000000000
-7.1261024411	12.3424147100	0.0000000000
0.0000000000	0.0000000000	22.9325370789

C N Fe H

25 24 6 1

Cartesian

3.563059807	0.493926167	5.995655537
0.308407784	6.907101631	6.023348808
10.688976288	0.986421466	5.985369205
6.818405628	6.907713413	6.024865150
2.389780998	2.425732613	6.006410122
-1.053900719	8.763304710	5.983641148
9.550601959	2.939362764	5.988440037
5.919831276	9.065413475	5.992951393
4.736394405	2.425196648	6.005313873
1.207371712	9.063715935	5.990995884
11.827176094	2.939648867	5.988306522
8.179944992	8.763982773	5.982931137
-1.052241683	3.577793837	5.987150669

-4.701608181	9.403356552	5.988581181
5.918787956	3.278076887	5.977197647
2.389810562	9.916520119	6.002383232
1.208039522	3.279495001	5.978482246
-2.424254894	9.402867317	5.988831520
8.178756714	3.578013420	5.986727715
4.736907005	9.917701721	6.002947807
0.310305119	5.431536198	6.013193607
-3.562839270	11.355127335	5.993645668
6.816997051	5.432410240	6.013116837
3.562927723	11.847090721	5.974947929
3.575768232	6.134004593	7.280381203
-0.921799779	4.899882317	6.003409386
-4.753645420	10.744729042	5.991153717
5.626338959	4.658200741	5.952506542
2.357083797	11.228024483	5.966990471
1.500632048	4.659530640	5.953944206
-2.372108936	10.744403839	5.990870953
8.049201965	4.899700642	6.001126766
4.769495487	11.228688240	5.967275620
0.007381439	2.735026121	5.991412640
-3.563148022	8.665129662	5.991068363
7.119011879	2.734437227	5.992191792
3.563799381	9.210711479	6.047337055
3.563240051	3.136530161	6.032454967
0.008264542	9.606165886	5.980133057
10.688853264	3.678659439	5.986330509
7.118933678	9.607905388	5.979488850
2.357659340	1.113758326	5.988716602
-0.922893286	7.441036224	5.990112305

9.498709679	1.598289728	5.989156723
5.624062061	7.683273315	6.011029720
4.768724918	1.113561988	5.987997055
1.504516602	7.680076122	6.005163193
11.879137993	1.598535895	5.989037037
8.050113678	7.442052841	5.988473415
3.565724134	4.949692249	5.973097801
3.570598125	7.393694878	6.043813229
3.586735249	7.406890392	3.104393244
5.026396751	6.228527546	4.454228878
3.573634148	5.093418598	3.095406294
2.117546797	6.246926308	4.437696457
3.570002556	6.122517586	8.367436409

CH2@Fe2_CN@Fe_4

1.0

14.2519006729	0.0000000000	0.0000000000
-7.1261024411	12.3424147100	0.0000000000
0.0000000000	0.0000000000	22.9325370789

C N Fe H

25 24 6 2

Cartesian

3.562808275	0.495111912	5.995361805
0.308886051	6.910648823	6.025303841
10.688885689	0.987053633	5.984303474
6.817762852	6.911055088	6.026817322
2.389083862	2.421628714	6.007944107
-1.054496288	8.765556335	5.984129906
9.550963402	2.939702988	5.988473415
5.921078205	9.065361023	5.995164394

4.736593246	2.421217918	6.006868839
1.206312180	9.064334869	5.993941307
11.827260971	2.940057755	5.988421917
8.180505753	8.765910149	5.983237267
-1.053017735	3.575920105	5.987728119
-4.701186180	9.402978897	5.988421917
5.918723106	3.279064655	5.979716301
2.387563705	9.922781944	6.005063057
1.208384633	3.279338121	5.981822014
-2.424394131	9.402435303	5.988778591
8.179429054	3.576466799	5.987091541
4.738941193	9.924023628	6.005567551
0.311818838	5.428303242	6.014752865
-3.562944174	11.354687691	5.992949009
6.815287590	5.429211140	6.014691353
3.562664509	11.846069336	5.974616528
3.604060411	6.154478550	7.359198093
-0.919216871	4.900232315	6.003403187
-4.753248215	10.745474815	5.991174221
5.622850418	4.660409927	5.953783035
2.355294228	11.231520653	5.969429970
1.505270243	4.663426399	5.959401608
-2.372681856	10.745393753	5.990908623
8.047403336	4.899914742	6.001316071
4.771568298	11.231938362	5.969672680
0.007331014	2.736673832	5.989613056
-3.563071728	8.664581299	5.991033554
7.118934155	2.735508442	5.990897655
3.563632488	9.225096703	6.032327175
3.562714815	3.127691031	6.016297817

0.007497787	9.605049133	5.978922844
10.688913345	3.678939819	5.986349106
7.119898319	9.607489586	5.979003429
2.356220961	1.111929655	5.991229534
-0.920446157	7.440350533	5.990192890
9.498986244	1.597446561	5.989121914
5.623188496	7.683705807	6.006194115
4.770450115	1.112082005	5.990545273
1.506118774	7.678627968	6.005536079
11.878611565	1.597404599	5.988987923
8.048510551	7.441679955	5.988800049
3.556252718	4.944006443	5.906589508
3.564473629	7.409779549	5.948516369
3.586839199	7.403957367	3.101188660
5.016140938	6.226893425	4.454597950
3.573520184	5.095634460	3.092266321
2.127292871	6.245116711	4.436838150
2.724506855	6.219217777	8.036451340
4.583616257	6.171833515	7.880813599

CH3@Fe2_CN@Fe_4

1.0

14.2519006729	0.0000000000	0.0000000000
-7.1261024411	12.3424147100	0.0000000000
0.0000000000	0.0000000000	22.9325370789

C N Fe H

25 24 6 3

Cartesian

3.563287497	0.488281995	6.009225845
0.310240984	6.913682938	5.979576111

10.689175606	1.002723098	5.977016926
6.819231987	6.914551735	5.976948261
2.392688274	2.413735867	5.954708576
-1.056183815	8.767623901	5.997928143
9.549048424	2.947629452	5.985357285
5.929070950	9.087858200	5.937933922
4.730713844	2.417008638	5.953271389
1.199722290	9.088661194	5.939376831
11.829851151	2.947118998	5.985805988
8.184830666	8.768126488	5.997816086
-1.048672199	3.575013876	6.003642559
-4.698808670	9.397470474	5.983067989
5.919672489	3.271900892	5.949672699
2.389903545	9.940917015	5.970601082
1.205346107	3.268005610	5.952388287
-2.423631430	9.397173882	5.983505249
8.174892426	3.576435089	6.002753735
4.736876488	9.940324783	5.970335960
0.318503141	5.433482170	5.994674206
-3.561600208	11.347030640	5.990849495
6.809810162	5.436320305	5.991912365
3.562925816	11.865566254	5.989416599
3.573438168	6.190811634	7.555062294
-0.912292838	4.897526264	6.027522564
-4.752122879	10.736097336	5.983438969
5.626519203	4.655635357	5.903599739
2.359174252	11.257952690	5.994698048
1.500463724	4.653294563	5.908224106
-2.371520996	10.736376762	5.983685017
8.041529655	4.898155689	6.025385857

4.767272949	11.256971359	5.995364666
0.008247375	2.721036434	6.001689911
-3.561486244	8.657147408	5.978754044
7.116489410	2.722742558	6.002955914
3.563536644	9.230417252	5.951633453
3.560923576	3.127846003	5.885122299
0.001668453	9.623970985	6.012870312
10.689598083	3.684889555	5.980928898
7.126916885	9.625022888	6.014748096
2.361037493	1.098825336	6.019498348
-0.920074940	7.446034908	6.021704197
9.496473312	1.610538840	5.978713036
5.643957615	7.702700138	5.849394798
4.764585495	1.102322817	6.018393040
1.486636639	7.700478077	5.852027893
11.881652832	1.609657049	5.978585720
8.050964355	7.447303295	6.020720005
3.552376270	4.960476398	5.905175209
3.559285641	7.393817425	5.870549202
3.584588051	7.374083996	3.131732702
5.066380978	6.204273224	4.435513020
3.575218678	5.097533703	3.101550579
2.078720093	6.216988564	4.415876865
3.588245392	5.141807079	7.929882526
4.491281509	6.647418022	7.956644535
2.667335510	6.638863087	7.980742931

COCO/Fe2_CN@Fe_4

1.0

14.2519006729	0.0000000000	0.0000000000
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-7.1261024411	12.3424147100	0.0000000000
0.0000000000	0.0000000000	22.9325370789
C N Fe O		
26 24 6 2		
Cartesian		
3.563712120	0.481101036	6.022435665
0.308000565	6.898276329	5.965960503
10.689328194	0.992898345	5.988257885
6.820838928	6.899151802	5.967149734
2.388550997	2.408947945	5.920845032
-1.050192833	8.757635117	5.999170780
9.552688599	2.944995880	5.988674164
5.917700291	9.057957649	5.912011623
4.737983704	2.409612656	5.920510292
1.211316109	9.057698250	5.910742760
11.826022148	2.945093155	5.988871574
8.179036140	8.757845879	5.998798847
-1.047724366	3.573436975	6.004717827
-4.698749542	9.394085884	5.988858700
5.920402050	3.264970779	5.926785946
2.400962830	9.903774261	5.928731441
1.206471562	3.264117956	5.926620960
-2.423641920	9.394012451	5.988955975
8.175105095	3.574111462	6.004081249
4.727546215	9.904288292	5.928678036
0.316692114	5.422584534	5.972861290
-3.561466217	11.345273972	5.997728348
6.811575890	5.423962116	5.974044323
3.563481331	11.844554901	5.982569218
3.570505619	7.696745396	8.025030136

3.549271345	5.637329102	7.391065598
-0.913474679	4.894165516	6.024046421
-4.751480579	10.733276367	5.984101772
5.633236885	4.644690037	5.845537186
2.360224247	11.230607986	5.964058876
1.493362427	4.643145084	5.843156815
-2.371364117	10.733578682	5.984255791
8.041972160	4.894460678	6.022212029
4.767562389	11.231016159	5.963961601
0.006055355	2.722684860	6.007871628
-3.561347246	8.652676582	5.987871170
7.120203495	2.723562717	6.008286476
3.564306259	9.193378448	5.912209988
3.563176632	3.112314224	5.789613247
0.021062374	9.603493690	5.997864723
10.689411163	3.686070204	5.986303329
7.108279705	9.604301453	5.998005390
2.358300209	1.097415328	6.031270981
-0.920496225	7.439346313	6.006900787
9.501259804	1.603928328	5.983014584
5.630081177	7.658329010	5.860265732
4.768961906	1.098291159	6.030533791
1.499536991	7.657068729	5.855406761
11.877344131	1.603890538	5.982922554
8.050462723	7.439956188	6.004604816
3.561837196	4.928758144	5.720853329
3.561418056	7.352889538	6.325250626
3.581539631	7.384101868	3.139550209
5.067651749	6.258827209	4.430210590
3.572642803	5.109770298	3.079819679

2.080677986	6.271182060	4.421494007
3.584600449	7.989144325	9.151323318
3.535319567	5.073470592	8.462165833

COCOH/Fe2_CN@Fe_4

1.0

14.2519006729	0.0000000000	0.0000000000
-7.1261024411	12.3424147100	0.0000000000
0.0000000000	0.0000000000	22.9325370789

C N Fe O H

26 24 6 2 1

Cartesian

3.561892271	0.522558987	5.968115807
0.303295135	6.928946495	5.954589367
10.687868118	0.997342467	5.993314743
6.823050022	6.930029392	5.960260868
2.399537563	2.453245640	5.828078747
-1.053797245	8.777451515	6.010123253
9.549025536	2.955252409	6.000173092
5.922843456	9.076853752	5.901857376
4.725713253	2.452771187	5.832272530
1.205273151	9.073827744	5.897054672
11.827561378	2.956214190	6.000531197
8.181186676	8.778616905	6.011752129
-1.049074769	3.598402500	5.998098373
-4.698785305	9.415251732	5.996794224
5.910746574	3.313998699	5.867105484
2.390255928	9.919320107	5.950571060
1.213461280	3.313368559	5.859500885
-2.425523043	9.415002823	5.996737957

8.173883438	3.597643614	5.998535633
4.738420963	9.922489166	5.953934193
0.299420595	5.461681843	5.959759235
-3.562323093	11.370620728	6.002313137
6.825293541	5.462162495	5.965034008
3.561635494	11.854994774	6.008854866
3.519361496	4.398186207	8.096254349
3.554419279	6.578868389	7.369692326
-0.929773569	4.918378353	6.007846355
-4.749923706	10.757184982	5.998786449
5.621842384	4.713340759	5.879521370
2.356207371	11.239392281	5.980405331
1.500604391	4.712605953	5.860248566
-2.374185562	10.757082939	5.999768734
8.054433823	4.917342186	6.004701614
4.768580914	11.242835999	5.982695580
0.027973056	2.761421204	5.948317528
-3.562266350	8.673628807	5.983204842
7.096404552	2.761977434	5.950730324
3.565114021	9.202268600	5.959289074
3.563342571	3.155881166	5.758097172
0.008709431	9.615691185	6.010148525
10.688034058	3.696890831	6.009589672
7.119809628	9.617823601	6.012513638
2.354448557	1.132085562	5.938651085
-0.924606562	7.456321239	6.030898571
9.498680115	1.613685727	5.984004498
5.641610146	7.693894863	5.795135975
4.769234180	1.131540298	5.941878319
1.484944344	7.691940784	5.786749840

11.876938820	1.614637136	5.984168530
8.050905228	7.457500458	6.033474445
3.562160730	4.937896252	6.442881584
3.567683220	7.405182838	5.828682899
3.579101563	7.276043415	3.125165462
5.007050514	6.074486732	4.449493408
3.574795723	5.005225658	3.022656918
2.134299278	6.080029011	4.439776897
3.482355595	4.250839233	9.268486023
3.551513672	7.021846294	8.608341217
3.532341242	6.311209679	9.294980049

COCOH/Fe2_CN@Fe_4

1.0

14.2519006729	0.0000000000	0.0000000000
-7.1261024411	12.3424147100	0.0000000000
0.0000000000	0.0000000000	22.9325370789

C N Fe O H

26 24 6 2 1

Cartesian

3.562885284	0.494376749	5.995639324
0.311987400	6.915087700	6.000436306
10.689468384	0.986195147	5.980507851
6.807197571	6.911113739	5.998301029
2.390146255	2.421502829	5.997785091
-1.055924892	8.767532349	5.984972477
9.553941727	2.939639330	5.985795021
5.924151421	9.084416389	5.970474720
4.733514786	2.422811031	5.996013641
1.201832294	9.082817078	5.965777397

11.827205658	2.938926697	5.986940384
8.181917191	8.765091896	5.983257771
-1.053770900	3.573310852	5.990514278
-4.697719097	9.401622772	5.984508038
5.923600197	3.261916161	5.961111069
2.387365341	9.928545952	6.000896454
1.203912020	3.266409159	5.963424206
-2.424795151	9.402232170	5.985507965
8.180012703	3.574788809	5.989090919
4.735563755	9.925977707	6.002904892
0.313169718	5.425460815	5.997744083
-3.562335253	11.356060982	5.993186951
6.807467461	5.429048538	5.994640827
3.562645912	11.851223946	5.973012924
2.576166391	6.191691875	7.911450386
3.862036705	6.157970428	7.516588211
-0.910431623	4.898353577	6.016678333
-4.751568317	10.741494179	5.989022732
5.627972603	4.646921635	5.887851238
2.351468086	11.249273300	5.973864079
1.497719526	4.659973621	5.885884285
-2.373812914	10.742713928	5.988868237
8.041587830	4.894921780	6.021853924
4.770736694	11.247306824	5.974739075
0.004821539	2.724444151	6.003277302
-3.561870575	8.660609245	5.984997272
7.125302315	2.716622114	6.001768112
3.558623314	9.211947441	6.027170658
3.560085058	3.141971588	5.998549461
0.002905846	9.619200706	6.001480103

10.689916611	3.680753708	5.982007980
7.125970364	9.625818253	5.995985508
2.353704214	1.100140452	5.995135307
-0.910300732	7.443256378	6.010313511
9.500344276	1.600395799	5.985817432
5.622569084	7.697172165	5.909190655
4.769192696	1.101044774	5.994132996
1.498825073	7.686299801	5.889590740
11.878141403	1.598981261	5.986104965
8.041467667	7.446259499	6.014331818
3.556076765	4.968853951	5.986489773
3.540314198	7.387980938	6.036466122
3.588591576	7.407270908	3.114003181
5.013327599	6.221492290	4.466612339
3.578697443	5.084255695	3.092183828
2.161905527	6.234096527	4.423115253
1.488035917	6.186018467	8.407002449
4.885412216	6.185770035	8.450326920
5.744888306	6.223458767	7.989302158

Fe2_CN@Fe13

1.0

14.2519006729	0.0000000000	0.0000000000
-7.1261024411	12.3424147100	0.0000000000
0.0000000000	0.0000000000	26.9325370789

C N Fe

24 24 15

Cartesian

3.563266993	0.489414632	9.997093201
0.306614399	6.905079365	10.032297134

10.688513756	0.989673078	9.990447044
6.818266869	6.905574322	10.031072617
2.390141726	2.423211813	9.981232643
-1.057488441	8.755398750	9.984816551
9.549995422	2.940082550	9.990708351
5.916165352	9.055667877	10.004325867
4.733186245	2.425379038	9.980820656
1.205805302	9.058131218	10.007615089
11.824913025	2.940852165	9.990915298
8.180756569	8.756620407	9.985011101
-1.055078268	3.580372810	9.985383034
-4.702452183	9.400211334	9.992673874
5.914170265	3.283525229	10.004367828
2.382659912	9.915158272	9.943060875
1.208009481	3.281206131	10.008818626
-2.426102638	9.399459839	9.993447304
8.178082466	3.579552174	9.986289024
4.739983559	9.913317680	9.946022034
0.309573412	5.430553436	10.025902748
-3.563051701	11.347552299	9.996082306
6.815926552	5.430567741	10.025352478
3.562941551	11.847670555	9.978094101
-0.926969767	4.902010441	9.978901863
-4.757219791	10.738795280	9.992249489
5.630125999	4.676231384	10.083862305
2.356172562	11.239953041	9.979928017
1.494276285	4.673556328	10.097977638
-2.370067358	10.737813950	9.992817879
8.050812721	4.903268814	9.984424591
4.769551277	11.237890244	9.982534409

0.009431839	2.734784126	9.966049194
-3.564533472	8.664095879	9.996565819
7.113477230	2.736233234	9.966533661
3.561187267	9.199786186	9.879809380
3.561011076	3.137298584	9.940437317
0.007005215	9.599368095	9.959422112
10.687147141	3.680577517	9.990946770
7.115118980	9.598483086	9.961103439
2.359083652	1.100278258	9.998885155
-0.930322409	7.434187889	9.958273888
9.496489525	1.602326393	9.990020752
5.634056091	7.657747746	10.124093056
4.765978336	1.101650119	9.999685287
1.488660812	7.659877777	10.143569946
11.879535675	1.603310704	9.990907669
8.053589821	7.433722496	9.965515137
3.555561781	5.036954403	9.951620102
3.554780483	7.297897339	10.031873703
2.298849106	6.355707645	4.424760818
4.739413261	6.287528038	4.423674107
1.495744705	7.569292068	6.408129215
5.552458763	4.994000435	6.359082699
4.999341965	6.241854668	8.409452438
2.057823658	6.245402336	8.419941902
3.516394138	8.330176353	7.770426750
3.522110701	4.194257259	7.574635506
3.574794292	8.346803665	5.301732540
3.465347767	4.280850410	5.143723965
1.466013432	5.014802933	6.367460728
5.567704678	7.555918694	6.393362045

3.521767378 6.292137623 6.515105247

CO/Fe2_CN@Fe13

1.0

14.2519006729	0.0000000000	0.0000000000
-7.1261024411	12.3424147100	0.0000000000
0.0000000000	0.0000000000	26.9325370789

C N Fe O

25 24 15 1

Cartesian

3.562050343	0.484207004	9.995810509
0.341056108	6.910479069	10.029423714
10.688126564	0.984606624	9.983311653
6.783317566	6.911318302	10.028187752
2.379612923	2.410738945	9.962957382
-1.050912857	8.755246162	9.983517647
9.552613258	2.936684132	9.985191345
5.919110775	9.081571579	9.990424156
4.743069172	2.411844254	9.960212708
1.202383041	9.082125664	9.996114731
11.822478294	2.937009096	9.984493256
8.173139572	8.757540703	9.985337257
-1.049746394	3.575184107	9.987589836
-4.700115204	9.397349358	9.989188194
5.920032501	3.260144711	9.988975525
2.371603489	9.938529015	9.919503212
1.202101469	3.259197950	9.994569778
-2.429194450	9.396496773	9.988464355
8.172419548	3.573699474	9.989231110
4.749844074	9.937117577	9.918236732

0.339994907	5.420077801	10.031550407
-3.563707829	11.351844788	9.997072220
6.783148766	5.419396400	10.029244423
3.561430931	11.860753059	9.969690323
3.566663504	6.035438061	11.502043724
-0.898092389	4.900143623	10.010738373
-4.752685547	10.737755775	9.989963531
5.610021591	4.647786140	10.023432732
2.347646713	11.247506142	10.010752678
1.512837410	4.645812988	10.032118797
-2.375449657	10.736878395	9.991283417
8.019577026	4.900561810	10.015249252
4.773944855	11.246153831	10.013063431
-0.003059149	2.719159842	9.979833603
-3.565049648	8.654649734	9.989432335
7.125473022	2.719888449	9.977251053
3.560234070	9.213634491	9.694378853
3.560894012	3.142710209	9.879726410
-0.002548218	9.612330437	9.967923164
10.687374115	3.680710554	9.983956337
7.124571800	9.612391472	9.967136383
2.350620508	1.096411467	10.008665085
-0.897725582	7.431969166	9.983412743
9.498519897	1.599516153	9.982760429
5.607223511	7.681923389	10.065831184
4.772445679	1.097210169	10.007526398
1.516661644	7.683630943	10.081317902
11.877519608	1.599863410	9.983863831
8.019985199	7.431920528	9.990264893
3.563013315	4.963624477	10.032567978

3.562488079	7.387864590	10.136549950
2.297341108	6.371059895	4.464920998
4.741895676	6.271462917	4.461328506
1.494899273	7.568727016	6.397571564
5.560805798	5.011026859	6.331642151
4.959526062	6.260362625	8.390072823
2.106458902	6.252969265	8.408875465
3.524959564	8.330025673	7.738354206
3.531806469	4.199002266	7.553532124
3.582213402	8.390087128	5.336423397
3.443209648	4.245136738	5.175496101
1.460174322	5.017795563	6.338077545
5.572548866	7.574847221	6.374664783
3.524473190	6.287404060	6.518311024
3.601968765	6.153892994	12.700042725

CHO/Fe2_CN@Fe13

1.0

14.2519006729	0.0000000000	0.0000000000
-7.1261024411	12.3424147100	0.0000000000
0.0000000000	0.0000000000	26.9325370789

C N Fe O H

25 24 15 1 1

Cartesian

3.560318708	0.512977302	9.994639397
0.298136711	6.907073498	10.009428024
10.687097549	0.970515907	9.999509811
6.821530342	6.907489777	10.009490013
2.384340763	2.449233055	9.883986473
-1.064601183	8.763548851	9.971081734

9.552883148	2.929897547	9.995800018
5.916337013	9.060451508	9.942863464
4.736137390	2.448825598	9.878308296
1.201569080	9.063730240	9.950963974
11.819614410	2.930787325	9.995759010
8.182991028	8.764398575	9.971328735
-1.061566472	3.578120470	9.973853111
-4.703743935	9.415373802	9.999322891
5.924557686	3.295403957	9.985946655
2.373766899	9.914135933	9.823387146
1.196211457	3.295945406	9.994478226
-2.428660870	9.414836884	9.999086380
8.181936264	3.576977253	9.974103928
4.744956970	9.911365509	9.819113731
0.286960840	5.426437378	10.017885208
-3.565834522	11.381606102	10.011249542
6.834175110	5.425298691	10.017580032
3.561598301	11.840723991	9.962123871
3.564423800	6.569912434	11.813662529
-0.953368545	4.902963161	9.962063789
-4.758221149	10.758463860	9.998744011
5.678004265	4.671666145	10.056845665
2.362803459	11.212141991	10.018427849
1.444636345	4.671992302	10.069745064
-2.374194622	10.757853508	9.998809814
8.073763847	4.902488708	9.970882416
4.758551598	11.209907532	10.015938759
-0.004877806	2.732987881	9.958785057
-3.566615105	8.678502083	10.014766693
7.125823975	2.731964588	9.951906204

3.557623386	9.216196060	9.441216469
3.559195995	3.166089058	9.549048424
-0.002504826	9.607082367	9.949008942
10.685648918	3.674961805	10.007367134
7.121315956	9.604831696	9.946087837
2.362071991	1.151367188	10.045757294
-0.938780308	7.439187527	9.967695236
9.495867729	1.593535542	9.993127823
5.635220528	7.667982578	10.007248878
4.757984638	1.151299238	10.040873528
1.481407642	7.672481060	10.027418137
11.876834869	1.594395399	9.993721008
8.056862831	7.438667297	9.973928452
3.567460060	5.089939117	9.978376389
3.549483776	7.414333820	10.194369316
2.307725191	6.412569523	4.429661274
4.769812584	6.294183254	4.423794270
1.473108768	7.514034748	6.387467861
5.528476715	4.981345654	6.351623058
4.951653957	6.323434830	8.378403664
2.121041775	6.300140858	8.406393051
3.518965721	8.314967155	7.676893711
3.537257910	4.203128338	7.701062202
3.592165947	8.367846489	5.298474312
3.439688683	4.288752079	5.195988178
1.488470316	4.989598274	6.373551846
5.587503910	7.537827015	6.325096130
3.525670052	6.263181210	6.481389999
3.569412947	5.403217316	12.257118225
3.541707516	7.431365967	12.540071487

CHOH/Fe2_CN@Fe13

1.0

14.2519006729	0.0000000000	0.0000000000
-7.1261024411	12.3424147100	0.0000000000
0.0000000000	0.0000000000	26.9325370789

C N Fe O H

25 24 15 1 2

Cartesian

3.555862188	0.468650818	10.014163017
0.322031260	6.899776459	9.979252815
10.677264214	0.990392685	9.981657982
6.779973507	6.913208961	10.030672073
2.386019707	2.415290833	9.909965515
-1.044636250	8.750445366	9.980838776
9.544796944	2.950253010	9.985671043
5.914011478	9.091710091	9.977283478
4.743875980	2.398676395	9.900535583
1.220609188	9.061518669	9.969519615
11.824483871	2.942726374	9.986254692
8.166072845	8.755654335	9.997985840
-1.045330882	3.572881937	9.998639107
-4.705236435	9.385282516	9.990830421
5.905931950	3.251467943	9.969973564
2.384778023	9.922126770	9.855019569
1.221439481	3.269627333	9.970274925
-2.427198172	9.386408806	9.987154007
8.161395073	3.577294111	10.004554749
4.751323223	9.945781708	9.845159531
0.326720715	5.423038006	9.993004799

-3.571051359	11.341640472	10.000647545
6.772819996	5.424179554	10.028518677
3.552755833	11.866615295	9.990552902
3.673129797	6.105296612	11.578916550
-0.913408518	4.891832352	9.996444702
-4.762060165	10.722776413	9.984368324
5.598456383	4.637769699	10.029665947
2.364632130	11.219937325	10.047008514
1.512432098	4.654592514	10.012687683
-2.376187086	10.723299026	9.988512993
8.010914803	4.898769379	10.022845268
4.756151676	11.237759590	10.038260460
0.015040636	2.721807241	9.975460052
-3.566215038	8.645742416	9.990397453
7.114745617	2.715520382	9.967350960
3.573309898	9.235627174	9.510210037
3.567896366	3.123598576	9.715720177
0.015122890	9.604296684	9.971702576
10.687133789	3.687742710	9.986722946
7.123003006	9.623234749	9.956823349
2.358750582	1.104904175	10.038376808
-0.919568777	7.432365894	9.942057610
9.488167763	1.611354589	9.971522331
5.612138748	7.705869675	10.082824707
4.761955261	1.089758158	10.025492668
1.510285378	7.670148373	10.049880981
11.873118401	1.605650663	9.973872185
8.021936417	7.436841488	9.996262550
3.593217611	4.960715294	10.009465218
3.622128963	7.412139416	10.116274834

2.302153111	6.394794464	4.469932079
4.743674278	6.267299175	4.455984592
1.492763996	7.551358223	6.420388699
5.566853046	5.020521641	6.311951160
4.926671982	6.249397755	8.362467766
2.177834511	6.274886131	8.433633804
3.534311771	8.354430199	7.710426807
3.518012047	4.168681145	7.573637009
3.594636440	8.411044121	5.335025787
3.441652060	4.225779057	5.199720860
1.461227417	5.024082184	6.346649170
5.577755451	7.592697144	6.356623173
3.526684761	6.288811684	6.486540318
2.658060789	6.250792980	12.486564636
4.595340252	6.005613804	12.177846909
1.814732552	6.408330917	12.012512207

CH/Fe2_CN@Fe13

1.0

14.2519006729	0.0000000000	0.0000000000
-7.1261024411	12.3424147100	0.0000000000
0.0000000000	0.0000000000	26.9325370789

C N Fe H

25 24 15 1

Cartesian

3.561793804	0.470403314	10.002779961
0.345368385	6.909483433	10.033868790
10.687836647	0.991591692	9.982258797
6.778173447	6.909911633	10.032805443
2.381487846	2.399566889	9.941102982

-1.046748161	8.755464554	9.988614082
9.548334122	2.941245794	9.984917641
5.916100502	9.086304665	9.980895996
4.741119862	2.400260687	9.937808990
1.205254078	9.085981369	9.987452507
11.826414108	2.941270590	9.984238625
8.168814659	8.757085800	9.990107536
-1.045560837	3.573250055	9.994194031
-4.705253124	9.390021324	9.988436699
5.916785240	3.252468824	9.979838371
2.374351978	9.938967705	9.890418053
1.204991341	3.252065897	9.984638214
-2.424641848	9.389548302	9.987659454
8.167591095	3.572099447	9.995195389
4.747261524	9.938373566	9.887697220
0.344938993	5.417893410	10.031955719
-3.564044476	11.337581635	9.997095108
6.777099133	5.416789532	10.030286789
3.561120033	11.866714478	9.974894524
3.573176622	6.101095200	11.423244476
-0.892783403	4.895959854	10.010361671
-4.757372856	10.727585793	9.987800598
5.608125687	4.631270409	10.026037216
2.358927250	11.244426727	10.013850212
1.514958620	4.631010056	10.031838417
-2.371353388	10.726939201	9.988806725
8.013936043	4.895979404	10.013611794
4.762471199	11.243735313	10.014417648
-0.000106812	2.714408159	9.981650352
-3.565164804	8.652306557	9.987604141

7.122942924	2.714321852	9.977824211
3.560189247	9.216773033	9.639623642
3.560695648	3.126885653	9.829372406
0.000891209	9.617104530	9.967460632
10.687126160	3.681888103	9.982348442
7.121058941	9.617306709	9.965238571
2.358700037	1.088084102	10.014970779
-0.892837524	7.433825493	9.985303879
9.495319366	1.605913281	9.979419708
5.605134010	7.695769787	10.065648079
4.763758183	1.088232279	10.012822151
1.517344952	7.697242737	10.079740524
11.880055428	1.605927110	9.980177879
8.014345169	7.433684826	9.991453171
3.563046217	4.952109814	10.057017326
3.560278416	7.401225567	10.199414253
2.301024914	6.389945030	4.471820831
4.746463776	6.274415970	4.470675468
1.475942612	7.543270111	6.399324894
5.574651718	5.022663116	6.346380711
4.914954185	6.287153244	8.425182343
2.154236555	6.263082981	8.445044518
3.521150112	8.349534035	7.715662479
3.536951303	4.184561729	7.543118000
3.585341454	8.401368141	5.340485573
3.435493231	4.250675678	5.177313328
1.442301035	5.031094551	6.358549595
5.592885971	7.557673931	6.371883869
3.526095390	6.282887936	6.516207218
3.611229420	6.101165771	12.530118942

CH2/Fe2_CN@Fe13

1.0

14.2519006729	0.0000000000	0.0000000000
-7.1261024411	12.3424147100	0.0000000000
0.0000000000	0.0000000000	26.9325370789

C N Fe H

25 24 15 2

Cartesian

3.562375784	0.462553293	10.012948990
0.350763321	6.912871838	10.028931618
10.687706947	0.999567509	9.982357025
6.770229340	6.911822319	10.033375740
2.382497787	2.399840832	9.896930695
-1.038018227	8.752455711	9.997893333
9.545089722	2.950936317	9.984898567
5.901273727	9.080084801	9.977744102
4.739377022	2.402155876	9.897201538
1.215074539	9.085722923	9.976805687
11.828134537	2.951434851	9.985424995
8.157247543	8.752763748	9.996348381
-1.036310315	3.579864025	10.005107880
-4.707236767	9.383676529	9.987227440
5.901328087	3.260452509	9.986102104
2.375312328	9.946534157	9.853785515
1.218847513	3.257328510	9.981317520
-2.424591064	9.382671356	9.987957954
8.157537460	3.579840660	10.004130363
4.741607666	9.941498756	9.855228424
0.351193190	5.422198772	10.031594276

-3.564327955	11.336742401	9.998060226
6.769635201	5.421940804	10.037570000
3.561489105	11.875951767	9.989317894
3.525681019	6.153941631	11.573741913
-0.886758447	4.900315762	10.011699677
-4.758651257	10.721456528	9.984305382
5.594437599	4.645779133	10.066704750
2.362452030	11.241309166	10.034950256
1.526722670	4.643346310	10.054779053
-2.371050835	10.720418930	9.983727455
8.007611275	4.901475906	10.013053894
4.758442879	11.236948013	10.035578728
0.011653423	2.721076727	9.977891922
-3.566104412	8.645010948	9.987417221
7.109392166	2.723305941	9.973378181
3.557179928	9.236960411	9.544432640
3.560366154	3.122977257	9.672645569
0.007432461	9.615889549	9.970523834
10.686660767	3.690195799	9.984469414
7.109375954	9.611962318	9.967484474
2.361893177	1.097128630	10.040670395
-0.888817310	7.434770584	9.990635872
9.494051933	1.613118052	9.973865509
5.593753338	7.689999580	10.075485229
4.761980057	1.098464131	10.038078308
1.524359226	7.696012497	10.075095177
11.881031036	1.613734126	9.973712921
8.008996964	7.433688641	9.993198395
3.557302237	4.951059818	10.057154655
3.547156334	7.423132896	10.128648758

2.298413754	6.396012783	4.457946301
4.736233711	6.268188477	4.457176685
1.497019291	7.542734623	6.402784348
5.561500549	5.037282467	6.351049900
4.884978294	6.260445118	8.431329727
2.187429667	6.236907482	8.433705330
3.541489124	8.353754044	7.711788177
3.541535616	4.171096802	7.604224682
3.586592197	8.409227371	5.333981514
3.424452305	4.242527962	5.197566986
1.463099241	5.016318798	6.351655483
5.575120926	7.567088604	6.376943111
3.526173353	6.282835007	6.490890026
4.426948547	6.148112774	12.188156128
2.599216938	6.114712238	12.156354904

CH3/Fe2_CN@Fe13

1.0

14.2519006729	0.0000000000	0.0000000000
-7.1261024411	12.3424147100	0.0000000000
0.0000000000	0.0000000000	26.9325370789

C N Fe H

25 24 15 3

Cartesian

3.562996149	0.469821662	10.014312744
0.332244873	6.908009052	10.000237465
10.688205719	1.000034690	9.984258652
6.792685032	6.907011509	10.002627373
2.385930538	2.396703720	9.906319618
-1.048131466	8.757815361	9.996797562

9.545702934	2.945194006	9.985416412
5.913698673	9.075606346	9.946112633
4.732879162	2.402685165	9.906164169
1.206423283	9.082883835	9.941936493
11.827875137	2.945726156	9.985268593
8.171085358	8.756641388	9.996901512
-1.044798970	3.573393822	10.005270958
-4.706552505	9.387660027	9.987837791
5.909682274	3.265096426	9.964569092
2.378012180	9.941894531	9.874786377
1.209019184	3.257745743	9.963092804
-2.423255682	9.387009621	9.987468719
8.166293144	3.574048281	10.004503250
4.742443085	9.936875343	9.878330231
0.335209846	5.422048569	10.007440567
-3.563891172	11.331542969	9.996606827
6.789175987	5.423225880	10.009385109
3.563107967	11.865767479	9.986178398
3.478836775	6.174799919	11.692312241
-0.902885675	4.894791603	10.019552231
-4.758423328	10.728876114	9.984964371
5.612892151	4.651352882	9.994599342
2.361157894	11.250792503	10.004903793
1.508325338	4.643619537	9.990808487
-2.370744467	10.727924347	9.984922409
8.026913643	4.896224976	10.020129204
4.763572693	11.245887756	10.009095192
0.005089045	2.717951775	9.991102219
-3.565100193	8.654362679	9.985435486
7.113745689	2.721720219	9.987037659

3.559287071	9.225163460	9.677911758
3.557565689	3.117186308	9.729786873
0.002301693	9.614487648	9.983265877
10.686647415	3.680755138	9.979835510
7.118072987	9.609908104	9.980349541
2.363661051	1.088844776	10.035567284
-0.905223131	7.435744762	9.995586395
9.493958473	1.606196761	9.979637146
5.612462997	7.677596569	9.987929344
4.759900570	1.093596697	10.034626961
1.509036064	7.685011387	9.983219147
11.881120682	1.606958866	9.979487419
8.029968262	7.433625698	9.997834206
3.544599533	4.960264683	9.993546486
3.546519756	7.387863636	10.055047035
2.298896074	6.390897751	4.460251331
4.739531517	6.275673389	4.459207535
1.497446060	7.560553074	6.397338390
5.556949615	5.010332108	6.349814892
4.960148811	6.247469425	8.396125793
2.107660055	6.248724461	8.405285835
3.531539917	8.342754364	7.735382080
3.533149481	4.193139076	7.617224216
3.582293510	8.404376984	5.330378056
3.437566996	4.266108036	5.180557728
1.473226547	5.000226021	6.369134903
5.569050789	7.573810101	6.382019043
3.525866985	6.287763119	6.506919384
3.652694225	5.116354942	11.997078896
4.325512886	6.705655575	12.164379120

2.526572227 6.456613064 12.140749931

2CO/Fe2_CN@Fe13

1.0

14.2519006729	0.0000000000	0.0000000000
-7.1261024411	12.3424147100	0.0000000000
0.0000000000	0.0000000000	26.9325370789

C N Fe O

26 24 15 2

Cartesian

3.560942173	0.503386796	10.001242638
0.297070503	6.895759583	9.979067802
10.684399605	0.971966445	10.000057220
6.825401306	6.897964478	9.977619171
2.385130882	2.440399170	9.827838898
-1.059250355	8.751827240	9.986082077
9.550291061	2.925813437	10.000762939
5.909260273	9.045855522	9.904535294
4.733603954	2.441503525	9.819905281
1.211057663	9.044160843	9.915555954
11.818805695	2.925777197	10.000571251
8.179131508	8.755340576	9.983914375
-1.053422451	3.570240021	9.990476608
-4.700606823	9.405169487	10.001962662
5.904240131	3.293107986	9.929976463
2.378701687	9.901391029	9.818137169
1.214558601	3.291156292	9.943934441
-2.432089329	9.403581619	10.003151894
8.171955109	3.570550919	9.990455627
4.740933895	9.901827812	9.815124512

0.300826550	5.424922466	9.989778519
-3.565234661	11.363001823	10.016330719
6.820191383	5.426849842	9.985668182
3.559051037	11.835075378	9.985510826
3.579650402	7.474452496	11.976692200
3.582841873	4.729314327	11.909768105
-0.928743958	4.896190166	9.984907150
-4.756971359	10.743525505	10.002861023
5.632092476	4.683981419	9.947679520
2.356547832	11.204885483	10.019138336
1.487850189	4.680141449	9.968496323
-2.374124765	10.741649628	10.002210617
8.047596931	4.897396564	9.991435051
4.761971474	11.205563545	10.015298843
0.011346698	2.736870050	9.977174759
-3.566769838	8.659923553	10.008583069
7.106363297	2.738617897	9.971633911
3.558682442	9.205619812	9.511269569
3.558695316	3.139129162	9.469783783
0.012525082	9.583738327	9.973523140
10.684512138	3.671762705	10.016409874
7.107256889	9.586227417	9.966021538
2.364797592	1.143982291	10.044136047
-0.934346437	7.427775860	9.973096848
9.493673325	1.590212226	9.988080025
5.628520489	7.637960434	9.915222168
4.756037235	1.144625545	10.037652016
1.493931770	7.637359619	9.938756943
11.875221252	1.590535283	9.988553047
8.054300308	7.429556847	9.983554840

3.560318232	4.962969303	10.159895897
3.562287331	7.380700111	10.214261055
2.268791914	6.444337845	4.441698074
4.774020195	6.260688782	4.433192730
1.491465092	7.577426910	6.390419960
5.548176289	4.995420933	6.316773891
4.924901962	6.282344341	8.380394936
2.166665077	6.278785229	8.399312019
3.534639835	8.283267021	7.729695320
3.551234007	4.213676929	7.679947376
3.587667942	8.372708321	5.290838718
3.425590754	4.282981873	5.184506893
1.496535063	5.001786709	6.308584690
5.557883739	7.590713024	6.336225033
3.528619528	6.272680759	6.466538906
3.595033169	7.525239944	13.148207664
3.608844042	4.567389011	13.069431305

2CO_coupled/Fe2_CN@Fe13

1.0

14.2519006729	0.0000000000	0.0000000000
-7.1261024411	12.3424147100	0.0000000000
0.0000000000	0.0000000000	26.9325370789

C N Fe O

26 24 15 2

Cartesian

3.562557936	0.465853482	10.009654045
0.311360121	6.904963017	9.988498688
10.688344002	0.981557310	9.984116554
6.814261436	6.906021595	9.985014915

2.383970976	2.396000624	9.911950111
-1.058873892	8.757722855	9.988728523
9.554594040	2.935110569	9.986753464
5.920195580	9.070887566	9.965996742
4.736386299	2.400587797	9.908118248
1.200513840	9.073709488	9.972667694
11.820825577	2.935968399	9.986474037
8.181170464	8.760178566	9.991220474
-1.057930827	3.572371721	9.994186401
-4.700154305	9.396539688	9.987863541
5.921042919	3.260255814	9.976497650
2.379696846	9.921431541	9.886514664
1.200507164	3.255738735	9.989816666
-2.429295778	9.395321846	9.987163544
8.181574821	3.571318626	9.995746613
4.740956306	9.918862343	9.884920120
0.315846920	5.417178631	9.993425369
-3.563456297	11.342944145	9.992014885
6.811880112	5.417312145	9.984810829
3.561747074	11.855673790	9.977540970
3.565048218	7.543808937	11.981563568
3.581751108	6.074472427	11.571516037
-0.925083995	4.892862320	9.997453690
-4.755115509	10.733162880	9.981446266
5.644304752	4.645586967	9.954111099
2.359342098	11.226906776	10.021997452
1.483161926	4.640471458	9.988471985
-2.372505665	10.731940269	9.982702255
8.051024437	4.893483639	10.004878998
4.762435436	11.224109650	10.024124146

-0.005532265	2.714643240	9.996311188
-3.564924240	8.654109001	9.990301132
7.127139091	2.716960907	9.997800827
3.559279442	9.191617966	9.621799469
3.558207273	3.102796555	9.614504814
-0.003301620	9.612594604	9.995371819
10.687588692	3.681073189	9.984672546
7.124312878	9.611779213	9.994277954
2.359596729	1.091873407	10.066577911
-0.926782131	7.436909199	9.978511810
9.498725891	1.598922968	9.980115891
5.638965130	7.671550274	9.960810661
4.762931824	1.096010327	10.065704346
1.485273361	7.674561501	9.979165077
11.877569199	1.599601150	9.981686592
8.049728394	7.437572956	9.986838341
3.551251650	4.938086033	9.928652763
3.557084084	7.356389999	10.172923088
2.304879904	6.369767189	4.448310852
4.738991261	6.274420738	4.441663742
1.487697601	7.563259125	6.395175934
5.568869591	4.995965481	6.325773239
5.013247490	6.246332645	8.348312378
2.049353123	6.251987934	8.368998528
3.520473480	8.335283279	7.742517471
3.524368286	4.195294857	7.596449852
3.585982323	8.382697105	5.322216034
3.455268383	4.268461227	5.162444115
1.455199957	5.006844997	6.349817753
5.577893734	7.570662498	6.370438099

3.525156021	6.289101601	6.513209820
3.571307659	8.272427559	12.926244736
3.618304729	4.980812550	12.155522346

COCHO_coupled/Fe2_CN@Fe13

1.0

14.2519006729	0.0000000000	0.0000000000
-7.1261024411	12.3424147100	0.0000000000
0.0000000000	0.0000000000	26.9325370789

C N Fe O H

26 24 15 2 1

Cartesian

3.572529554	0.504815996	10.007834435
0.306271076	6.918811798	9.979516983
10.689993858	0.991284490	9.994388580
6.888616562	6.928822517	9.910129547
2.384642124	2.432108879	9.904028893
-1.043416023	8.768528938	9.990665436
9.545089722	2.944203615	9.993397713
5.958392143	9.070324898	9.826090813
4.729606628	2.457616806	9.907974243
1.210446835	9.075357437	9.950907707
11.822216034	2.953401089	9.988193512
8.206449509	8.774573326	10.023280144
-1.050452471	3.586424828	9.999615669
-4.683423996	9.412445068	9.998567581
5.905453682	3.313123941	9.961113930
2.392935753	9.921767235	9.860051155
1.205123425	3.277223110	9.961956978
-2.411675692	9.410247803	9.988385201

8.168929100	3.580443859	10.011411667
4.758858204	9.919210434	9.814342499
0.319843531	5.438471794	9.991365433
-3.545542479	11.365148544	9.996520042
6.831514359	5.446693897	9.982117653
3.571151733	11.855756760	10.012607574
3.598999262	4.946818352	12.061652184
3.474490881	6.450447559	11.992363930
-0.912899613	4.906930447	9.987278938
-4.738933563	10.747081757	9.973655701
5.636894226	4.707722664	9.985079765
2.373585224	11.231850624	10.031863213
1.500005484	4.671893120	10.012322426
-2.359040260	10.745646477	9.999550819
8.051064491	4.906304359	10.002613068
4.777510643	11.220732689	10.028429985
0.006760955	2.734712601	9.981788635
-3.549257517	8.665885925	9.987442017
7.103230000	2.749660254	9.979932785
3.572353840	9.217524529	9.563486099
3.552104950	3.175988197	9.753849983
0.013592243	9.623793602	9.980399132
10.681624413	3.695673704	9.991422653
7.138535976	9.610995293	10.032660484
2.365131378	1.117523432	10.012545586
-0.932229519	7.446784019	9.963919640
9.495148659	1.610256314	9.981076241
5.765726566	7.685673714	9.634829521
4.767818928	1.140992284	10.015898705
1.469368935	7.685547829	10.007987022

11.877754211	1.618350029	9.980335236
8.108684540	7.444861889	10.037560463
3.486257553	5.016997814	10.196321487
3.577533245	7.350726604	10.181791306
2.275799990	6.395149708	4.459569454
4.752880096	6.261519909	4.449228764
1.465707302	7.576087475	6.395412445
5.579425812	5.030100346	6.311512947
4.920574188	6.262335777	8.389779091
2.075326443	6.222543716	8.388809204
3.463545799	8.317220688	7.713166237
3.538001060	4.217018604	7.628671646
3.597414494	8.359352112	5.279728889
3.449320555	4.259971619	5.201815128
1.440359116	5.035535812	6.328524113
5.580378532	7.572813988	6.371746063
3.516619205	6.285754204	6.501906395
3.606197357	4.118275642	12.956400871
4.484984875	7.321280956	11.918075562
2.497446537	6.884101868	12.253250122