

## Supporting Information

### Breaking scaling relations for efficient CO<sub>2</sub> electrochemical reduction through dual-atom catalysts

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#### Computational details

The scaling relations on transition-metal surface are mainly reported by Norskov et al, hence, in the calculation of scaling relations of binding energies, to compare the scaling relations of dual-atom catalysts with that of transition-metals, we used the same calculation equations reported by Norskov et al.<sup>1</sup> The binding energies of \*CO, \*COOH, and \*CHO are calculated through

$$E_b(\text{CO}) = E(*\text{CO}) + \Delta E_{\text{sol}}(\text{CO}) - E^* - E(\text{CO}_{(\text{g})})$$

$$E_b(\text{COOH}) = E(*\text{COOH}) + \Delta E_{\text{sol}}(\text{COOH}) - E^* - E(\text{CO}_{2(\text{g})}) - 1/2E(\text{H}_2)$$

$$E_b(\text{CHO}) = E(*\text{CHO}) + \Delta E_{\text{sol}}(\text{CHO}) - E^* - E(\text{CO}_{(\text{g})}) - 1/2E(\text{H}_2)$$

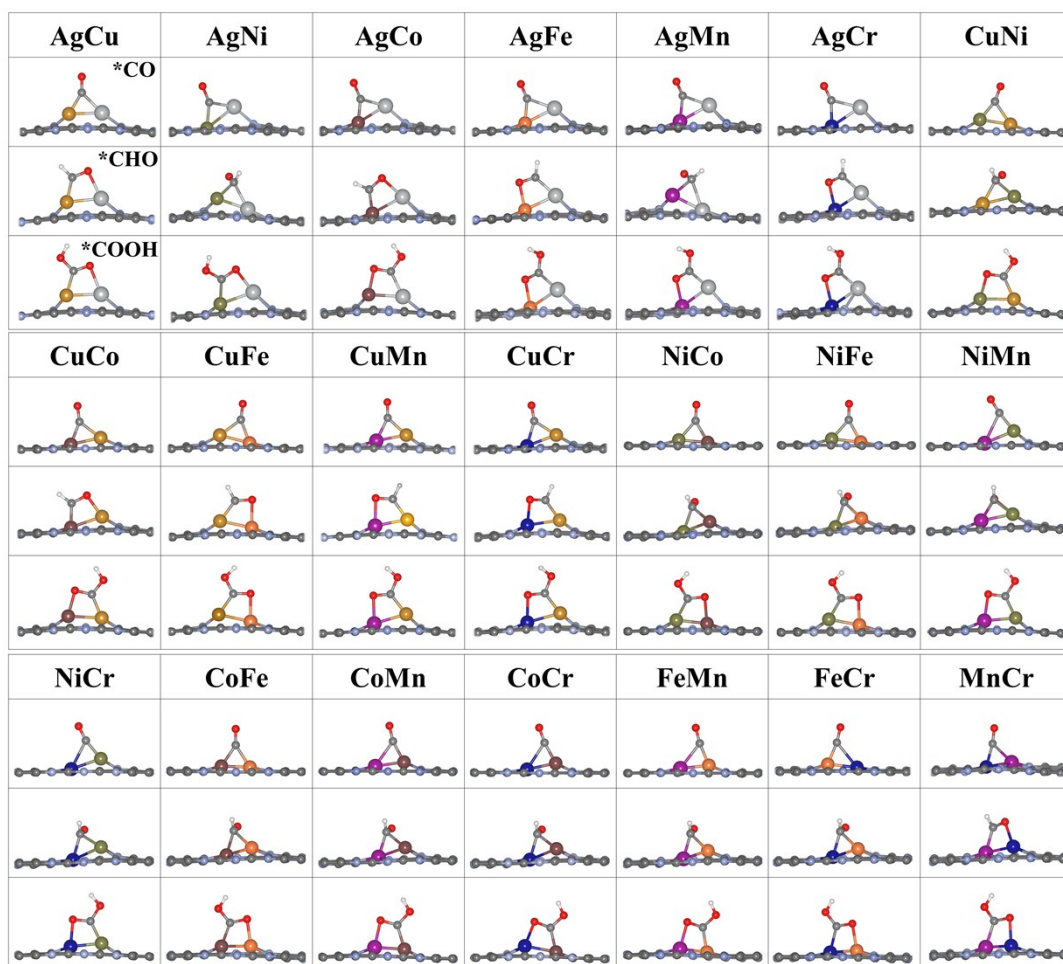
$E_b(\text{CO})$ ,  $E_b(\text{COOH})$ , and  $E_b(\text{CHO})$  are the binding energies of \*CO, \*COOH, and \*CHO, respectively. The  $\Delta E_{\text{sol}}$  indicates a solvation correction to binding energy. For \*CO, \*COOH, and \*CHO, the solvation correction is -0.1 eV, -0.25 eV and -0.1 eV, respectively.

For gas-phase species, the standard ideal-gas method was used to calculate the free energy.<sup>2</sup> The energy corrections of gas-phase species, including zero point energies, heat capacities, and entropies, are listed below:

**Table S1.** Free energy corrections for gas-phase species.

Molecule	ZPE (eV)	$\int C_p dT$ (eV)	-TS (eV)
CO <sub>2</sub>	0.31	0.10	-0.66
CO	0.13	0.09	-0.61
H <sub>2</sub>	0.28	0.09	-0.40
H <sub>2</sub> O	0.57	0.10	-0.67
CH <sub>3</sub> OH	1.37	0.12	-0.81
HCOOH	0.90	0.11	-0.99
CH <sub>4</sub>	1.20	0.11	-0.58
HCHO	0.71	0.11	-0.68

The dissolution potentials were calculated by  $U_{\text{diss}} = U_{\text{diss(Metal,Bulk)}} - (\mu_{\text{Metal,dim}} - \mu_{\text{Metal,Bulk}})/ne$ , where  $U_{\text{diss(Metal,Bulk)}}$ ,  $\mu_{\text{Metal,dim}}$ ,  $\mu_{\text{Metal,Bulk}}$ , and  $n$  are the dissolution potential of bulk metals, the chemical potential of metal atom in dimer system, the chemical potential of metal atom in bulk, and the number of electrons involved in the dissolution, respectively.<sup>3</sup> Computational hydrogen electrode (CHE)<sup>4</sup> model was used to calculate the Gibbs free energy change of CO<sub>2</sub>RR elementary reactions. At electrode potential  $U = 0$  V (vs. reversible hydrogen electrode), the free energy can be calculated by  $\Delta G = \Delta E - T\Delta S + \Delta ZPE$ .  $\Delta E$  is reaction energy of hydrogenation.  $T\Delta S$  is the gas-phase entropy contribution at 298 K.  $\Delta ZPE$  is the zero-point energy correction. The electrode potential,  $U$  (vs. reversible hydrogen electrode), is considered by  $\Delta G_n(U) = \Delta G_n(U=0) + neU$  when  $n$  electrons are transferred. The Poisson–Boltzmann (PB) implicit solvation model, VaspSol,<sup>5</sup> was used to describe the effect of solvation as implemented in VASP, with a dielectric constant  $\epsilon=80$  for water. The solvation energy was directly contained in the total energy.

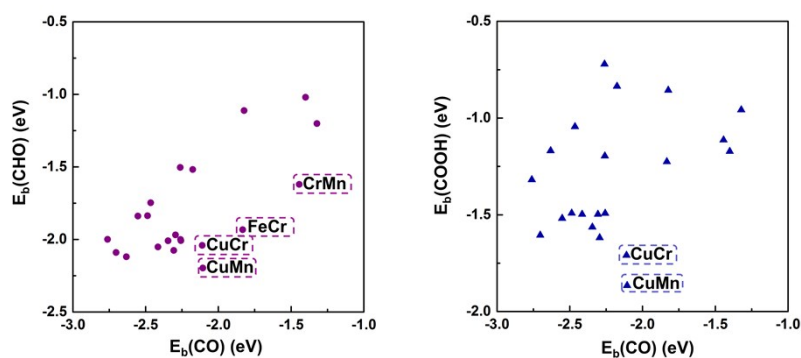


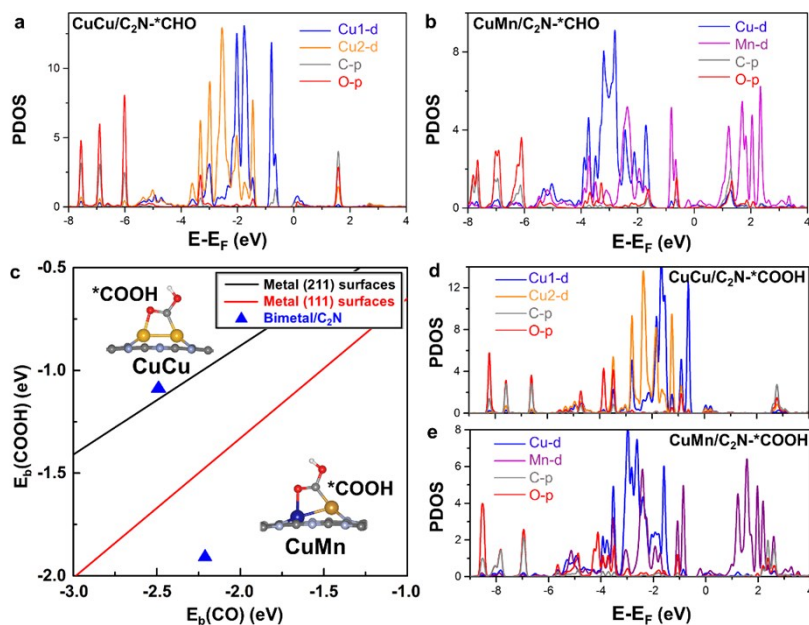
**Figure S1.** Optimized geometries of \*CO, \*CHO and \*COOH adsorbed M<sub>1</sub>M<sub>2</sub>/C<sub>2</sub>N.

**Table S2.** Binding energies of \*CO, \*CHO, and \*COOH without solvation correction.

Metal dimers	*CO (eV)	*CHO (eV)	*COOH (eV)	Metal dimers	*CO (eV)	*CHO (eV)	*COOH (eV)
CuCr	-2.05	-2.02	-1.49	NiCr	-2.36	-1.91	-1.38
CuMn	-2.12	-2.10	-1.66	NiMn	-2.25	-1.94	-1.30
CuFe	-2.65	-1.99	-1.48	NiFe	-2.46	-1.78	-1.30
CuCo	-2.70	-1.89	-1.14	NiCo	-2.59	-2.04	-1.00
CuNi	-2.48	-1.72	-0.91	CoFe	-2.40	-2.02	-1.33
CuAg	-1.78	-1.08	-0.71	CoCr	-2.30	-1.94	-1.03
AgNi	-2.19	-1.33	-0.57	CoMn	-2.30	-1.97	-1.35
AgCo	-2.05	-1.43	-0.55	FeCr	-1.78	-1.83	-1.10
AgFe	-2.51	-1.75	-1.35	FeMn	-2.34	-1.95	-1.47
AgMn	-1.33	-1.00	-0.92	CrMn	-1.37	-1.60	-1.04
AgCr	-1.35	-1.14	-0.74				

Considering strict solvation corrections may have effect on scaling relations,<sup>6</sup> we used implicit solvation models implemented by VASPsol to calculate the scaling relations of \*CO, \*CHO and \*COOH, as shown in Fig. S2. Comparing the scaling relations with constant solvation corrections and solvation corrections calculated by VASPsol (Fig. 1d, 1e and Fig. S2), we can find that the four metal dimers (CuMn, CuCr, FeCr and MnCr) approach the desired low overpotential region with both solvation corrections. Because of the strong ability of dual-sites to stabilize \*CHO and \*COOH, the solvation effect has very limited impacts on scaling relations.

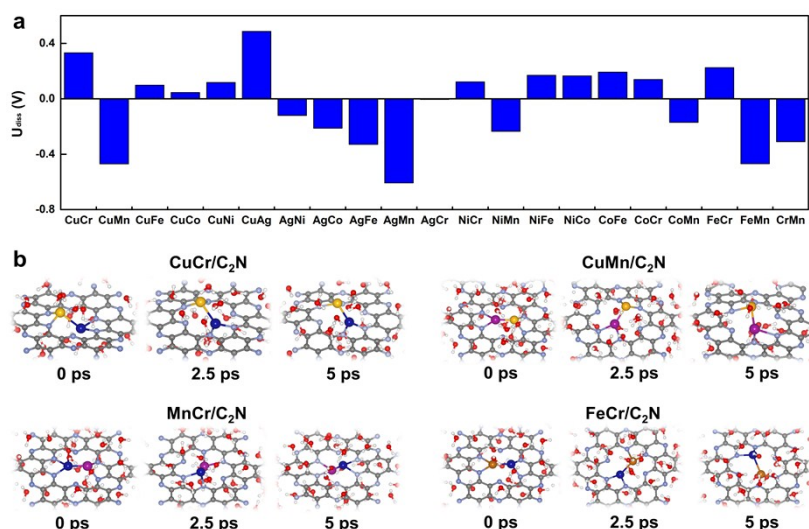
**Figure S2.** Scaling relations of binding energies of \*CO, \*CHO and \*COOH with solvation corrections calculated by VASPsol.



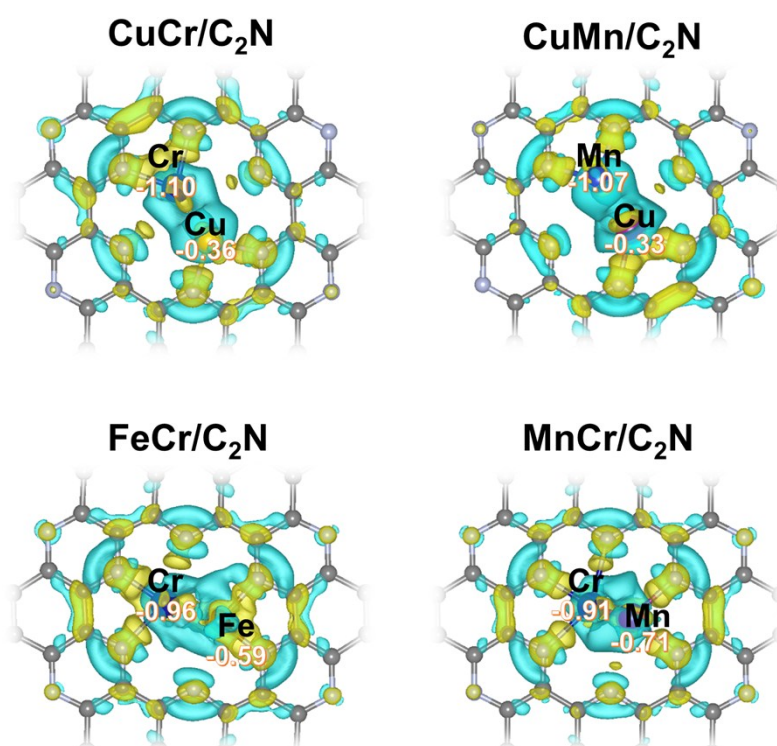
**Figure S3.** Projected density of states (PDOS) of the (a) CuCu/C<sub>2</sub>N and (b) CuMn/C<sub>2</sub>N with adsorbed \*CHO species. (c) Relationship between binding energies E<sub>b</sub>(COOH) and E<sub>b</sub>(CO) for the C<sub>2</sub>N supported CuCu and CuMn dimers. Projected density of states (PDOS) of the (d) CuCu/C<sub>2</sub>N and (e) CuMn/C<sub>2</sub>N with adsorbed \*COOH species.

The projected density of states (PDOS) of the CuCu/C<sub>2</sub>N with \*CHO adsorbate (CuCu/C<sub>2</sub>N-\*CHO) is compared to the CuMn/C<sub>2</sub>N-\*CHO (Figure S2a and S2b). The sharp peaks at around -8~-6 eV correspond to the covalent C-O bond without much mixing with the metal atoms. For CuMn/C<sub>2</sub>N-\*CHO, the O-2p states are delocalized and have strong hybridization with Mn-3d states in a broad energy range from -4 to 0 eV. In contrast, the O in CHO\* adsorbate and the Cu in CuCu/C<sub>2</sub>N have much weaker hybridization.

The scaling relations between \*COOH and \*CO on CuCu/C<sub>2</sub>N and CuMn/C<sub>2</sub>N are shown in Figure S2c. The CuCu/C<sub>2</sub>N still follow the linear scaling relationship of pure metal surfaces, indicating the high limiting potential for CO<sub>2</sub> reduction. Similar to the PDOS analysis in \*CHO adsorbate, the hybridization between Mn-3d states and O-2p states in CuMn/C<sub>2</sub>N-\*COOH is strong, and the hybridization between Cu-3d states and O-2p states in CuCu/C<sub>2</sub>N-\*COOH is weak (Figure S2d and S2e).



**Figure S4.** (a) Dissolution potentials ( $U_{\text{diss}}$ ) of TM atoms on  $C_2N$  at pH 0 (b) Ab initio molecular dynamics simulations of structural evolution of CuCr/ $C_2N$ , CuMn/ $C_2N$ , FeCr/ $C_2N$ , and MnCr/ $C_2N$  in acidic aqueous solution in 5 picoseconds at 300 K. In order to simulate the electrical double layer, a charged aqueous interface model was used. Two H atoms were located in bulk water as solvated  $H^+$  in solution, and electrons entered in slab spontaneously.



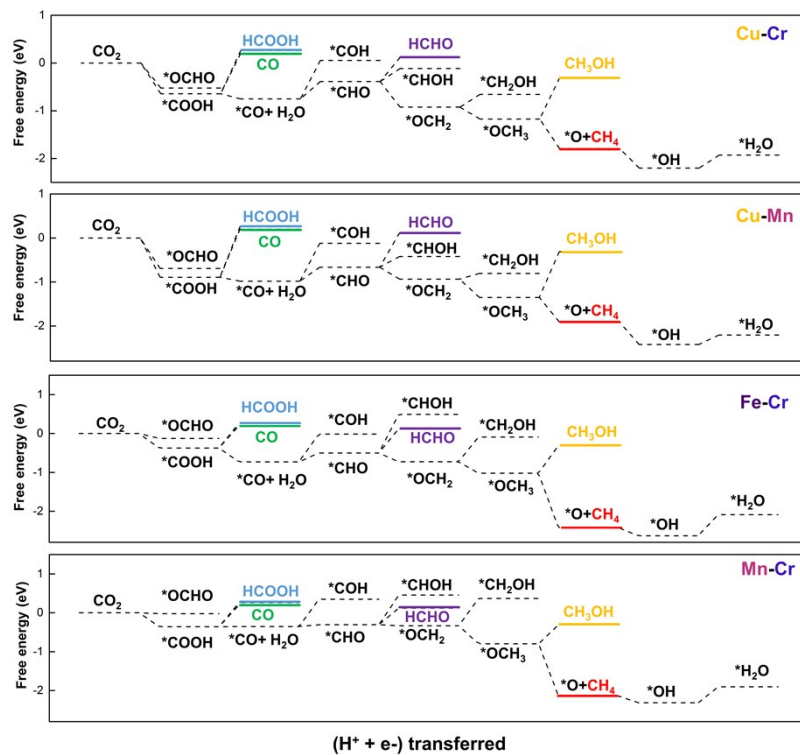
**Figure S5.** Difference charge density and Bader charge for CuCr/ $C_2N$ , CuMn/ $C_2N$ , FeCr/ $C_2N$ , and MnCr/ $C_2N$ . Charge depletion and accumulation are displayed in cyan and yellow, respectively. Negative charges indicate that electrons are transferred from the metal atoms to  $C_2N$ .

**Table S3.** Free energy corrections for intermediates.

Metal dimers	Adsorbate	ZPE (eV)	TS (eV)	$\int C_p dT$ (eV)
CuCr	*COOH	0.645	0.172	0.099
	*OCHO	0.650	0.203	0.098
	*CO	0.193	0.144	0.068
	*COH	0.497	0.128	0.069
	*CHO	0.480	0.122	0.066
	*CHOH	0.777	0.171	0.084
	*OCH <sub>2</sub>	0.790	0.154	0.074
	*CH <sub>2</sub> OH	1.094	0.172	0.089
	*OCH <sub>3</sub>	1.411	0.221	0.102
	*O	0.077	0.051	0.028
*OH	0.374	0.070	0.041	
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Metal dimers	Adsorbate	ZPE (eV)	TS (eV)	$\int C_p dT$ (eV)
CuMn	*COOH	0.647	0.174	0.099
	*OCHO	0.651	0.199	0.097
	*CO	0.193	0.076	0.045
	*COH	0.488	0.150	0.074
	*CHO	0.473	0.134	0.070
	*CHOH	0.775	0.181	0.085
	*OCH <sub>2</sub>	0.731	0.082	0.046
	*CH <sub>2</sub> OH	1.052	0.106	0.060
	*OCH <sub>3</sub>	1.104	0.189	0.095
	*O	0.077	0.051	0.028
*OH	0.367	0.078	0.044	

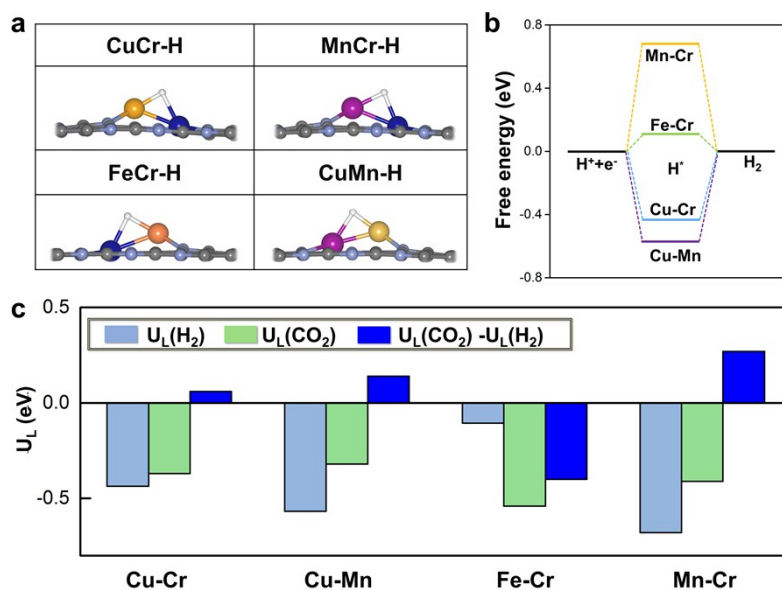
Metal dimers	Adsorbate	ZPE (eV)	TS (eV)	$\int C_p dT$ (eV)
FeCr	*COOH	0.604	0.161	0.083
	*OCHO	0.626	0.209	0.100
	*CO	0.203	0.141	0.067
	*COH	0.499	0.138	0.070
	*CHO	0.477	0.113	0.063
	*CHOH	0.766	0.141	0.070
	*OCH <sub>2</sub>	0.788	0.137	0.072
	*CH <sub>2</sub> OH	1.102	0.171	0.087
	*OCH <sub>3</sub>	1.103	0.230	0.100
	*O	0.078	0.049	0.028
*OH	0.365	0.076	0.044	

Metal dimers	Adsorbate	ZPE (eV)	TS (eV)	$\int C_p dT$ (eV)
CrMn	*COOH	0.605	0.162	0.081
	*OCHO	0.629	0.203	0.099
	*CO	0.196	0.131	0.066
	*COH	0.494	0.171	0.073
	*CHO	0.464	0.128	0.069
	*CHOH	0.768	0.153	0.081
	*OCH <sub>2</sub>	0.776	0.148	0.075
	*CH <sub>2</sub> OH	1.071	0.207	0.098
	*OCH <sub>3</sub>	1.107	0.193	0.095
	*O	0.075	0.052	0.029
*OH	0.364	0.077	0.044	



**Figure S6.** Free energy profiles for the CO<sub>2</sub> reduction reaction to CO, HCOOH, HCHO, CH<sub>4</sub> and CH<sub>3</sub>OH on M<sub>1</sub>M<sub>2</sub>/C<sub>2</sub>N (M<sub>1</sub>M<sub>2</sub> = CuCr, CuMn, FeCr, and MnCr), at zero applied voltage (vs. RHE).





**Figure S7.** (a) Optimized geometries of  $*H$  adsorbed  $M_1M_2/C_2N$ . (b) Free energy diagrams of HER (c) Calculated limiting potentials for HER  $U_L(H_2)$ , limiting potentials for CO<sub>2</sub>RR  $U_L(CO_2)$  and  $U_L(CO_2) - U_L(H_2)$  on  $M_1M_2/C_2N$  ( $M_1M_2 = CuCr, CuMn, FeCr, \text{ and } MnCr$ ).

## References

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- (2) A. A. Peterson and J. K. Nørskov, *J. Phys. Chem. Lett.*, 2012, **3**, 251-258.
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- (4) A. A. Peterson, F. Abild-Pedersen, F. Studt, J. Rossmeisl and J. K. Nørskov, *Energy Environ. Sci.*, 2010, **3**, 1311-1315.
- (5) K. Mathew, R. Sundararaman, K. Letchworth-weaver, T. A. Arias and R. G. Hennig, *J. Chem. Phys.* 2014, **140**, 084106.
- (6) . F. Calle-Vallejo, A. Krabbe and J. M. Garcia-Lastra, *Chem. Sci.*, 2017, **8**, 124-130.

## Atoms Coordinate

C<sub>2</sub>N-AgCu\*CO

16.6396408081	0.0000000000	0.0000000000
-8.3201839081	14.4105558332	0.0000000000
0.0000000000	0.0000000000	18.0000000000

C	N	Cu	Ag	O
49	24	1	1	1

Cartesian

-1.393503070	4.703249931	8.928036690
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2.755599022	2.339499950	9.113263130
3.477998734	3.574681520	9.201477051
4.943076134	3.548417807	9.163704872
3.469318867	1.070594072	9.018261909
0.732141733	5.990228653	9.170269012
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6.954201221	11.905037880	9.083971024
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5.617490768	14.289181709	9.004242897
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3.791506767	7.334587097	12.943072319

C<sub>2</sub>N-AgCu\*CHO

C	N	Cu	Ag	O	H
49	24	1	1	1	1

Cartesian

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6.908545494	11.916549683	9.082079887
5.506076336	9.482851982	9.287189484
5.566971779	14.302865982	8.964863777
2.854357719	7.843017101	10.209095955
5.088743210	6.620684624	10.469879150
4.146448612	6.926592350	12.494970322
2.379055500	7.820550919	12.803435326

C<sub>2</sub>N-AgCu\*COOH

C	N	Cu	Ag	O	H
49	24	1	1	2	1

Cartesian

-1.453732967	4.718145847	8.875386238
-0.738563538	3.488175869	8.964486122
1.431513309	4.748782635	9.127386093
0.723519802	3.506174564	9.046133995
-0.734000921	5.994921207	8.885897636

5.590611458	2.335691690	8.941698074
2.703848839	2.359987736	9.049697876
3.422874928	3.591989756	9.143154144
4.887937546	3.568485975	9.112806320
3.420891762	1.085013986	8.961786270
0.684228659	6.004316330	9.067157745
4.845618725	1.079148889	8.889444351
6.913277626	4.688114166	9.057366371
7.594985485	3.453273535	8.889353752
9.775054932	4.700118065	8.813123703
9.059364319	3.460954428	8.813646317
7.640798092	5.944714546	9.061397552
13.933403015	2.320574999	8.889497757
11.038038254	2.319249392	8.789327621
11.751881599	3.555703640	8.786195755
13.217009544	3.557447433	8.816255569
11.768967628	1.049189329	8.828333855
9.050142288	5.972901821	8.890434265
13.198486328	1.047532082	8.898227692
-5.659492493	11.939029694	8.857926369
-4.943599701	10.702504158	8.771759987
-2.766874313	11.939606667	8.698266029
-3.481008291	10.704060555	8.696969986
-4.926024437	13.209335327	8.853300095
1.344798565	9.574272156	8.955162048
-1.504930496	9.559097290	8.685323715
-0.787302494	10.800121307	8.692091942
0.675662994	10.810423851	8.786627769
-0.782888412	8.285983086	8.768754005
-3.496986866	13.207880020	8.768321991
0.622195721	8.323133469	8.941103935
2.684206009	11.911910057	8.922132492
3.384226322	10.678582191	9.109439850
5.567173481	11.896029472	9.086957932
4.845311165	10.660928726	9.172584534
3.429430962	13.174447060	8.907857895
9.731669426	9.542007446	8.901432037
6.845965385	9.516919136	9.175590515
7.552020550	10.756024361	9.080586433
9.013987541	10.772928238	8.981406212
7.599765301	8.261168480	9.132497787
4.851886749	13.171161652	8.997677803
9.016746521	8.268114090	8.951868057
3.239690781	7.518577576	12.109446526

6.930901527	2.293987513	8.850456238
5.573512077	4.717987061	9.206928253
-1.448227644	7.126307964	8.759340286
2.775313616	4.770052433	9.196344376
1.368534803	2.337680340	9.018179893
1.335715771	7.186659813	9.150804520
15.270106316	2.307274103	8.963532448
13.849810600	4.734689236	8.801046371
6.949325085	7.090900898	9.225557327
11.110742569	4.729356766	8.789327621
9.700894356	2.289131165	8.792280197
9.722146988	7.128210545	8.853912354
2.682319641	9.523447037	9.188225746
1.347892284	11.966410637	8.790300369
-5.606406212	14.360090256	8.942939758
-1.430070877	11.971122742	8.681471825
-2.839828491	9.530536652	8.673336029
-2.792450905	14.342350006	8.785296440
11.065454483	9.525176048	8.790984154
9.643910408	11.953454971	8.957123756
2.746253014	14.322406769	8.824122429
6.901614666	11.923048973	9.054810524
5.502165318	9.487462997	9.238517761
5.558835030	14.308428764	8.984250069
2.832159519	7.865987778	10.305414200
5.077719688	6.624791622	10.393398285
4.288475990	6.928710461	12.491118431
2.361348629	7.900558472	13.071924210
2.740556240	7.619898319	13.942026138

C<sub>2</sub>N-AgNi\*CO

C	N	Ag	Co	O
49	24	1	1	1

Cartesian

-1.531915188	4.746289730	8.933021545
-0.805896521	3.515685558	8.985294342
1.338479757	4.791437626	9.185165405
0.655029774	3.544131994	9.058446884
-0.834089279	6.029909611	9.025308609
5.527460575	2.451062441	8.969561577
2.656399012	2.435254335	9.028007507
3.365698814	3.685168028	9.090126038
4.823804855	3.697517872	9.035118103
3.374006987	1.169877768	8.972352028

0.570254803	6.021220207	9.252791405
4.797445297	1.176275969	8.953506470
6.885271072	4.778324127	8.950086594
7.543624878	3.523092747	8.900712013
9.742365837	4.735438347	8.794026375
9.011068344	3.505382061	8.846712112
7.635464191	5.985424042	8.927082062
13.877285004	2.328860998	8.913906097
10.975040436	2.333141088	8.857332230
11.697427750	3.561799288	8.808389664
13.157981873	3.562419176	8.844264030
11.706859589	1.060126901	8.918010712
9.041204453	6.021695614	8.814258575
13.143101692	1.056019902	8.938890457
-5.692458153	12.015579224	8.863811493
-4.969708920	10.784211159	8.807273865
-2.790213585	12.021847725	8.883197784
-3.506660223	10.786934853	8.830169678
-4.958066463	13.291547775	8.894627571
1.307592869	9.584215164	9.230706215
-1.550532341	9.613497734	8.933238029
-0.828278542	10.848064423	8.982162476
0.633364201	10.829359055	9.080675125
-0.848773479	8.332053185	9.032382011
-3.521924019	13.293665886	8.892864227
0.549171925	8.351277351	9.271530151
2.646475315	11.923798561	9.078246117
3.344731331	10.670526505	9.160056114
5.518511772	11.893737793	9.051480293
4.810925961	10.643564224	9.100961685
3.377207279	13.183886528	9.023741722
9.714944839	9.603194237	8.816705704
6.844225407	9.545782089	8.995697975
7.523158073	10.801950455	8.968157768
8.986613274	10.831002235	8.894592285
7.603840351	8.330598831	8.944883347
4.800329208	13.173683167	9.027000427
9.014450073	8.317110062	8.827055931
4.954906940	7.054456711	11.091383934
6.870331287	2.376041412	8.913545609
5.514761925	4.882022381	9.031913757
-1.534197807	7.177422047	8.960273743
2.690566063	4.844641685	9.182232857
1.319596171	2.391806364	8.999279976



1.205493927	7.190031528	9.494729996
15.216217995	2.328846693	8.972153664
13.774224281	4.746635437	8.847990036
6.925396442	7.150071144	9.052794456
11.075342178	4.743320942	8.767979622
9.635866165	2.323457003	8.868995667
9.728900909	7.173603535	8.780255318
2.658158302	9.522726059	9.266147614
1.306683540	11.977722168	9.031067848
2.674339056	0.024642050	8.937917709
-1.451055050	12.030032158	8.948304176
-2.884074688	9.605557442	8.844623566
5.491055489	0.030017188	8.917181969
11.050251007	9.601536751	8.773830414
9.608432770	12.016976357	8.907624245
2.688861847	14.333502769	8.965295792
6.855763435	11.951164246	8.993070602
5.486366272	9.465746880	9.058427811
5.505071640	14.313529968	8.988821983
2.929791451	7.254965782	10.763837814
5.078618526	6.926332951	9.165258408
5.507169247	7.007262707	12.293802261

C<sub>2</sub>N-AgNi\*CHO

C	N	Ag	Ni	O	H
49	24	1	1	1	1
Cartesian					
-1.491239309			4.734487534		8.892395973
-0.773349166			3.503811359		8.963352203
1.400030851			4.763567924		9.129636765
0.682893515			3.521781206		9.077814102
-0.774327517			6.006953716		8.904222488
5.547323227			2.330316544		9.084258080
2.657615662			2.366573572		9.172260284
3.390177965			3.598301411		9.274463654
4.848958969			3.558931828		9.311382294
3.363035440			1.085619330		9.109962463
0.652088881			6.023294926		9.010764122
4.787563324			1.076093912		9.028440475
6.912879944			4.647533894		9.256788254
7.567505360			3.425043106		8.997983932
9.730368614			4.705176353		8.909567833
9.022575378			3.456487179		8.862839699
7.608435631			5.903529167		9.280692101

13.899706841	2.339135885	8.826569557
11.007596016	2.343185425	8.727696419
11.714175224	3.580835819	8.779625893
13.178596497	3.579538822	8.798219681
11.738648415	1.079768538	8.703845978
9.003276825	5.965682030	9.070757866
13.165532112	1.067404270	8.782793999
-5.737540722	11.930974960	9.042606354
-5.021930218	10.688799858	8.978112221
-2.847859383	11.933755875	8.833355904
-3.556094170	10.694765091	8.873009682
-5.001851082	13.206625938	9.023112297
1.294687748	9.599015236	8.792838097
-1.566730499	9.568408012	8.776709557
-0.859210968	10.813566208	8.725859642
0.608338356	10.835354805	8.703378677
-0.828364134	8.298808098	8.808119774
-3.574452877	13.202793121	8.918747902
0.589481831	8.335700035	8.854434013
2.618254185	11.958931923	8.717165947
3.324222088	10.731122971	8.836469650
5.508568764	11.913465500	8.962595940
4.776372433	10.691566467	8.977499962
3.377514362	13.208629608	8.720009804
9.643737793	9.530694962	9.121409416
6.748041630	9.498847961	9.240768433
7.469904423	10.743112564	9.163259506
8.932353973	10.762841225	9.150354385
7.487997055	8.239869118	9.344087601
4.803615570	13.189520836	8.835929871
8.919205666	8.253473282	9.183617592
4.491510391	7.390410423	11.679803848
6.884943008	2.271997213	8.950985909
5.574927330	4.691961765	9.490356445
-1.492772579	7.141813755	8.825345993
2.738756180	4.779505730	9.249444008
1.327975392	2.351961374	9.099017143
1.307186604	7.195637226	8.984807968
15.233432770	2.322808743	8.917110443
13.812196732	4.753869057	8.818973541
6.863915443	7.030895710	9.513197899
11.065399170	4.748378754	8.854523659
9.672033310	2.296552658	8.755632401
9.653116226	7.134594440	9.077022552

2.638896465	9.578163147	8.861364365
1.272871017	11.999165535	8.654057503
-5.672075272	14.362842560	9.110861778
-1.513785839	11.976886749	8.748521805
-2.901211977	9.527423859	8.837964058
-2.862413406	14.333459854	8.923913956
10.981616020	9.512941360	9.024461746
9.566204071	11.944059372	9.121157646
2.706465721	14.360450745	8.655858040
6.842177868	11.915959358	9.045432091
5.402667999	9.505058289	9.124199867
5.518417358	14.322406769	8.848619461
3.481650352	7.717025280	9.676206589
5.337137222	6.331508636	10.467162132
4.228183746	6.224106312	12.105720520
4.536033154	8.265563011	12.356711388

C<sub>2</sub>N-AgNi\*COOH

C	N	Ag	Ni	O	H
49	24	1	1	2	1

Cartesian

-1.471986294	4.697452068	9.007056236
-0.751417160	3.467150927	9.071477890
1.414841175	4.725495338	9.241524696
0.711531401	3.485927820	9.142829895
-0.760066271	5.973060131	9.069120407
5.581075668	2.342983484	8.943533897
2.697234631	2.349857330	9.101106644
3.421859980	3.589366913	9.152189255
4.873752117	3.578702927	9.046745300
3.412263870	1.078774214	9.027845383
0.655284643	5.972425938	9.254484177
4.836376190	1.076281190	8.965278625
6.920766354	4.677190781	8.831988335
7.586258888	3.433228493	8.782938004
9.773457527	4.678934574	8.715366364
9.052951813	3.438747644	8.743103981
7.644476414	5.912405968	8.803152084
13.923610687	2.296494961	8.979840279
11.029153824	2.296250105	8.833301544
11.743828773	3.529793739	8.810550690
13.206511497	3.531912088	8.893331528
11.758758545	1.029201865	8.927927971
9.054451942	5.954715729	8.727516174

13.189751625	1.025512695	8.989613533
-5.667654037	11.925671577	8.931132317
-4.950371742	10.690052986	8.871767998
-2.770942211	11.929620743	8.920601845
-3.483512163	10.692257881	8.886834145
-4.932055950	13.201336861	8.956098557
1.353227615	9.550105095	9.226404190
-1.509089947	9.545263290	8.956476212
-0.794990063	10.784441948	8.987598419
0.669706345	10.787570000	9.077418327
-0.789144039	8.271802902	9.037116051
-3.501071930	13.198786736	8.929457664
0.616605759	8.298866272	9.230130196
2.675670147	11.899429321	9.109565735
3.377985477	10.656678200	9.228006363
5.559819698	11.871560097	9.122112274
4.846135139	10.632526398	9.188783646
3.417583942	13.157212257	9.054324150
9.720804214	9.525348663	8.860931396
6.839843273	9.485819817	9.054882050
7.542745113	10.735691071	9.031608582
9.004970551	10.755692482	8.954604149
7.580837250	8.241757393	8.947817802
4.843850613	13.148220062	9.085121155
9.001837730	8.243846893	8.834039688
5.441977024	6.934892654	11.607677460
6.919120789	2.275167465	8.835371971
5.562137604	4.758870125	9.018270493
-1.463827372	7.115283966	8.990621567
2.763732195	4.759100437	9.259037971
1.362927675	2.321684599	9.098928452
1.297245979	7.145964146	9.402534485
15.260938644	2.285370111	9.059165955
13.833455086	4.710623741	8.908289909
6.911854267	7.055566788	8.950626373
11.108564377	4.703590870	8.742239952
9.691742897	2.267486572	8.792172432
9.724193573	7.114058971	8.736246109
2.696805000	9.508127213	9.329022408
1.334489346	11.944059372	9.045215607
-5.613994598	14.348994255	9.013535500
-1.432932854	11.956769943	8.963711739
-2.845044613	9.518733978	8.897472382
-2.799590111	14.338719368	8.924021721

11.057899475	9.512955666	8.825076103
9.635149002	11.936840057	8.977121353
2.734680176	14.305186272	8.968283653
6.896107197	11.898753166	9.064943314
5.495726109	9.455817223	9.158885956
5.550881386	14.285054207	9.059147835
3.044434071	7.430918694	10.656827927
5.289844513	6.494866371	9.801395416
6.629022121	6.734989166	12.230135918
4.489164829	7.381907940	12.315941811
6.510482788	6.978686333	13.180572510

C<sub>2</sub>N-AgCo\*CO

C	N	Ag	Co	O
49	24	1	1	1

Cartesian

-1.531915188	4.746289730	8.933021545
-0.805896521	3.515685558	8.985294342
1.338479757	4.791437626	9.185165405
0.655029774	3.544131994	9.058446884
-0.834089279	6.029909611	9.025308609
5.527460575	2.451062441	8.969561577
2.656399012	2.435254335	9.028007507
3.365698814	3.685168028	9.090126038
4.823804855	3.697517872	9.035118103
3.374006987	1.169877768	8.972352028
0.570254803	6.021220207	9.252791405
4.797445297	1.176275969	8.953506470
6.885271072	4.778324127	8.950086594
7.543624878	3.523092747	8.900712013
9.742365837	4.735438347	8.794026375
9.011068344	3.505382061	8.846712112
7.635464191	5.985424042	8.927082062
13.877285004	2.328860998	8.913906097
10.975040436	2.333141088	8.857332230
11.697427750	3.561799288	8.808389664
13.157981873	3.562419176	8.844264030
11.706859589	1.060126901	8.918010712
9.041204453	6.021695614	8.814258575
13.143101692	1.056019902	8.938890457
-5.692458153	12.015579224	8.863811493
-4.969708920	10.784211159	8.807273865
-2.790213585	12.021847725	8.883197784
-3.506660223	10.786934853	8.830169678

-4.958066463	13.291547775	8.894627571
1.307592869	9.584215164	9.230706215
-1.550532341	9.613497734	8.933238029
-0.828278542	10.848064423	8.982162476
0.633364201	10.829359055	9.080675125
-0.848773479	8.332053185	9.032382011
-3.521924019	13.293665886	8.892864227
0.549171925	8.351277351	9.271530151
2.646475315	11.923798561	9.078246117
3.344731331	10.670526505	9.160056114
5.518511772	11.893737793	9.051480293
4.810925961	10.643564224	9.100961685
3.377207279	13.183886528	9.023741722
9.714944839	9.603194237	8.816705704
6.844225407	9.545782089	8.995697975
7.523158073	10.801950455	8.968157768
8.986613274	10.831002235	8.894592285
7.603840351	8.330598831	8.944883347
4.800329208	13.173683167	9.027000427
9.014450073	8.317110062	8.827055931
4.954906940	7.054456711	11.271383286
6.870331287	2.376041412	8.913545609
5.514761925	4.882022381	9.031913757
-1.534197807	7.177422047	8.960273743
2.690566063	4.844641685	9.182232857
1.319596171	2.391806364	8.999279976
1.205493927	7.190031528	9.494729996
15.216217995	2.328846693	8.972153664
13.774224281	4.746635437	8.847990036
6.925396442	7.150071144	9.052794456
11.075342178	4.743320942	8.767979622
9.635866165	2.323457003	8.868995667
9.728900909	7.173603535	8.780255318
2.658158302	9.522726059	9.266147614
1.306683540	11.977722168	9.031067848
2.674339056	0.024642050	8.937917709
-1.451055050	12.030032158	8.948304176
-2.884074688	9.605557442	8.844623566
5.491055489	0.030017188	8.917181969
11.050251007	9.601536751	8.773830414
9.608432770	12.016976357	8.907624245
2.688861847	14.333502769	8.965295792
6.855763435	11.951164246	8.993070602
5.486366272	9.465746880	9.058427811

5.505071640	14.313529968	8.988821983
2.929791451	7.254965782	10.763837814
5.078618526	6.926332951	9.525258064
5.507169247	7.007262707	12.473801613

C<sub>2</sub>N-AgCo\*CHO

C	N	Ag	Co	O	H
49	24	1	1	1	1

Cartesian

-1.477935076	4.701357365	9.009107590
-0.753771663	3.472266674	9.065987587
1.403975010	4.739848137	9.253026009
0.707645655	3.497268915	9.145026207
-0.771639347	5.979991436	9.077633858
5.573704243	2.368461132	9.021492004
2.696310759	2.369412422	9.120599747
3.417174816	3.610449791	9.179280281
4.867645264	3.607524157	9.099827766
3.410482883	1.098170757	9.053135872
0.639768124	5.978117943	9.277488708
4.834578514	1.099510908	9.018323898
6.924833775	4.699195862	8.939321518
7.585975647	3.450146437	8.912322044
9.776777267	4.684021473	8.813987732
9.052700996	3.448748589	8.864658356
7.651698112	5.921196461	8.869823456
13.924118042	2.292560816	8.982071877
11.025094032	2.296538115	8.901918411
11.742647171	3.527113199	8.866169930
13.204339981	3.528150797	8.916299820
11.756088257	1.025844216	8.963208199
9.061515808	5.964730740	8.804051399
13.189660072	1.020339370	8.994329453
-5.667995453	11.944592476	8.924435616
-4.949040413	10.709391594	8.874072075
-2.769304276	11.949031830	8.938008308
-3.483288288	10.712244987	8.896986008
-4.932913780	13.219855309	8.961948395
1.345565319	9.551272392	9.254267693
-1.514323235	9.556692123	8.973629951
-0.797310829	10.794198036	9.008711815
0.666544437	10.791056633	9.099989891
-0.799427509	8.280535698	9.058391571
-3.499541283	13.220085144	8.954225540

0.603302002	8.308650970	9.267155647
2.676469803	11.894068718	9.117414474
3.376155853	10.647570610	9.228258133
5.554362297	11.859915733	9.099450111
4.841726303	10.618403435	9.168246269
3.415462017	13.151635170	9.063179970
9.726919174	9.536776543	8.857511520
6.847913742	9.489942551	9.018090248
7.543867588	10.740980148	8.999298096
9.007330894	10.766674042	8.932968140
7.593840599	8.256355286	8.917920113
4.840215206	13.140453339	9.074357986
9.013675690	8.255273819	8.837369919
5.520403385	6.813296318	11.251205444
6.916982174	2.296999454	8.952281952
5.558450699	4.790155411	9.073512077
-1.474934340	7.123800755	8.998794556
2.755312681	4.782012939	9.270648003
1.361837506	2.335187435	9.102977753
1.280298233	7.152607441	9.448001862
15.262779236	2.287488461	9.047790527
13.827073097	4.709629059	8.926074028
6.913185120	7.075280190	8.918622017
11.110302925	4.704671860	8.812115669
9.686817169	2.273250818	8.898570061
9.737504959	7.118785858	8.774873734
2.692004204	9.500937462	9.341729164
1.334780693	11.943929672	9.060750008
-5.615392685	14.368996620	9.017117500
-1.430686951	11.969537735	8.984069824
-2.849554539	9.536026955	8.908326149
-2.798625469	14.361084938	8.975250244
11.064846039	9.529196739	8.831753731
9.632261276	11.950399399	8.955827713
2.732133865	14.302419662	9.001638412
6.890033245	11.898954391	9.037998199
5.499762535	9.439231873	9.127313614
5.549126625	14.276191711	9.043902397
2.993002892	7.361718655	10.704545975
5.160616875	6.668917179	9.495306015
4.635723114	7.164265633	12.080087662
6.532915115	6.581200123	11.665872574

C<sub>2</sub>N-AgCo\*COOH



C	N	Ag	Co	O	H
49	24	1	1	2	1
Cartesian					
-1.507138610			4.745079041		8.823293686
-0.788541317			3.514590502		8.908074379
1.375637054			4.775125027		9.062154770
0.669764519			3.532474041		8.999892235
-0.791649818			6.019635201		8.809829712
5.538153172			2.379427671		9.035172462
2.650684357			2.389587164		9.077327728
3.372422457			3.627554893		9.169614792
4.827501297			3.610017300		9.191898346
3.366911888			1.116169572		9.022734642
0.628277302			6.029578209		8.963964462
4.791172981			1.113935947		8.965403557
6.888816833			4.710883141		9.142560959
7.552453995			3.472208977		8.998685837
9.730526924			4.727440834		8.920494080
9.013439178			3.485538721		8.919504166
7.606986523			5.953908443		9.147707939
13.884264946			2.347090483		8.851931572
10.989341736			2.348574638		8.828244209
11.702293396			3.583285570		8.826264381
13.165510178			3.584020376		8.809955597
11.719139099			1.080186367		8.815985680
9.011387825			5.999244213		9.005561829
13.149732590			1.076007366		8.856395721
-5.713189602			11.964277267		8.928773880
-4.999841690			10.727519989		8.835534096
-2.822584152			11.969493866		8.730144501
-3.537666559			10.731698990		8.731962204
-4.976825714			13.239423752		8.923698425
1.302899837			9.598251343		8.852742195
-1.559176683			9.587602615		8.658018112
-0.842555046			10.828034401		8.659440041
0.623829365			10.836248398		8.714375496
-0.832424641			8.313593864		8.707229614
-3.549353123			13.239151001		8.828639984
0.579806328			8.344676971		8.845361710
2.629968643			11.949334145		8.826984406
3.331959724			10.715991974		8.987489700
5.515099049			11.928553581		9.022158623
4.791680336			10.696148872		9.089567184
3.375924587			13.206481934		8.838215828

9.671150208	9.568984032	8.983133316
6.785155296	9.541055679	9.195011139
7.496302128	10.785349846	9.099845886
8.957212448	10.801489830	9.040662766
7.528571129	8.290320396	9.211571693
4.800961018	13.199680328	8.924094200
8.949272156	8.289902687	9.053442001
3.907223225	7.157492638	12.030407906
6.878336430	2.316554308	8.967257500
5.530464172	4.774447441	9.320075989
-1.502640009	7.156425953	8.699148178
2.715235710	4.802778721	9.172836304
1.318631768	2.365319967	9.014507294
1.283774376	7.203188419	9.010296822
15.220552444	2.333270788	8.907137871
13.795515060	4.760627747	8.780147552
6.872699738	7.097760677	9.334170341
11.064483643	4.757284641	8.866260529
9.653728485	2.315084457	8.867214203
9.674506187	7.161296844	8.981333733
2.642175674	9.561129570	9.033209801
1.290152073	11.996095657	8.712809563
-5.657773972	14.386921883	9.010332108
-1.485964775	11.999078751	8.679132462
-2.894964457	9.559286118	8.679528236
-2.847179890	14.378578186	8.857403755
11.003860474	9.550004959	8.870111465
9.592683792	11.981282234	9.021924019
2.694419861	14.356819153	8.790750504
6.850555420	11.950731277	9.035063744
5.438368320	9.522307396	9.202230453
5.508823395	14.336024284	8.917200089
3.184542179	7.685106277	10.166255951
5.378734589	6.409642220	10.308221817
4.995329857	6.530128956	12.224951744
3.181885242	7.477824211	13.112261772
3.659126759	7.143687248	13.913333893

C<sub>2</sub>N-AgFe\*CO

C	N	Ag	Fe	O
49	24	1	1	1

Cartesian

-1.505807996	4.767069340	9.005543709
-0.781694770	3.539218187	9.066761971

1.386784077	4.811526299	9.212526321
0.682584763	3.565949678	9.134963989
-0.798680544	6.043772697	9.065429688
5.544741631	2.404675007	8.918352127
2.662714005	2.422875643	9.079919815
3.390142918	3.660180330	9.113021851
4.839190006	3.639775038	9.022158623
3.372135639	1.149976730	9.000198364
0.619474411	6.052318096	9.242730141
4.795964718	1.143737078	8.924741745
6.896421432	4.740193844	8.893692017
7.556297302	3.494631767	8.821224213
9.742306709	4.740842342	8.762328148
9.023056030	3.501563311	8.778743744
7.614215851	5.971647739	8.870130539
13.896936417	2.357970476	8.966556549
10.999434471	2.359368324	8.828747749
11.713551521	3.592205763	8.817947388
13.176490784	3.594194412	8.891280174
11.730353355	1.090216160	8.900261879
9.021836281	6.018698692	8.783946037
13.162519455	1.085215688	8.964845657
-5.716775894	11.996686935	8.897274017
-4.995841026	10.761169434	8.836739540
-2.818516731	11.999194145	8.855622292
-3.532259703	10.763575554	8.839008331
-4.980728626	13.272092819	8.917253494
1.289254665	9.625285149	9.206261635
-1.560841322	9.615357399	8.917811394
-0.843487740	10.855183601	8.927802086
0.618196964	10.861048698	9.025415421
-0.843623877	8.342990875	9.019889832
-3.548671722	13.267597198	8.872812271
0.558022976	8.377965927	9.218646049
2.632796764	11.963686943	9.057275772
3.332833290	10.722836494	9.200537682
5.514708519	11.923409462	9.086363792
4.794068813	10.684980392	9.154205322
3.379335880	13.217174530	9.002843857
9.680518150	9.590513229	8.853750229
6.800314426	9.543909073	9.034938812
7.500519753	10.794240952	9.007920265
8.959756851	10.819070816	8.935452461
7.548837662	8.306892395	8.949510574

4.803997040	13.205199242	9.045180321
8.968406677	8.309069633	8.845002174
4.989189625	6.866254807	11.311074257
6.886713505	2.338040829	8.834400177
5.533124924	4.814855099	9.032615662
-1.510869503	7.182264328	8.978597641
2.741533041	4.841413498	9.192438126
1.328598142	2.400135756	9.087354660
1.253365040	7.231505394	9.392220497
15.235036850	2.354238033	9.046907425
13.798633575	4.774303913	8.910449982
6.877216816	7.121725559	8.982162476
11.076405525	4.767184734	8.772822380
9.662331581	2.329639196	8.800109863
9.693082809	7.176038742	8.772678375
2.634853363	9.581016541	9.334061623
1.290766239	12.015435219	8.983566284
2.662192345	0.011672550	8.985834122
-1.480574131	12.028101921	8.886653900
-2.895131588	9.588164330	8.860068321
-2.844127655	14.404387474	8.866673470
11.016557693	9.581217766	8.806409836
9.586843491	12.003993034	8.948393822
2.702172279	14.369961739	8.921429634
6.847975254	11.955948830	9.028638840
5.452063084	9.501556396	9.119771957
5.516528130	14.338907242	9.029501915
3.085770130	7.661357403	10.592531204
5.043905258	6.676150799	9.489636421
5.459046364	6.758839130	12.391830444

C<sub>2</sub>N-AgFe\*CHO

C	N	Ag	Fe	O	H
49	24	1	1	1	1

Cartesian

-1.519237041	4.801309109	8.976059914
-0.815889716	3.563514233	8.892738342
1.364247084	4.772603035	9.006480217
0.652076483	3.541811943	8.884457588
-0.770401478	6.051511288	9.067535400
5.522820473	2.351831675	8.736515999
2.606423855	2.352091074	8.769348145
3.349512100	3.548642635	8.852489471
4.780562401	3.548282146	8.828370094

3.347610474	1.089423656	8.725139618
0.662704706	6.035659313	9.116711617
4.782122135	1.088948131	8.714141846
6.767363071	4.772905827	8.931456566
7.478572369	3.542503834	8.813754082
9.648906708	4.801539898	8.904077530
8.945871353	3.563571930	8.824248314
7.467220306	6.036523819	9.033929825
13.830848694	2.444044590	8.838576317
10.938738823	2.444059134	8.809218407
11.648321152	3.686911821	8.867609978
13.121403694	3.686724424	8.887914658
11.671013832	1.177832365	8.813555717
8.899734497	6.053024292	8.983854294
13.098187447	1.178797841	8.823348045
-5.702648163	11.948123932	8.867358208
-4.991737843	10.705990791	8.943462372
-2.807350636	11.947200775	8.873981476
-3.519354343	10.705861092	8.953037262
-4.968347549	13.215402603	8.788067818
1.364457130	9.627202988	9.249300003
-1.517752171	9.592977524	9.070451736
-0.815449238	10.831291199	9.006749153
0.646101475	10.851912498	9.067500114
-0.762680054	8.338019371	9.139266014
-3.540841103	13.214898109	8.785871506
0.668927670	8.346637726	9.230832100
2.608726025	12.046965599	9.006389618
3.342821121	10.852027893	9.199151993
5.520195961	12.047253609	8.995284081
4.787532806	10.849563599	9.183635712
3.347144604	13.305957794	8.899109840
9.644784927	9.593409538	9.026063919
6.761733055	9.626640320	9.198036194
7.482115269	10.852892876	9.034541130
8.943267822	10.832760811	8.977536201
7.458242416	8.345268250	9.163601875
4.780907154	13.306894302	8.899973869
8.889518738	8.338034630	9.072018623
4.206536293	6.864770889	11.980691910
6.864407539	2.352609873	8.726165771
5.404518127	4.761853218	8.948466301
-1.453562737	7.197366714	9.084311485
2.728689671	4.761405945	9.009305954

1.264744639	2.352047682	8.783027649
1.366773605	7.182898521	9.229320526
15.168219566	2.400942802	8.830349922
13.779296875	4.847884178	8.962577820
6.760896206	7.181947231	9.156401634
10.989835739	4.849137783	8.915904045
9.601926804	2.400798559	8.778059959
9.582280159	7.198462009	9.006174088
2.708140373	9.671702385	9.386622429
1.269866467	12.039413452	8.975267410
-5.663780212	14.356286049	8.748900414
-1.472869396	11.993084908	8.901665688
-2.856900692	9.544370651	9.044028282
-2.846306324	14.356083870	8.735777855
10.983926773	9.543952942	9.012725830
9.602375031	11.994698524	8.888363838
10.973917007	0.035810232	8.841959953
6.857816219	12.040725708	8.953703880
5.420251846	9.664698601	9.334061623
13.794418335	0.036300190	8.852561951
4.036365986	8.377807617	10.625021935
4.080427170	6.090232372	9.554597855
4.225111008	5.670986176	11.595563889
4.306511402	7.010187626	13.086108208

C<sub>2</sub>N-AgFe\*COOH

C	N	Ag	Fe	O	H
49	24	1	1	2	1

Cartesian

-1.481856108	4.807606220	9.020682335
-0.756744742	3.587421417	9.010223389
1.450538635	4.843272686	9.087677956
0.716769695	3.606429100	9.025289536
-0.750767231	6.067881584	9.075635910
5.546108246	2.330028296	8.714573860
2.647489548	2.396590710	8.908433914
3.405561209	3.602898359	8.917451859
4.821912289	3.543209791	8.796006203
3.348774433	1.110578299	8.843292236
0.689026594	6.086903572	9.144180298
4.776713848	1.083356738	8.749601364
6.853457451	4.707539558	8.800127983
7.537154198	3.472050428	8.716841698
9.692296028	4.764979839	8.848728180

9.001075745	3.514532804	8.749998093
7.509286880	5.960407734	8.927477837
13.902783394	2.423120499	8.925264359
11.003642082	2.421189547	8.782559395
11.702309608	3.663437128	8.855567932
13.175974846	3.663854837	8.914949417
11.736566544	1.157816052	8.813250542
8.931250572	6.017574310	8.923769951
13.164714813	1.147498131	8.893890381
-5.764505863	11.951912880	8.930141449
-5.052148342	10.702893257	8.945963860
-2.873076916	11.945903778	8.834615707
-3.579256773	10.704852104	8.915831566
-5.026220322	13.228688240	8.868096352
1.286607265	9.669814110	9.185850143
-1.571033001	9.604361534	8.976311684
-0.870385647	10.850356102	8.899991989
0.594733715	10.890590668	8.963153839
-0.816143990	8.355571747	9.062603951
-3.600053310	13.212203026	8.799066544
0.602068901	8.392030716	9.172620773
2.591553211	12.039443016	8.956259727
3.301455498	10.828308105	9.182070732
5.490870953	11.988443375	9.050742149
4.750853062	10.778188705	9.167634010
3.360364914	13.286489487	8.884457588
9.593576431	9.563449860	9.029303551
6.706324100	9.553838730	9.148823738
7.440425873	10.792325020	9.076319695
8.897035599	10.800351143	9.030617714
7.405837536	8.276342392	9.100782394
4.789119720	13.267971992	8.958600044
8.843160629	8.294081688	9.045486450
4.205638885	6.835431099	11.990807533
6.890118122	2.295169353	8.660952568
5.486411095	4.739156246	8.810837746
-1.471208811	7.193144321	9.038124084
2.827535152	4.842724800	9.049464226
1.318231702	2.409617901	8.966159821
1.337602139	7.262847900	9.217223167
15.242806435	2.407355309	8.968319893
13.817635536	4.834337711	8.967167854
6.716329098	7.079387188	9.061650276
11.031210899	4.822463989	8.887248039

9.669893265	2.361414433	8.717958450
9.583105087	7.175794125	8.989937782
2.619517326	9.684412003	9.389754295
1.248218536	12.063854218	8.887193680
-5.692184448	14.390525818	8.888580322
-1.537364483	12.002941132	8.819747925
-2.909831524	9.546935081	8.977157593
-2.880450249	14.336832047	8.728487968
10.935523987	9.532107353	8.991917610
9.540267944	11.977218628	8.976635933
11.017588615	0.030752126	8.800020218
6.824646473	11.976901054	9.027954102
5.362580776	9.576592445	9.218699455
5.510319710	14.397672653	8.956602097
3.425744057	8.259957314	10.747187614
4.621933937	6.303148270	9.411785126
4.778374672	5.827369213	11.499713898
4.120756626	6.931491852	13.326516151
4.554622173	6.134271145	13.721615791

C<sub>2</sub>N-AgMn\*CO

C	N	Ag	Mn	O
49	24	1	1	1

Cartesian

-1.508902431	4.756261349	8.965025902
-0.781627893	3.530658245	9.016883850
1.384563446	4.799406528	9.179333687
0.680854559	3.557533979	9.084185600
-0.800086260	6.034535408	9.035964012
5.544434071	2.399732351	8.950446129
2.661224842	2.416549444	9.044748306
3.388046503	3.651332140	9.090791702
4.834173203	3.633247137	9.020286560
3.374648571	1.142108560	8.983440399
0.618335009	6.038123608	9.218394279
4.799234867	1.136805534	8.951490402
6.889465332	4.740481853	8.918208122
7.555390358	3.494530916	8.872451782
9.739460945	4.736922264	8.789633751
9.018447876	3.498133659	8.830781937
7.611844063	5.971316814	8.881595612
13.895471573	2.349324226	8.934173584
10.993917465	2.352062225	8.860409737
11.709715843	3.584582567	8.824535370



13.172198296	3.584568024	8.869985580
11.725094795	1.083558440	8.921015739
9.020930290	6.011939526	8.796797752
13.158400536	1.074364543	8.947314262
-5.710960388	11.989755630	8.875512123
-4.989992142	10.755419731	8.828495979
-2.811569214	11.992522240	8.895708084
-3.526293993	10.756528854	8.852364540
-4.974638939	13.264887810	8.909207344
1.300652981	9.611797333	9.214325905
-1.556398153	9.606047630	8.936982155
-0.838020802	10.845168114	8.974205971
0.621824741	10.848856926	9.066473961
-0.840312719	8.333394051	9.021563530
-3.542739391	13.261414528	8.904780388
0.563340664	8.361407280	9.220319748
2.633455276	11.953700066	9.083789825
3.339838505	10.709693909	9.189539909
5.514584064	11.912903786	9.050166130
4.798686028	10.674244881	9.122220039
3.377954483	13.210891724	9.023435593
9.687091827	9.585295677	8.822231293
6.807943821	9.540147781	8.987075806
7.502284050	10.789832115	8.954423904
8.964491844	10.813811302	8.888436317
7.556642056	8.308794975	8.912879944
4.802508831	13.194030762	9.027071953
8.974480629	8.304745674	8.818254471
4.971646786	7.073219299	11.421287537
6.886248112	2.335273743	8.890487671
5.523423672	4.813529015	9.020969391
-1.508173227	7.172349930	8.965025902
2.738712549	4.836528301	9.171720505
1.328448534	2.389126062	9.034020424
1.254130840	7.214731216	9.385182381
15.232768059	2.344366789	8.997444153
13.797262192	4.765556335	8.880479813
6.881093979	7.125529766	8.964593887
11.074050903	4.760138035	8.779985428
9.656757355	2.324509144	8.856900215
9.696045876	7.169698238	8.766683578
2.645869255	9.561706543	9.306593895
1.295052528	12.004929543	9.033534050
2.665462494	0.005058105	8.952965736

-1.475806713	12.019124031	8.947673798
-2.890280724	9.581521034	8.866007805
-2.837804794	14.397961617	8.918153763
11.023121834	9.575325012	8.791343689
9.590952873	11.998056412	8.904257774
2.697971344	14.360955238	8.961803436
6.850413322	11.951322556	8.979156494
5.455382347	9.488054276	9.080927849
5.514414787	14.330202103	8.992223740
3.012913704	7.635836601	10.708182335
5.000291824	6.728806973	9.509561539
5.504464149	7.074516296	12.477869987

C<sub>2</sub>N-AgMn\*CHO

C	N	Ag	Mn	O	H
49	24	1	1	1	1

Cartesian

-1.494641900	4.731475353	8.920224190
-0.772558570	3.501491308	8.971829414
1.399506807	4.759748936	9.068759918
0.685872078	3.519792557	9.044370651
-0.778013229	6.003884315	8.888256073
5.550600529	2.341816187	9.137555122
2.661633492	2.367942572	9.127764702
3.391075850	3.600866556	9.225702286
4.839291573	3.565387726	9.304074287
3.374874115	1.091167212	9.074897766
0.649900913	6.013453007	8.945837975
4.801058292	1.084048510	9.044154167
6.906564713	4.674121380	9.328284264
7.572105885	3.436326742	9.144215584
9.740061760	4.705161572	9.056195259
9.026950836	3.458792686	9.040805817
7.613725185	5.918372154	9.329112053
13.899506569	2.333948135	8.906543732
11.005374908	2.335129738	8.895077705
11.716555595	3.571958780	8.925714493
13.178056717	3.572031021	8.905464172
11.735287666	1.071929216	8.833643913
9.017210960	5.971835613	9.160398483
13.165132523	1.063570976	8.868869781
-5.714686394	11.938742638	8.969202042
-4.998950958	10.698656082	8.923049927
-2.822866440	11.942257881	8.823654175

-3.534746408	10.703209877	8.843274117
-4.977765560	13.214652061	8.973432541
1.313524246	9.585930824	8.742996216
-1.552179098	9.568046570	8.755488396
-0.841140270	10.810914993	8.717561722
0.624296188	10.825613022	8.693225861
-0.820543528	8.296675682	8.777735710
-3.549185753	13.211453438	8.910665512
0.598717213	8.325757027	8.792406082
2.631282806	11.949650764	8.731224060
3.340286732	10.715141296	8.798058510
5.520565510	11.911621094	8.913743973
4.795998573	10.683337212	8.919269562
3.382406235	13.201942444	8.772390366
9.668338776	9.541055679	9.036828041
6.779857159	9.512854576	9.135953903
7.493731976	10.759309769	9.048779488
8.954982758	10.774484634	9.037044525
7.522690296	8.273705482	9.266615868
4.809504986	13.186148643	8.849718094
8.943889618	8.266283989	9.134081841
4.304630280	7.385337353	11.699316025
6.895500660	2.284231663	9.083771706
5.547279835	4.715868473	9.496997833
-1.490692377	7.141266346	8.815770149
2.739596128	4.783641815	9.179045677
1.332218766	2.348128080	9.061056137
1.307395458	7.181702137	8.888256073
15.236495018	2.319523096	8.951273918
13.808428764	4.749502659	8.899884224
6.877850533	7.078003883	9.492929459
11.073711395	4.741879940	8.992547989
9.672141075	2.293742657	8.948267937
9.674241066	7.135415554	9.109277725
2.657659054	9.561576843	8.792280197
1.287481785	11.989020348	8.677512169
-5.654961586	14.366143227	9.044442177
-1.488543034	11.978961945	8.749205589
-2.886876822	9.533028603	8.807076454
-2.841056347	14.345520973	8.950265884
11.004843712	9.521385193	8.965169907
9.589481354	11.954895973	9.014165878
2.704960823	14.353086472	8.770157814
6.857395172	11.926233292	8.958744049

5.432461739	9.502334595	9.042101860
5.521786690	14.319567680	8.881757736
3.509109020	7.586638451	9.411875725
5.372321129	6.417582512	10.523754120
4.221562862	6.158481121	12.082932472
3.924309731	8.216625214	12.314321518

C<sub>2</sub>N-AgMn\*COOH

C	N	Ag	Mn	O	H
49	24	1	1	2	1

Cartesian

-1.501332641	4.793613911	9.018936157
-0.780880213	3.566338778	9.004571915
1.413232565	4.814595699	9.057329178
0.687809229	3.578631163	9.006408691
-0.769486427	6.054565907	9.067176819
5.534202099	2.345980883	8.719200134
2.637040138	2.389183760	8.888472557
3.382723331	3.603230000	8.889552116
4.812560081	3.561943531	8.782020569
3.351270676	1.109511971	8.833896637
0.666447878	6.067651272	9.124595642
4.779001713	1.092392206	8.752391815
6.833740234	4.726244450	8.783964157
7.524199486	3.492873907	8.718875885
9.687163353	4.764706135	8.835731506
8.987730026	3.519749403	8.749782562
7.513320923	5.983536720	8.897364616
13.878963470	2.409877300	8.927441597
10.981711388	2.408565760	8.788517952
11.686477661	3.648896933	8.857656479
13.156697273	3.650496244	8.919774055
11.714984894	1.143780231	8.817984581
8.936874390	6.023396015	8.898156166
13.143465042	1.138015985	8.895689964
-5.741293907	11.957850456	8.932445526
-5.027097225	10.712706566	8.946882248
-2.848575115	11.953095436	8.834795952
-3.558474064	10.713931084	8.915741920
-5.004172802	13.230301857	8.866638184
1.296833515	9.647492409	9.189431190
-1.560366154	9.598942757	8.974169731
-0.854835510	10.840571404	8.898461342
0.608154297	10.868959427	8.964269638

-0.813006878	8.343711853	9.058284760
-3.577273846	13.220301628	8.801010132
0.608525276	8.373440742	9.167327881
2.602768421	12.019037247	8.960778236
3.316131592	10.811677933	9.189377785
5.500089645	11.985043526	9.052289963
4.763749123	10.768907547	9.168695450
3.359459400	13.271084785	8.887536049
9.623386383	9.573321342	9.022392273
6.733097553	9.567383766	9.134567261
7.461209297	10.804803848	9.072108269
8.919149399	10.810034752	9.028997421
7.447061062	8.295840263	9.071387291
4.787347317	13.259974480	8.960490227
8.880059242	8.306373596	9.023544312
4.188614845	6.890421391	12.085721970
6.878394604	2.314090252	8.671751976
5.474238396	4.749632359	8.784755707
-1.479960918	7.189195633	9.032219887
2.775561571	4.819221497	9.014058113
1.306351423	2.388664961	8.950697899
1.332852840	7.232945919	9.199908257
15.218404770	2.388952971	8.966628075
13.798383713	4.821368217	8.972820282
6.762444496	7.117013454	9.025775909
11.024307251	4.812491417	8.879418373
9.647004128	2.359094620	8.726759911
9.602239609	7.175822735	8.966753960
2.632371902	9.664280891	9.407358170
1.260332108	12.042555809	8.891819954
-5.679538727	14.386461258	8.880929947
-1.513137341	12.000404358	8.818470001
-2.897609711	9.550494194	8.975664139
-2.866473675	14.350867271	8.735903740
10.963086128	9.541112900	8.989146233
9.563323975	11.985475540	8.980830193
11.005665779	0.011197002	8.804699898
6.833348751	11.986584663	9.027773857
5.389929295	9.571304321	9.208044052
5.498847961	14.393536568	8.956241608
3.380939484	8.334100723	10.880154610
4.536703110	6.404194832	9.448668480
4.773381233	5.924237251	11.516652107
4.135375977	6.888937473	13.423086166

4.595640182

6.073256969

13.746456146

C<sub>2</sub>N-AgCr\*CO

C	N	Ag	Cr	O
49	24	1	1	1

Cartesian

-1.520675302	4.760282040	9.019691467
-0.780613184	3.542791843	9.051713943
1.384978294	4.829006195	9.107351303
0.685437918	3.585447073	9.076769829
-0.817757845	6.046294212	9.054396629
5.542195320	2.444246531	8.969759941
2.666873217	2.456798077	9.038591385
3.397280693	3.696062326	9.040607452
4.830926895	3.686796665	8.994564056
3.373790264	1.175728440	9.001800537
0.609241009	6.054652691	9.147203445
4.794042110	1.174388289	8.977319717
6.907610893	4.760584831	8.926019669
7.556496620	3.509445906	8.921844482
9.748688698	4.739790440	8.864315987
9.020269394	3.502759218	8.902529716
7.633508682	5.968434334	8.876735687
13.902619362	2.341239929	9.009341240
10.991271973	2.345174074	8.945531845
11.709299088	3.574495077	8.921772003
13.170619011	3.571685076	8.964557648
11.726668358	1.075877666	8.988497734
9.039299965	6.018251419	8.838899612
13.162619591	1.058815598	9.010656357
-5.726934910	12.013157845	8.921411514
-5.001432419	10.780998230	8.886077881
-2.819815159	12.018158913	8.949186325
-3.538500547	10.784269333	8.916552544
-4.987010956	13.293752670	8.952768326
1.290827274	9.613339424	9.141965866
-1.574577570	9.621423721	8.979911804
-0.849552631	10.858742714	9.000701904
0.612198353	10.852935791	9.057131767
-0.861053944	8.343294144	9.038304329
-3.552091122	13.292484283	8.952965736
0.550727367	8.366048813	9.152351379
2.629036427	11.942387581	9.065340042
3.334780216	10.691364288	9.112554550

5.500182629	11.878592491	9.029339790
4.784435749	10.635667801	9.054216385
3.376091003	13.200545311	9.034703255
9.685693741	9.591896057	8.851409912
6.808509827	9.516659737	8.942328453
7.491261482	10.774801254	8.947278023
8.955747604	10.815093040	8.907192230
7.560659885	8.309126854	8.875043869
4.796386242	13.170598984	9.034955978
8.982967377	8.302151680	8.832077980
5.072988510	6.831785202	11.118707657
6.879225731	2.354151487	8.947764397
5.529029846	4.887743473	8.989199638
-1.530354023	7.179872513	9.015965462
2.743428946	4.888709068	9.070253372
1.337816238	2.417860746	9.046673775
1.258141041	7.227498531	9.251405716
15.241327286	2.349194527	9.047879219
13.787071228	4.758394718	8.971325874
6.870353222	7.115514278	8.891712189
11.083053589	4.754258156	8.871822357
9.653437614	2.324869394	8.934011459
9.716238022	7.178359032	8.808947563
2.635170460	9.541675568	9.187416077
1.294552326	12.007004738	9.040391922
2.660086870	0.039211124	8.983421326
-1.483453274	12.036632538	8.984718323
-2.907661438	9.605687141	8.932104111
5.472927094	0.019627178	8.959644318
11.021331787	9.595312119	8.841294289
9.573505402	12.006860733	8.931978226
2.699419975	14.351904869	9.005112648
6.837027550	11.931392670	8.986248016
5.442005634	9.431536674	9.005435944
5.512052536	14.309509277	9.028530121
3.064795971	7.633472919	10.612331390
5.005506992	6.794014931	9.210078239
5.592880726	6.672144890	12.171761513

C<sub>2</sub>N-AgCr\*CHO

C	N	Ag	Cr	O	H
49	24	1	1	1	1

Cartesian

-1.486474156	4.818746090	9.027647972
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-0.762219429	3.597105265	9.017568588
1.444614410	4.850362778	9.095022202
0.710795879	3.615161896	9.035496712
-0.753546000	6.075893879	9.075689316
5.539643764	2.329379797	8.717129707
2.638005018	2.398896217	8.919648170
3.400502443	3.599929810	8.924112320
4.811246395	3.535658598	8.800866127
3.341220140	1.112739801	8.851302147
0.686314821	6.094800472	9.146933556
4.769634247	1.084206939	8.755362511
6.846102715	4.712928772	8.805545807
7.528475761	3.480019569	8.722025871
9.681962013	4.774779320	8.862731934
8.991865158	3.524144650	8.764505386
7.496823311	5.967584133	8.929836273
13.895160675	2.436003685	8.938241959
10.995870590	2.434274435	8.814131737
11.694055557	3.676982880	8.882532120
13.168119431	3.677948236	8.935056686
11.728255272	1.172039270	8.842949867
8.919178009	6.026234627	8.928018570
13.157351494	1.161923051	8.907281876
-5.772193909	11.956150055	8.923319817
-5.059743881	10.705904007	8.935416222
-2.881588459	11.949434280	8.840610504
-3.587552071	10.707201004	8.909910202
-5.034016609	13.231758118	8.869950294
1.278561592	9.681472778	9.196109772
-1.576865196	9.611120224	8.974295616
-0.877407551	10.858742714	8.912034035
0.585947990	10.902234077	8.981982231
-0.819663048	8.363944054	9.059723854
-3.608747482	13.214465141	8.805150032
0.598897934	8.403487206	9.176741600
2.581303120	12.055208206	8.977392197
3.293910503	10.845873833	9.190296173
5.483507633	12.003704071	9.042713165
4.739928722	10.795754433	9.165707588
3.350448132	13.301044464	8.905482292
9.582943916	9.570424080	9.013284683
6.694809437	9.565366745	9.137772560
7.431415558	10.802052498	9.059669495
8.886602402	10.808017731	9.013859749



7.394081593	8.285695076	9.091979980
4.780882835	13.282670975	8.960760117
8.830864906	8.304168701	9.035387993
4.276929855	6.855619907	11.951622009
6.884551525	2.298353910	8.667072296
5.478632450	4.729457855	8.827685356
-1.472756624	7.202511311	9.033371925
2.824931145	4.847321987	9.054989815
1.310460448	2.413998604	8.980290413
1.333575249	7.271436691	9.223812103
15.235651016	2.418509245	8.976564407
13.811835289	4.846860886	8.983619690
6.707726002	7.090281963	9.055530548
11.020162582	4.834510803	8.908811569
9.662679672	2.372409821	8.743373871
9.569841385	7.183575630	8.986410141
2.613318443	9.698203087	9.395261765
1.237002850	12.078697205	8.912952423
-5.699481964	14.394200325	8.894322395
-1.547081947	12.010463715	8.836038589
-2.915156126	9.549731255	8.967311859
-2.888595581	14.338171959	8.734968185
10.924548149	9.536416054	8.977463722
9.533130646	11.983587265	8.966267586
11.008193970	0.046675790	8.836596489
6.815510273	11.988458633	9.012546539
5.352663517	9.593423843	9.216107368
13.823131561	0.000432317	8.955827713
3.457876205	8.252867699	10.707029343
4.569327831	6.275321484	9.441828728
4.863245010	5.852977276	11.485224724
4.251728058	6.907627583	13.068395615

C<sub>2</sub>N-AgCr\*COOH

C	N	Ag	Cr	O	H
49	24	1	1	2	1

Cartesian

-1.481631517	4.808110714	9.020700455
-0.756495237	3.587277412	9.010151863
1.449972153	4.843128681	9.087858200
0.716262341	3.607192516	9.025415421
-0.750916958	6.067132473	9.075617790
5.545317650	2.330647945	8.714214325
2.646740437	2.396331310	8.908452034

3.406959057	3.601313114	8.917595863
4.819391727	3.540255785	8.795501709
3.348649979	1.110419750	8.843310356
0.689110041	6.086759567	9.144107819
4.776597977	1.083443284	8.749620438
6.857268333	4.708231449	8.799695969
7.537029266	3.472958326	8.716553688
9.692304611	4.765109539	8.848799706
9.001116753	3.514662504	8.750105858
7.509977341	5.958433628	8.927514076
13.902584076	2.422832251	8.925264359
11.003841400	2.421074390	8.782559395
11.702383995	3.663509130	8.855567932
13.175991058	3.664114237	8.914968491
11.736375809	1.157888055	8.813285828
8.931749344	6.017747402	8.923913956
13.164863586	1.147901654	8.893890381
-5.764672279	11.952115059	8.930160522
-5.051815033	10.702921867	8.945945740
-2.872935295	11.946004868	8.834615707
-3.579739571	10.704910278	8.915831566
-5.026386738	13.228572845	8.868185997
1.285184860	9.669425011	9.185688019
-1.571240425	9.604317665	8.976311684
-0.869952679	10.850212097	8.899955750
0.594576359	10.890056610	8.963352203
-0.816659927	8.355111122	9.062585831
-3.600003242	13.212203026	8.799030304
0.602509499	8.393544197	9.172403336
2.592061043	12.039313316	8.956421852
3.302562237	10.829359055	9.181943893
5.491203308	11.988645554	9.050724030
4.749322414	10.778562546	9.167364120
3.360339642	13.286128998	8.884475708
9.593601227	9.563147545	9.029196739
6.706799507	9.553506851	9.148752213
7.440982819	10.791964531	9.076302528
8.896410942	10.800423622	9.030672073
7.406228542	8.277337074	9.100926399
4.789310932	13.267899513	8.958581924
8.842736244	8.294816971	9.045611382
4.205854893	6.834739208	11.991293907
6.890483856	2.294564009	8.661149979
5.488158226	4.735438347	8.810946465

-1.470984221	7.193965912	9.038177490
2.827102900	4.842523098	9.048923492
1.319396257	2.409300804	8.966087341
1.337885380	7.262156487	9.217350006
15.242857933	2.407672405	8.968338013
13.817626953	4.834035397	8.967095375
6.717536449	7.079863071	9.060606003
11.030971527	4.822305202	8.887176514
9.669776917	2.361645222	8.717975616
9.583003998	7.174987316	8.989883423
2.619949818	9.683605194	9.389879227
1.248185158	12.063854218	8.887122154
-5.691968918	14.390698433	8.888525963
-1.537647247	12.002882957	8.819747925
-2.909440517	9.546921730	8.977121353
-2.880549431	14.336917877	8.728542328
10.935298920	9.532150269	8.991917610
9.540460587	11.977146149	8.976582527
11.017729759	0.030824179	8.799965858
6.824048519	11.976986885	9.027972221
5.362980843	9.575986862	9.218861580
5.510162354	14.397370338	8.956602097
3.424636841	8.261845589	10.748250008
4.617890358	6.310411453	9.412271500
4.778308392	5.826303005	11.500577927
4.120632648	6.931909561	13.326066017
4.554581165	6.134371758	13.721597672

C<sub>2</sub>N-CuNi\*CO

C	N	Cu	Ni	O
49	24	1	1	1

Cartesian

-1.415087223	4.711992264	8.949636459
-0.697430134	3.478117228	8.977319717
1.471282482	4.738060951	9.011555672
0.762115479	3.494314909	9.012078285
-0.698807716	5.986822128	8.947170258
5.632202148	2.336743832	9.064800262
2.742303133	2.353906631	9.057095528
3.465746880	3.592320919	9.058896065
4.920551300	3.576411724	9.096336365
3.457789660	1.080618739	9.057726860
0.729056358	5.993220329	8.993951797
4.884148121	1.074782491	9.045018196

6.967050552	4.676369667	9.119483948
7.641536236	3.436744690	9.067445755
9.819931984	4.689396858	9.029934883
9.103817940	3.448402882	9.031104088
7.687638760	5.925058842	9.118512154
13.975234985	2.310746908	8.959608078
11.080162048	2.310963154	8.973522186
11.793479919	3.546999931	8.973954201
13.257195473	3.549694538	8.954567909
11.809576035	1.042027354	8.953056335
9.098330498	5.961344242	9.065070152
13.241375923	1.039736032	8.960003853
-5.625905037	11.930369377	9.033425331
-4.907416344	10.692977905	9.002898216
-2.730025768	11.931666374	8.960940361
-3.443527460	10.695831299	8.961929321
-4.890340805	13.203873634	9.032544136
1.389834404	9.560020447	8.976275444
-1.468472958	9.553074837	8.917451859
-0.752832890	10.792584419	8.915975571
0.712820053	10.801749229	8.925461769
-0.743601799	8.279181480	8.928270340
-3.459455967	13.200458527	9.002016068
0.670476437	8.313809395	8.977733612
2.720247746	11.909661293	8.942760468
3.428719997	10.670080185	8.990243912
5.609138966	11.890755653	9.014490128
4.886577606	10.654906273	9.009954453
3.466270447	13.167414665	8.947458267
9.765041351	9.530204773	9.044567108
6.875517368	9.499740601	9.059993744
7.586432457	10.745273590	9.059778214
9.046751022	10.762436867	9.059291840
7.616430283	8.247608185	9.096209526
4.893693924	13.163163185	8.979570389
9.045808792	8.251382828	9.063540459
4.258571625	7.061373711	11.223846436
6.972443104	2.276651621	9.055799484
5.607614517	4.742442131	9.167526245
-1.415813684	7.124809265	8.919540405
2.813393116	4.766089916	9.018737793
1.409368873	2.328054190	9.028745651
1.394711971	7.165807247	9.033408165
15.312662125	2.296941757	8.974728584

13.886194229	4.726806164	8.943191528
6.950315475	7.069328308	9.167003632
11.154439926	4.719586372	9.001367569
9.745182037	2.277761221	9.002321243
9.768213272	7.121047974	9.052325249
2.746315479	9.507076263	9.030221939
1.376204491	11.961150169	8.914536476
-5.570290089	14.353878975	9.056951523
-1.393638611	11.963931084	8.933706284
-2.803345680	9.522509575	8.936063766
-2.754297733	14.335721970	9.015011787
11.101537704	9.514757156	9.014616013
9.677746773	11.944189072	9.058643341
2.784332275	14.319251060	8.939880371
6.942698479	11.912817001	9.033678055
5.532799244	9.478211403	9.017981529
5.601939201	14.298874855	8.977986336
3.276401997	7.641860485	9.533213615
5.226504803	6.515372753	9.893321991
3.902170181	7.258208275	12.334085464

C<sub>2</sub>N-CuNi\*CHO

C	N	Cu	Ni	O	H
49	24	1	1	1	1

Cartesian

-1.422358155	4.682537079	9.005166054
-0.697820306	3.453518391	9.064980507
1.460982561	4.732555866	9.144324303
0.761350393	3.481575727	9.103715897
-0.714623213	5.969745636	9.025091171
5.632317543	2.357235670	9.022644043
2.752628326	2.358935833	9.087408066
3.468475580	3.605924368	9.102509499
4.929993629	3.603143215	9.061056137
3.469994545	1.090432286	9.041472435
0.706434965	5.974991322	9.161279678
4.895097256	1.093112707	9.014418602
6.975618362	4.694295883	8.965836525
7.644223213	3.445290089	8.960472107
9.837337494	4.667607784	8.887643814
9.111139297	3.434972048	8.937215805
7.714495659	5.923156738	8.921321869
13.980386734	2.271017075	9.041975021
11.077384949	2.268365622	8.987921715

11.797634125	3.499689817	8.941752434
13.259609222	3.504099607	8.973720551
11.807672501	0.993939221	9.048761368
9.126884460	5.951545238	8.870418549
13.243323326	0.994429231	9.074610710
-5.603692055	11.940917969	8.924201965
-4.885044575	10.709593773	8.854829788
-2.701763630	11.943065643	8.913204193
-3.422811270	10.712259293	8.858861923
-4.868825912	13.213730812	8.958240509
1.382222652	9.522509575	9.180450439
-1.465494156	9.544860840	8.913492203
-0.736326218	10.777251244	8.964486122
0.726814747	10.769671440	9.063809395
-0.763085842	8.264281273	8.980020523
-3.433615208	13.215502739	8.945640564
0.637529850	8.298418999	9.144162178
2.741913795	11.842998505	9.157373428
3.447699547	10.590577126	9.244764328
5.619581699	11.843762398	9.154853821
4.909774303	10.592968941	9.179765701
3.480508327	13.113417625	9.132911682
9.799360275	9.530997276	8.869194031
6.925977707	9.486497879	9.014147758
7.616316795	10.735301971	9.028601646
9.076710701	10.761269569	8.954675674
7.676140785	8.249063492	8.937323570
4.902956009	13.115046501	9.150192261
9.093580246	8.247608185	8.868887901
4.415926456	7.310994148	11.264382362
6.976643562	2.292171717	8.987544060
5.614310265	4.773467541	9.044712067
-1.432885170	7.103712082	8.946198463
2.804249763	4.772099018	9.131148338
1.419360995	2.323745489	9.082475662
1.356982231	7.157867432	9.283464432
15.316915512	2.267299175	9.081665993
13.882400513	4.686399460	8.954981804
6.998121262	7.078436375	8.961660385
11.171079636	4.679727077	8.886221886
9.738526344	2.255136728	8.982432365
9.809413910	7.104505062	8.834706306
2.740693569	9.425570488	9.346464157
1.405058861	11.918293953	9.090432167

-5.552660465	14.360090256	9.008783340
-1.364777565	11.957116127	8.957592010
-2.797705173	9.532683372	8.851464272
-2.736375809	14.353504181	8.971632004
11.134832382	9.527034760	8.819514275
9.697914124	11.946206093	8.973449707
2.791696548	14.262631416	9.080225945
6.954220295	11.888939857	9.085140228
5.580214977	9.433293343	9.079596519
5.605935097	14.257659912	9.126485825
5.171546936	6.745898247	9.556074142
3.027123928	7.642234802	10.084733963
3.436019659	6.576573849	11.657015800
5.040797710	7.844991207	12.009725571

C<sub>2</sub>N-CuNi\*COOH

C	N	Cu	Ni	O	H
49	24	1	1	2	1

Cartesian

-1.480723023	4.740453243	8.889030457
-0.762158990	3.512126207	8.975358009
1.406303406	4.779477119	9.111059189
0.698243141	3.535831451	9.059796333
-0.763753414	6.018208504	8.886329651
5.561257362	2.372121572	9.031895638
2.678522587	2.391662359	9.109188080
3.401899576	3.627684593	9.183869362
4.857577324	3.609887600	9.177965164
3.387977362	1.114699721	9.045125961
0.658744574	6.029923916	9.028403282
4.810999393	1.110145926	8.984286308
6.914000988	4.700723648	9.093348503
7.575958252	3.459628582	8.961533546
9.753265381	4.714514256	8.886834145
9.038024902	3.472612619	8.886797905
7.625156403	5.939844131	9.084743500
13.912336349	2.337204695	8.908488274
11.016648293	2.336066484	8.839116096
11.729300499	3.571814775	8.837027550
13.192989349	3.574178219	8.849448204
11.746703148	1.067029595	8.856036186
9.030298233	5.987787724	8.959301949
13.177087784	1.062893748	8.912772179
-5.703014374	11.959939957	8.943408012

-4.987095833	10.721842766	8.866169930
-2.808399677	11.964609146	8.785619736
-3.523115158	10.726842880	8.786142349
-4.966218472	13.236182213	8.943389893
1.311244965	9.594115257	8.914265633
-1.544134140	9.582990646	8.737020493
-0.827146053	10.824460030	8.738154411
0.638281345	10.834302902	8.793126106
-0.818888187	8.309688568	8.786808014
-3.536349297	13.234698296	8.864658356
0.591744900	8.347112656	8.908649445
2.649162769	11.933150291	8.902476311
3.350903034	10.696235657	9.046925545
5.530258179	11.908408165	9.074141502
4.806599140	10.674201012	9.128232002
3.397665501	13.192460060	8.905158043
9.685254097	9.556259155	8.983890533
6.801896572	9.519843102	9.180576324
7.510862827	10.764397621	9.108774185
8.970830917	10.786921501	9.043002129
7.542374134	8.267767906	9.165168762
4.820654392	13.184938431	8.990442276
8.966153145	8.275218964	9.028674126
3.607457638	7.270586491	11.671955109
6.901565552	2.305861950	8.950284004
5.562170982	4.772444725	9.262151718
-1.483229876	7.149552345	8.781875610
2.750477791	4.807159901	9.192419052
1.345380068	2.368475914	9.065285683
1.315988541	7.210768223	9.070164680
15.249796867	2.328010798	8.973828316
13.822254181	4.753336430	8.829431534
6.877434254	7.077312469	9.233657837
11.087329865	4.745295525	8.852489471
9.680202484	2.302633762	8.854290009
9.694724083	7.148154259	8.944902420
2.656960011	9.536243439	9.089171410
1.309869289	11.990620613	8.795286179
-5.642498970	14.388507843	9.026280403
-1.471496105	11.994914055	8.749728203
-2.879847288	9.554141045	8.749259949
-2.830324173	14.370969772	8.886311531
11.020626068	9.542439461	8.888274193
9.600786209	11.970301628	9.025019646



2.718930244	14.343849182	8.841923714
6.864640713	11.931177139	9.075078011
5.455183506	9.495806694	9.205757141
5.533151627	14.319769859	8.982864380
3.028684139	7.782506943	9.966221809
5.211653709	6.529509068	9.986346245
4.607851505	6.500688553	11.846015930
2.960356236	7.674470901	12.783725739
3.418322563	7.272358894	13.563684464

C<sub>2</sub>N-CuFe\*CO

C	N	Fe	Cu	O
49	24	1	1	1
Cartesian				
-1.402640820			4.708072662	8.982917786
-0.680923581			3.479327679	9.031733513
1.480408907			4.754503727	9.085301399
0.777631760			3.505338907	9.074592590
-0.690804243			5.990741730	8.995050430
5.642618179			2.331988335	9.043128014
2.760789394			2.371026516	9.098586082
3.486537457			3.607898712	9.141227722
4.941692352			3.571065426	9.166302681
3.466866732			1.089164257	9.052253723
0.732084751			5.993796825	9.051462173
4.890986919			1.076713562	9.009989738
7.000728607			4.660431385	9.141300201
7.662451267			3.423198700	8.995032310
9.842205048			4.677190781	8.917236328
9.124993324			3.435188293	8.918370247
7.718722820			5.904509068	9.137430191
13.997682571			2.300400257	8.973863602
11.102234840			2.298584700	8.889120102
11.814947128			3.532733440	8.891513824
13.276413918			3.535889387	8.925966263
11.830068588			1.031060815	8.918153763
9.121086121			5.949945450	8.989452362
13.260694504			1.024114966	8.969202042
-5.633992195			11.933626175	8.984466553
-4.912116528			10.696767807	8.946053505
-2.734701633			11.932790756	8.926181793
-3.447221518			10.698684692	8.926469803
-4.897237778			13.209450722	8.988083839
1.372154713			9.562858582	9.020105362

-1.472990513	9.553606987	8.942004204
-0.756177425	10.794889450	8.938097954
0.709125519	10.805899620	8.963640213
-0.749857426	8.279066086	8.973252296
-3.465055466	13.202663422	8.950139999
0.658370495	8.326562881	9.025289536
2.720530987	11.899112701	8.976347923
3.429218292	10.665352821	9.034901619
5.606609821	11.870436668	9.054000854
4.876519203	10.637166023	9.066005707
3.475065231	13.157255173	8.964792252
9.766763687	9.523360252	8.998505592
6.872706890	9.473859787	9.124128342
7.580758095	10.720920563	9.081432343
9.043956757	10.750476837	9.039491653
7.632137775	8.232275009	9.153269768
4.899900913	13.146619797	9.014004707
9.055675507	8.244783401	9.030833244
3.851202011	7.308183670	11.114892006
6.986079216	2.268682718	8.972820282
5.649271011	4.719889164	9.278063774
-1.420273066	7.119967461	8.963244438
2.829641581	4.792532921	9.112301826
1.427871704	2.341629028	9.070775986
1.405552387	7.179050922	9.087515831
-1.306660652	2.292935610	9.025794029
13.902308464	4.717540741	8.930250168
6.991093159	7.045507908	9.269459724
11.175655365	4.708173275	8.892323494
9.764549255	2.264820814	8.891136169
9.782341003	7.112978458	8.962812424
2.739744186	9.489726067	9.078318596
1.377826691	11.966064453	8.947134018
-5.569434166	14.366776466	9.036359787
-1.397823811	11.965127945	8.926218033
-2.807330847	9.524512291	8.930610657
-2.754213810	14.333127975	8.954766273
11.103807449	9.515952110	8.947332382
9.667147636	11.937099457	9.028169632
2.799542427	14.308759689	8.915273666
6.939462662	11.889631271	9.051444054
5.518306255	9.449823380	9.094211578
5.614537239	14.281639099	9.014796257
3.293533325	7.630432606	9.388925552

5.206778526	6.527318954	9.961199760
3.728091717	7.378290653	12.292290688

C<sub>2</sub>N-CuFe\*CHO

C	N	Fe	Cu	O	H
49	24	1	1	1	1

Cartesian

-1.396983266	4.704729557	8.928702354
-0.675041318	3.477353573	9.003959656
1.483537197	4.751448154	9.128412247
0.783987999	3.502226114	9.079092026
-0.684714317	5.988811016	8.946864128
5.647085667	2.336758137	9.041183472
2.769184113	2.370089769	9.129708290
3.491878748	3.607581615	9.197225571
4.947291374	3.574855328	9.189414024
3.475544214	1.089610934	9.075870514
0.737176180	5.988119125	9.063719749
4.898715973	1.078053713	9.016434669
7.006252289	4.663111687	9.106865883
7.666620255	3.424855947	8.953632355
9.846472740	4.677234173	8.854793549
9.129043579	3.435116053	8.868149757
7.724771023	5.904466152	9.103536606
14.002348900	2.299377203	8.939718246
11.106462479	2.296538115	8.848854065
11.819604874	3.530831337	8.830566406
13.281538963	3.533353090	8.865072250
11.835109711	1.029417992	8.898714066
9.126085281	5.950651646	8.936712265
13.265270233	1.022760391	8.953722000
-5.621778488	11.930974960	8.992332458
-4.901110172	10.694736481	8.918370247
-2.721339703	11.932617188	8.890955925
-3.435589790	10.696724892	8.873909950
-4.883975983	13.208642960	8.998596191
1.385001183	9.559631348	9.003186226
-1.459429264	9.549775124	8.859581947
-0.741501808	10.792007446	8.877258301
0.719949245	10.801072121	8.924183846
-0.738542557	8.277827263	8.895239830
-3.452051640	13.202793121	8.940923691
0.668520451	8.320713043	8.992134094
2.729258060	11.896591187	8.995446205

3.441050053	10.664085388	9.093779564
5.616544724	11.869715691	9.106884003
4.886129379	10.637468338	9.151686668
3.483485222	13.156246185	8.981136322
9.774758339	9.523230553	8.990262032
6.883830070	9.474248886	9.196128845
7.591773510	10.719969749	9.131814957
9.053590775	10.749698639	9.067031860
7.640390873	8.231496811	9.179622650
4.907538414	13.145640373	9.039780617
9.060617447	8.244091988	9.016272545
4.295479774	7.000907421	11.611116409
6.988841534	2.272112370	8.944217682
5.658273697	4.726835251	9.282527924
-1.409873247	7.114376068	8.872830391
2.832329035	4.791999340	9.207828522
1.434552550	2.339481831	9.087282181
1.410752296	7.174770832	9.105263710
-1.302076459	2.291854858	9.005723953
13.909347534	4.714571953	8.855477333
6.998480320	7.040752411	9.285894394
11.179914474	4.706271172	8.821782112
9.768601418	2.264287233	8.853425980
9.786624908	7.113828659	8.917181969
2.748430252	9.487621307	9.123929977
1.392103195	11.963816643	8.926830292
-5.557744980	14.363793373	9.063702583
-1.385543823	11.963196754	8.883702278
-2.795691252	9.524065971	8.848746300
-2.744137764	14.336399078	8.947026253
11.110763550	9.514915466	8.911782265
9.680567741	11.935903549	9.061830521
2.806513786	14.305474281	8.911295891
6.948713779	11.889977455	9.103518486
5.528481960	9.450067520	9.216665268
5.620360374	14.281811714	9.023903847
3.251093388	7.650506496	9.632213593
5.281740189	6.493194580	10.109879494
3.205525875	7.633862019	11.685977936
4.723742962	6.687939167	12.600864410

C<sub>2</sub>N-CuFe\*COOH

C	N	Cu	Fe	O	H
49	24	1	1	2	1

## Cartesian

-1.380002022	4.694108963	8.970479965
-0.657918930	3.466949224	9.031931877
1.503612995	4.741837025	9.149166107
0.802924395	3.492571115	9.099683762
-0.666884661	5.977700233	8.996742249
5.665289879	2.324566841	8.991324425
2.787563086	2.359843731	9.117828369
3.510981560	3.596226454	9.184823990
4.966310501	3.561021328	9.161315918
3.492857933	1.079163313	9.045882225
0.756803274	5.977556229	9.099810600
4.915090084	1.066035271	8.967275620
7.020480156	4.650401592	9.073854446
7.682819366	3.414754152	8.903016090
9.862955093	4.666555882	8.822358131
9.145825386	3.424438000	8.822052002
7.739521980	5.895084858	9.072359085
14.020137787	2.289088011	8.945927620
11.124457359	2.286494017	8.820558548
11.837409973	3.521521807	8.821980476
13.299401283	3.523625851	8.878643990
11.853746414	1.019244194	8.877059937
9.140820503	5.939051151	8.901521683
13.283150673	1.012456775	8.945657730
-5.608183861	11.918840408	8.960616112
-4.886025429	10.682559013	8.894483566
-2.706097603	11.919532776	8.865630150
-3.420123100	10.683135986	8.864658356
-4.869382858	13.197173119	8.962091446
1.402672768	9.548707962	9.031302452
-1.443363190	9.536416054	8.889768600
-0.725227356	10.779441833	8.889858246
0.735831738	10.789126396	8.942813873
-0.721528053	8.266341209	8.942921638
-3.437766075	13.189750671	8.896535873
0.686375141	8.309356689	9.031986237
2.744759083	11.886259079	8.995553970
3.456691742	10.653594017	9.096588135
5.632045269	11.857336998	9.096047401
4.900572300	10.625911713	9.144900322
3.499858856	13.145841599	8.969399452
9.790142059	9.511139870	8.963261604
6.897167683	9.460457802	9.179568291

7.605776310	10.705832481	9.112733841
9.067817688	10.736151695	9.041669846
7.655591965	8.218339920	9.155916214
4.923679352	13.134688377	9.030402184
9.075843811	8.231727600	8.986895561
4.400949955	7.019684315	11.693069458
7.005007267	2.261290073	8.885051727
5.676836014	4.711459160	9.266958237
-1.392725706	7.102170467	8.932157516
2.854534864	4.782589436	9.211679459
1.451933026	2.329610348	9.091818810
1.429938316	7.164741039	9.141300201
-1.284621239	2.281248808	9.018737793
-2.713245392	4.705046654	8.890686035
7.014862537	7.028316498	9.261989594
11.197111130	4.696573257	8.808137894
9.786505699	2.253681183	8.805959702
9.800569534	7.103078365	8.881649971
2.765943050	9.476799965	9.137177467
1.408211231	11.952547073	8.931672096
-5.541138172	14.353130341	9.034559250
-1.370326042	11.950242043	8.868419647
-2.779983044	9.510260582	8.867609978
-2.730318069	14.324106216	8.889570236
11.125356674	9.502954483	8.886384010
9.694552422	11.923178673	9.031608582
2.824452400	14.295386314	8.888724327
6.963823318	11.877064705	9.087479591
5.541377544	9.435916901	9.206585884
5.637167931	14.270427704	9.017855644
3.285936832	7.635605812	9.636174202
5.324206352	6.460194588	10.155258179
4.958767414	6.733634949	12.888396263
3.299905777	7.648820400	11.699945450
4.365396976	7.092731476	13.593762398

C<sub>2</sub>N-CuMn\*CO

C	N	Cu	Mn	O
49	24	1	1	1

Cartesian

-1.409945488	4.714057446	8.970235825
-0.686761141	3.486802578	9.025318146
1.483729124	4.758618355	9.113168716
0.773391247	3.513318062	9.078723907

-0.699887037	5.990887642	8.981279373
5.634988785	2.333661556	9.030290604
2.747245312	2.361753464	9.082768440
3.478218079	3.593366623	9.102005005
4.925714493	3.565088511	9.089695930
3.457555294	1.086457372	9.044480324
0.724780560	6.003565311	9.103022575
4.883271694	1.077818155	9.002698898
6.983694553	4.675673008	9.082338333
7.649848938	3.430800438	9.022496223
9.829675674	4.683934689	8.984993935
9.113197327	3.442421675	8.985530853
7.696670532	5.911147118	9.079505920
13.989929199	2.304916382	8.973912239
11.090934753	2.305402040	8.939628601
11.803744316	3.540396690	8.941638947
13.267103195	3.542835712	8.942200661
11.820577621	1.037086010	8.935791016
9.107856750	5.956994534	9.019079208
13.254097939	1.030139446	8.969521523
-5.636394501	11.936088562	8.972785950
-4.917314053	10.700110435	8.915346146
-2.742888927	11.938540459	8.862573624
-3.455765009	10.703683853	8.861331940
-4.900523186	13.210393906	8.976742744
1.360613346	9.575939178	9.034819603
-1.482911587	9.560281754	8.848638535
-0.766306400	10.801820755	8.846377373
0.696393490	10.815894127	8.903988838
-0.764031887	8.286662102	8.911615372
-3.470517635	13.205934525	8.920466423
0.642188549	8.331717491	9.039081573
2.716686249	11.908694267	8.965614319
3.418177128	10.668823242	9.088792801
5.598817348	11.871740341	9.060266495
4.875464439	10.633916855	9.096386909
3.467260838	13.162235260	8.955305099
9.762170792	9.529335022	8.991293907
6.881300449	9.488559723	9.087078094
7.582551003	10.737410545	9.066822052
9.041899681	10.759652138	9.031863213
7.629045486	8.248655319	9.078598022
4.891820431	13.149714470	9.009455681
9.050338745	8.250417709	9.019532204

4.289223671	7.039945602	11.321666718
6.981080055	2.272501230	9.005517960
5.617064476	4.737966537	9.142726898
-1.423957348	7.124742031	8.902166367
2.835661650	4.782678604	9.112967491
1.415550590	2.341992140	9.068511963
1.366151333	7.190373421	9.184752464
-1.312104106	2.300564051	9.018084526
13.891990662	4.722477436	8.930747986
6.959189415	7.063676357	9.134743690
11.163668633	4.713997841	8.960149765
9.754448891	2.272443771	8.958699226
9.776327133	7.115197659	8.998062134
2.711465359	9.520176888	9.177011490
1.372608185	11.968421936	8.888762474
-5.576025009	14.362762451	9.035202026
-1.406966686	11.972362518	8.841407776
-2.817149401	9.529902458	8.842450142
-2.759988308	14.336969376	8.937945366
11.097959518	9.519100189	8.929534912
9.667510986	11.944665909	9.026857376
2.791196823	14.316766739	8.919330597
6.934176445	11.900688171	9.050222397
5.530135155	9.450973511	9.097473145
5.606554985	14.284223557	9.007723808
3.069716454	7.763609409	10.026150703
5.039905548	6.622231483	9.586334229
4.313068390	7.012757778	12.508782387

C<sub>2</sub>N-CuMn\*CHO

C	N	Cu	Mn	O	H
49	24	1	1	1	1

Cartesian

-1.472444534	4.728593349	8.960111618
-0.751842260	3.501693010	9.041183472
1.419673443	4.776465416	9.172871590
0.709275484	3.529231548	9.109313965
-0.759127140	6.006103516	8.978940010
5.566433430	2.349871635	8.948105812
2.682948589	2.375810623	9.077724457
3.412973881	3.607437849	9.122796059
4.861272335	3.579337120	9.058877945
3.390698671	1.101629257	9.001349449
0.662330866	6.020542622	9.148374557



4.816041946	1.092853308	8.927477837
6.911813259	4.693647385	8.977518082
7.579535007	3.448676586	8.888507843
9.762134552	4.699815750	8.851302147
9.045596123	3.458518982	8.847018242
7.624791145	5.929410458	8.983008385
13.924741745	2.319523096	8.962524414
11.025417328	2.319033146	8.851158142
11.738868713	3.554896832	8.853515625
13.203498840	3.557418585	8.892432213
11.755556107	1.049391031	8.891550064
9.037071228	5.974040031	8.897507668
13.188161850	1.044001579	8.963405609
-5.702739239	11.949953079	8.920169830
-4.983010769	10.713671684	8.847107887
-2.808240414	11.953065872	8.787258148
-3.521792173	10.716770172	8.789544106
-4.966799736	13.224941254	8.916498184
1.293157578	9.590599060	9.048203468
-1.546638250	9.572283745	8.794152260
-0.829292774	10.815323830	8.793089867
0.632349014	10.828063011	8.878427505
-0.826309204	8.300466537	8.878751755
-3.536414623	13.219797134	8.840951920
0.575787544	8.347228050	9.047700882
2.652749062	11.917428970	8.980560303
3.350979805	10.679446220	9.151541710
5.532188892	11.884342194	9.117504120
4.807023525	10.645711899	9.179874420
3.402790546	13.173755646	8.962038040
9.695045471	9.544255257	8.940635681
6.815598488	9.502536774	9.135305405
7.517610073	10.750461578	9.090251923
8.974975586	10.774325371	9.012906075
7.563740730	8.261773109	9.072396278
4.825555801	13.163422585	9.045827866
8.981328964	8.266255379	8.962703705
3.863049984	7.274808884	11.728457451
6.912830353	2.290701866	8.876573563
5.549424648	4.753624439	9.091223717
-1.484178066	7.135833263	8.866098404
2.773782253	4.796510220	9.189197540
1.349240661	2.358244181	9.079236031
1.300381184	7.212554932	9.244170189

15.262069702	2.315343857	9.035657883
13.830307961	4.737398148	8.884026527
6.890945911	7.078493595	9.101627350
11.097098351	4.729443550	8.846298218
9.687458038	2.287618160	8.839493752
9.706403732	7.130314350	8.891045570
2.637841702	9.530766487	9.246294022
1.311875343	11.980374336	8.866260529
-5.642640114	14.376619339	8.993969917
-1.470605850	11.986454964	8.774855614
-2.881577253	9.541776657	8.778185844
-2.826762676	14.353504181	8.845146179
11.029545784	9.532237053	8.856054306
9.601844788	11.959710121	9.000953674
2.726933479	14.327075958	8.883629799
6.866371632	11.914604187	9.089909554
5.466198921	9.462749481	9.198233604
5.539982796	14.298571587	9.039887428
2.935401917	7.814268112	10.204596519
4.993781090	6.619330406	9.741545677
4.958095551	6.635542393	11.796947479
3.423748493	7.532772064	12.728699684

C<sub>2</sub>N-CuMn\*COOH

C	N	Cu	Mn	O	H
49	24	1	1	2	1

Cartesian

-1.497612357	4.743191242	8.983619690
-0.774672270	3.517141104	9.049878120
1.399331570	4.791495323	9.154278755
0.688492298	3.544823647	9.097560883
-0.782980204	6.020586014	9.000251770
5.543694496	2.364728928	8.902223587
2.661317348	2.391979218	9.042947769
3.391075850	3.623490810	9.071567535
4.837085724	3.595865965	8.991215706
3.369807243	1.116832495	8.972891808
0.641023397	6.033440590	9.151559830
4.794610023	1.106860280	8.899614334
6.883567810	4.710291862	8.902511597
7.554942131	3.465104580	8.842122078
9.737057686	4.714917660	8.826138496
9.020777702	3.473722219	8.824733734
7.597642422	5.947380543	8.906076431

13.900256157	2.335504293	8.987921715
11.000257492	2.334250689	8.871084213
11.713668823	3.570388079	8.871767998
13.177906036	3.573241472	8.922599792
11.730462074	1.065213799	8.922456741
9.011670113	5.988811016	8.847000122
13.163426399	1.058830023	8.988462448
-5.722957134	11.963211060	8.912394524
-5.002154350	10.726915359	8.848152161
-2.826735973	11.965819359	8.803350449
-3.540437460	10.729436874	8.806661606
-4.986643314	13.238617897	8.909567833
1.277091503	9.603295326	9.067319870
-1.565765619	9.585181236	8.821800232
-0.848045826	10.827947617	8.819585800
0.612406254	10.840096474	8.903987885
-0.845985651	8.314457893	8.905878067
-3.555726051	13.232810020	8.842391968
0.557624817	8.356954575	9.066401482
2.630601406	11.932300568	9.000611305
3.331069469	10.692949295	9.155879974
5.510133743	11.896461487	9.104435921
4.785691261	10.657614708	9.161694527
3.379785538	13.189707756	8.984753609
9.674112320	9.558291435	8.910036087
6.792819023	9.515851974	9.082223892
7.494846344	10.763719559	9.052703857
8.953335762	10.787570000	8.981891632
7.539503574	8.277005196	9.001925468
4.802932262	13.177415848	9.053838730
8.959138870	8.280622482	8.912969589
3.869407177	7.249763012	11.758068085
6.888844490	2.305962563	8.838000298
5.521744251	4.771334648	8.994779587
-1.506491899	7.150071144	8.899361610
2.754388571	4.814451218	9.144611359
1.327442527	2.373288870	9.058571815
1.281469345	7.223147392	9.250289917
15.237935066	2.331037045	9.050004005
13.804883003	4.753509521	8.918891907
6.863922596	7.095959187	9.004050255
11.072063446	4.744444847	8.841581345
9.662822723	2.302763462	8.839241982
9.682701111	7.145142555	8.847072601

2.620428085	9.543663979	9.255474091
1.290950298	11.994193077	8.896409988
-5.662840843	14.390828133	8.973702431
-1.489658833	11.998934746	8.797769547
-2.900688410	9.554818153	8.803584099
-2.847138405	14.367266655	8.834309578
11.009386063	9.545911789	8.843580246
9.580944061	11.972851753	8.978670120
2.702374458	14.342350006	8.918603897
6.844299316	11.928308487	9.066366196
5.442962646	9.472274780	9.153900146
5.516545296	14.313688278	9.053423882
2.883834839	7.844818592	10.281311989
4.926221848	6.661351681	9.584945679
4.965011120	6.607945919	11.654784203
3.420031071	7.494368076	13.002947807
4.067364216	7.104230881	13.641084671

C<sub>2</sub>N-NiCo\*CO

C	N	Co	Ni	O
49	24	1	1	1

Cartesian

-1.397432804	4.714701653	9.014291763
-0.680141687	3.484025717	9.021329880
1.485075951	4.760599136	8.982684135
0.777673483	3.512155056	9.015066147
-0.681286812	5.998927116	9.012815475
5.638241768	2.343286037	9.026891708
2.756978989	2.372380972	9.023237228
3.481779099	3.609656811	9.005723953
4.933379650	3.590188265	9.046332359
3.462748528	1.092233658	9.023903847
0.751228571	6.008971214	8.999657631
4.887625694	1.085186958	9.014273643
6.990478039	4.673055172	9.095327377
7.655230045	3.427608490	9.050760269
9.836638451	4.679626465	9.036144257
9.119925499	3.438200235	9.035675049
7.702847481	5.906843662	9.095454216
13.996875763	2.301826954	9.025956154
11.098307610	2.298815012	9.022734642
11.812150955	3.535644293	9.023633957
13.276546478	3.541192293	9.022518158
11.825734138	1.027559042	9.019835472

9.113855362	5.953793049	9.051300049
13.259263992	1.023711443	9.024623871
-5.637320042	11.935989380	9.025415421
-4.917907715	10.696105957	9.021545410
-2.738778591	11.936738968	9.025506020
-3.452637911	10.701062202	9.028241158
-4.900724411	13.211396217	9.023670197
1.362395763	9.562182426	9.051227570
-1.478149414	9.556893349	9.044495583
-0.761203289	10.797685623	9.042965889
0.704257965	10.808854103	9.043470383
-0.755906105	8.281818390	9.044604301
-3.467168808	13.208226204	9.017208099
0.652803898	8.334561348	9.051389694
2.719000816	11.885335922	9.012167931
3.426001072	10.639226913	9.000089645
5.600820065	11.866602898	9.014543533
4.874181747	10.629053116	8.983763695
3.472544670	13.148680687	9.012257576
9.758060455	9.522322655	9.017675400
6.869827747	9.476799965	9.007452011
7.578261852	10.723399162	9.024137497
9.039587975	10.752854347	9.025289536
7.612403870	8.229623795	9.047736168
4.896773338	13.143507004	9.019475937
9.044444084	8.242766380	9.028907776
4.029972076	7.208909512	10.888775826
6.981778145	2.274057627	9.030726433
5.628646374	4.752932549	9.118116379
-1.418741941	7.121725559	9.033893585
2.829267502	4.787100315	8.943120003
1.425251007	2.347638130	9.015011787
1.422682762	7.200191021	9.043704033
-1.305920362	2.297042608	9.025919914
13.904056549	4.722296238	9.015930176
6.952704906	7.046343803	9.118097305
11.170920372	4.708850861	9.027162552
9.761580467	2.267861128	9.025775909
9.776166916	7.113785267	9.032274246
2.729794025	9.461826324	9.043722153
1.378017902	11.962533951	9.032400131
-5.573011398	14.370033264	9.026477814
-1.402599335	11.967924118	9.031715393
-2.812198400	9.527956963	9.035927773

-2.756875992	14.338920593	9.009036064
11.097735405	9.515692711	9.014453888
9.662704468	11.938943863	9.027287483
2.796704292	14.303903580	9.013049126
6.933064461	11.888578415	9.014183044
5.524230003	9.452387810	8.944883347
5.611965179	14.278944969	9.024605751
3.245368958	7.653676987	9.283499718
5.106871605	6.583375931	9.464814186
3.980726242	7.242212296	12.071105957

C<sub>2</sub>N- NiCo \*CHO

C	N	Co	Ni	O	H
49	24	1	1	1	1

Cartesian

-1.446726322	4.657736778	9.075870514
-0.721631169	3.428300142	9.097919464
1.433161736	4.713130951	9.160794258
0.742390037	3.460320234	9.116603851
-0.740713835	5.950204849	9.114624023
5.616002083	2.364080429	9.017730713
2.743384838	2.357451677	9.066383362
3.445853949	3.608504295	9.081665993
4.913470268	3.616775751	9.037241936
3.466525555	1.088861704	9.029034615
0.681950331	5.950479031	9.207953453
4.889372826	1.092392206	9.022193909
6.938587189	4.708461761	8.966861725
7.622148991	3.455103636	8.968788147
9.815905571	4.656252384	8.901539803
9.089218140	3.425994396	8.952300072
7.693030357	5.935837746	8.914086342
13.957572937	2.240380287	9.060534477
11.049863815	2.238679886	9.005795479
11.771651268	3.473304272	8.973341942
13.236322403	3.473678827	9.018989563
11.782271385	0.961241663	9.056610107
9.112915993	5.942481041	8.861886024
13.220319748	0.958532512	9.067734718
-5.595979214	11.940644264	8.927909851
-4.872024536	10.714046478	8.901377678
-2.693377018	11.941969872	9.008225441
-3.418734789	10.714565277	8.961192131
-4.861537457	13.212576866	8.973845482

1.362589359	9.489883423	9.233909607
-1.478971481	9.528720856	9.058824539
-0.740061760	10.759108543	9.094320297
0.717247009	10.738400459	9.160919189
-0.789617538	8.242420197	9.111401558
-3.426060200	13.214407921	8.998038292
0.615899086	8.271212578	9.225594521
2.738255501	11.796365738	9.171540260
3.454540730	10.541666985	9.212867737
5.610148907	11.798801422	9.067986488
4.897837162	10.541220665	9.105245590
3.469176769	13.074422836	9.122345924
9.825567245	9.528230667	8.837081909
6.974790573	9.479969978	8.926145554
7.629295826	10.730863571	8.934065819
9.089248657	10.756528854	8.890811920
7.723122597	8.264324188	8.869733810
4.888105869	13.071858406	9.096443176
9.132675171	8.238140106	8.820467949
4.507347584	7.537224770	11.095685959
6.953856468	2.305328846	8.993105888
5.588876724	4.782128811	9.013157845
-1.463393450	7.082571983	9.079038620
2.776436806	4.767444134	9.126288414
1.406989932	2.308628559	9.074016571
1.344985008	7.131957054	9.324485779
15.295359612	2.241144180	9.092754364
13.858364105	4.657361984	9.029988289
7.010866165	7.105614662	8.931726456
11.153599739	4.655531883	8.913275719
9.708642006	2.240149736	8.995229721
9.823066711	7.087053299	8.815842628
2.731152058	9.364771843	9.331056595
1.407105923	11.886273384	9.164033890
-5.551421165	14.356502533	8.997983932
-1.358395100	11.946465492	9.068094254
-2.807464361	9.528346062	8.987832069
-2.734488010	14.358072281	9.015048027
-5.482993603	9.527034760	8.842140198
9.705410004	11.944837570	8.923391342
2.774891853	14.221359253	9.092681885
6.944529533	11.874370575	8.993771553
5.612497807	9.378908157	9.007487297
5.585627556	14.222656250	9.079938889

3.068564415	7.655910015	9.989999771
5.187453747	7.428469181	9.242244720
3.731389999	6.580983639	11.463461876
5.196664810	8.026376724	11.809278488

C<sub>2</sub>N- NiCo \*COOH

C	N	Co	Ni	O	H
49	24	1	1	2	1
Cartesian					
-1.399794579			4.676974773		9.043326378
-0.679857850			3.448114634		9.084456444
1.487589836			4.717079163		9.144180298
0.780386686			3.470623970		9.130356789
-0.681967974			5.959298134		9.048510551
5.643750191			2.305040359		9.035496712
2.759500504			2.330489635		9.130266190
3.486206532			3.567462683		9.140687943
4.936525822			3.542489290		9.107478142
3.469388485			1.051567078		9.083429337
0.745105982			5.962050438		9.113346100
4.893750191			1.042791009		9.034235954
6.984847069			4.638628483		9.037836075
7.653159142			3.397504568		8.980451584
9.833578110			4.650171280		8.954099655
9.118086815			3.408038855		8.950265884
7.698971748			5.881019592		9.017009735
13.994155884			2.275354624		9.019871712
11.097318649			2.272227526		8.953091621
11.809131622			3.507385015		8.963478088
13.273261070			3.511232615		8.992746353
11.826399803			1.003723979		8.962937355
9.108572960			5.922940254		8.974295616
13.256901741			0.998493016		8.996706009
-5.621861458			11.895467758		9.008262634
-4.903188705			10.658133507		8.979084015
-2.724567413			11.897196770		8.961425781
-3.437810421			10.660626411		8.962920189
-4.885214806			13.172574043		9.022356033
1.391174316			9.526025772		9.010278702
-1.461009026			9.517724991		8.959770203
-0.745336056			10.758531570		8.949348450
0.719309807			10.767999649		8.958618164
-0.736611366			8.245114326		8.993574142
-3.455121040			13.167530060		8.988156319



0.673355579	8.286054611	9.043722153
2.726895809	11.863936424	8.965979576
3.437132835	10.624412537	9.006875992
5.613783360	11.845361710	9.010368347
4.889407158	10.609454155	9.014183044
3.478892803	13.128059387	8.965638161
9.769849777	9.490748405	8.993160248
6.880826950	9.451783180	9.026909828
7.589986324	10.699809074	9.026280403
9.051677704	10.721655846	9.017495155
7.623727322	8.204246521	9.033390045
4.903920650	13.120004654	8.995103836
9.050526619	8.209722519	8.997786522
4.689476013	7.219213486	11.399417877
6.984923363	2.237570286	8.989379883
5.625436306	4.713361263	9.162125587
-1.407917023	7.085684776	9.004788399
2.835325241	4.751448154	9.147384644
1.426782608	2.304406404	9.127547264
1.419089794	7.146122456	9.147438049
15.329811096	2.264013529	9.067824364
13.904314995	4.690491676	9.000018120
6.949002266	7.023214817	9.068039894
11.168259621	4.680980682	8.958563805
9.760115623	2.238463640	8.944992065
9.779420853	7.081894875	8.968266487
2.752715588	9.449072838	9.051876068
1.387752533	11.928121567	8.943426132
-5.562044144	14.325532913	9.071387291
-1.388471127	11.928812981	8.947656631
-2.796181679	9.488370895	8.959464073
-2.748014450	14.302246094	8.990316391
11.106771469	9.478946686	8.973252296
9.681043625	11.905338287	9.024948120
2.799642563	14.278122902	8.948160172
6.947591305	11.866645813	9.014993668
5.533399105	9.429907799	9.015858650
5.614429474	14.257674217	9.010746002
3.260271072	7.611410141	9.558449745
5.236181259	6.489793777	9.813276291
5.470716476	7.160144329	12.504384041
3.567791939	7.826286316	11.521548271
4.992374420	7.624322891	13.232430458

C<sub>2</sub>N-NiFe\*CO

C	N	Fe	Ni	O
49	24	1	1	1
Cartesian				
-1.401509404			4.713260651	9.008855820
-0.682271481			3.483535767	9.017135620
1.478986025			4.760627747	8.995553970
0.776342154			3.511059761	9.015048027
-0.686594963			5.998667717	9.007991791
5.637801170			2.345288992	9.032327652
2.757835865			2.376660824	9.028727531
3.481945038			3.614470005	9.027881622
4.933446407			3.589842319	9.066114426
3.462123871			1.094986081	9.026153564
0.740220547			6.001780510	9.004212379
4.885945320			1.084639311	9.016937256
6.995461464			4.669034481	9.097667694
7.656636238			3.425806999	9.043344498
9.838775635			4.678343773	9.024479866
9.121872902			3.436557293	9.023544312
7.708514214			5.903889179	9.097811699
13.995834351			2.302763462	9.019242287
11.099580765			2.299578905	9.011303902
11.812334061			3.534433842	9.012942314
13.275531769			3.539232492	9.013733864
11.826948166			1.029951215	9.010350227
9.115785599			5.952842236	9.044388771
13.257973671			1.024532914	9.017208099
-5.639924526			11.934649467	9.021311760
-4.918556213			10.697027206	9.016650200
-2.739843369			11.936422348	9.015516281
-3.452903509			10.701090813	9.019188881
-4.901647568			13.213370323	9.019835472
1.362179756			9.564112663	9.041058540
-1.477657795			9.556619644	9.030833244
-0.760945320			10.798074722	9.027881622
0.704141617			10.809286118	9.029772758
-0.754933357			8.282034874	9.032976151
-3.469115734			13.207707405	9.011879921
0.652379513			8.334662437	9.042174339
2.715905666			11.891850471	9.004571915
3.426382065			10.654646873	9.002105713
5.601052761			11.868850708	9.012528419
4.870512962			10.635378838	8.994312286

3.471538067	13.153882980	9.004517555
9.757570267	9.523143768	9.019926071
6.864794254	9.474076271	9.028134346
7.574452877	10.720257759	9.028152466
9.036460876	10.751038551	9.026622772
7.612045288	8.229522705	9.066959381
4.896032810	13.146029472	9.013086319
9.041931152	8.241612434	9.034235954
4.027950287	7.208866596	10.922993660
6.981277943	2.271752119	9.027125359
5.634237289	4.752558231	9.143135071
-1.423018456	7.121811867	9.024372101
2.826804399	4.795228004	8.977157593
1.424951196	2.348128080	9.014345169
1.419179916	7.192423344	9.045989990
-1.307376266	2.296480656	9.021581650
13.901950836	4.721388340	9.008118629
6.955757618	7.041170597	9.143316269
11.172185898	4.708879948	9.015605927
9.762178421	2.266679764	9.013031960
9.777356148	7.114808559	9.029141426
2.734685421	9.471366882	9.044639587
1.374981403	11.967908859	9.019889832
-5.573660851	14.371099472	9.025181770
-1.403406143	11.967967033	9.018719673
-2.812148571	9.528043747	9.025271416
-2.758847713	14.340117455	9.006515503
11.095530510	9.515649796	9.012311935
9.661182404	11.937978745	9.025271416
2.796297073	14.307088852	9.003761292
6.932573795	11.888650894	9.012078285
5.514646530	9.450975418	8.976798058
5.611583710	14.280788422	9.018737793
3.266243935	7.646053791	9.268434525
5.120068073	6.576112747	9.500904083
4.011635780	7.220351219	12.107520103

C<sub>2</sub>N- NiFe \*CHO

C	N	Fe	Ni	O	H
49	24	1	1	1	1

Cartesian

-1.457708478	4.655632496	9.058608055
-0.727754593	3.427464247	9.087911606
1.417720079	4.718491554	9.166374207

0.735626101	3.463793278	9.114137650
-0.760373592	5.947452545	9.102527618
5.612524033	2.380133867	9.033227921
2.744765282	2.376415968	9.076608658
3.445187807	3.631935596	9.101754189
4.912928581	3.636763096	9.055206299
3.467165709	1.105217576	9.035874367
0.656075716	5.943964958	9.209177971
4.887683868	1.107681751	9.033803940
6.946532249	4.716516972	8.964918137
7.623963356	3.460925579	8.970191956
9.822437286	4.652692795	8.879796028
9.090048790	3.425965548	8.945190430
7.709595203	5.936774731	8.904941559
13.956075668	2.232685089	9.051462173
11.046152115	2.230811834	8.999586105
11.771018982	3.462208033	8.956835747
13.232994080	3.464023829	9.003582001
11.779910088	0.951961279	9.050651550
9.126635551	5.943158150	8.840826035
13.219138145	0.952076614	9.059418678
-5.596470356	11.953484535	8.925731659
-4.869021416	10.728759766	8.896391869
-2.690681934	11.953469276	9.016775131
-3.418726683	10.728240967	8.961011887
-4.862328529	13.226627350	8.976870537
1.361424446	9.477375984	9.232722282
-1.485694408	9.533736229	9.060696602
-0.741467476	10.760621071	9.101736069
0.716881275	10.731598854	9.162576675
-0.802055120	8.242520332	9.115236282
-3.425096512	13.227838516	9.006948471
0.603061676	8.271399498	9.240263939
2.744121075	11.786725044	9.154062271
3.459856033	10.533900261	9.185184479
5.612269402	11.792705536	9.053459167
4.899018288	10.534649849	9.084797859
3.469376564	13.064884186	9.108953476
9.834760666	9.534038544	8.825993538
6.981787205	9.477418900	8.920025826
7.633380413	10.729004860	8.924958229
9.092584610	10.760204315	8.882351875
7.739378452	8.266111374	8.873819351
4.887881279	13.066021919	9.083033562

9.147768021	8.241166115	8.810766220
4.521408558	7.491399765	11.162088394
6.949529648	2.315214157	8.999351501
5.595890045	4.799118519	9.014885902
-1.480408192	7.087140083	9.073872566
2.764796972	4.790457726	9.145782471
1.408736587	2.317390442	9.074501991
1.316648006	7.120255470	9.357083321
15.294635773	2.237671137	9.085914612
13.848333359	4.650646687	9.009143829
7.034520149	7.106608868	8.950697899
11.157734871	4.646899700	8.887499809
9.705529213	2.237181187	8.995590210
9.837177277	7.088321686	8.798850060
2.735346317	9.353329659	9.288827896
1.409086704	11.874859810	9.150083542
-5.551188469	14.372295380	8.998505592
-1.355159283	11.952388763	9.080388069
-2.812173843	9.537943840	8.984736443
-2.735419750	14.372483253	9.026280403
-5.475755692	9.539024353	8.832564354
9.704968452	11.951539040	8.919666290
2.773003578	14.213274956	9.082026482
6.944488049	11.873173714	8.980793953
5.617497921	9.368374825	8.990081787
5.584979057	14.215652466	9.066743851
3.097037315	7.560886860	9.944856644
5.223087311	7.434852600	9.321660042
3.691612720	6.593679428	11.564027786
5.184226990	8.002642632	11.886354446

C<sub>2</sub>N- NiFe \*COOH

C	N	Fe	Ni	O	H
49	24	1	1	2	1

Cartesian

-1.389228463	4.686629772	9.059345245
-0.675040722	3.454440594	9.079848289
1.492914915	4.719326973	9.143837929
0.786992550	3.471200228	9.119502068
-0.666301727	5.965191841	9.065897942
5.646829128	2.297229767	9.020627975
2.763519287	2.326872349	9.109169960
3.485465527	3.561511278	9.134495735
4.937017441	3.531868696	9.105659485

3.472358704	1.049218178	9.058247566
0.760771990	5.963880539	9.117018700
4.897119999	1.035686612	9.009899139
6.980030060	4.638354301	9.063467026
7.656787395	3.398427010	8.993789673
9.832404137	4.658457279	8.988552094
9.121282578	3.415503502	8.965908051
7.689578533	5.890026569	9.049446106
13.997257233	2.287877560	9.008316040
11.102758408	2.286177158	8.947296143
11.813631058	3.523308992	8.980451584
13.279983521	3.526190758	9.005075455
11.832455635	1.017587066	8.936190605
9.102615356	5.929396152	9.013715744
13.261343956	1.013105273	8.969885826
-5.620064259	11.890740395	8.993142128
-4.898129940	10.652657509	8.977355957
-2.719657898	11.892382622	8.942057610
-3.431005001	10.653334618	8.958906174
-4.881995201	13.169244766	9.003221512
1.400526047	9.534729958	8.978706360
-1.447988510	9.515520096	8.956133842
-0.736250877	10.760059357	8.922978401
0.724750519	10.774888039	8.918640137
-0.718150139	8.249711990	8.998811722
-3.451326370	13.160901070	8.967473984
0.694670677	8.291185379	9.031661987
2.726803780	11.885048866	8.914770126
3.443505287	10.654933929	8.967222214
5.619681835	11.860103607	8.971037865
4.885238171	10.631430626	8.990495682
3.480682373	13.144530296	8.917829514
9.768644333	9.492838860	8.998235703
6.870061398	9.459880829	9.028962135
7.587207317	10.701479912	9.005022049
9.048474312	10.721237183	9.002214432
7.615465641	8.211726189	9.048527718
4.906949043	13.136547089	8.949906349
9.044219971	8.216380119	9.017009735
4.639799595	7.148932457	11.510280609
6.988950253	2.240279436	8.981441498
5.625577927	4.696313858	9.180450439
-1.392376184	7.089863777	9.023345947
2.843012571	4.748508453	9.157392502

1.426308513	2.304046154	9.108756065
1.445954323	7.147923946	9.128862381
-1.306177616	2.273164511	9.049482346
13.912876129	4.703562260	9.026244164
6.942013264	7.032092094	9.087515831
11.167601585	4.693474770	8.994438171
9.767420769	2.248407125	8.939016342
9.769711494	7.086894989	9.000089645
2.766018391	9.472692490	9.012311935
1.387395382	11.943180084	8.888112068
-5.558916569	14.321383476	9.048888206
-1.384543896	11.928697586	8.915867805
-2.785565615	9.483155251	8.965403557
-2.744636536	14.296799660	8.966033936
11.105440140	9.475805283	8.982810020
9.683156013	11.904272079	9.001044273
2.802961349	14.296178818	8.908091545
6.949620724	11.876906395	8.982810020
5.519888401	9.440196991	9.031967163
5.618556023	14.270960808	8.972802162
3.367720604	7.640880585	9.533267975
5.283846378	6.445942402	9.949031830
5.320605755	7.022941113	12.674861908
3.542873383	7.811198711	11.559455872
4.805056572	7.496860981	13.371191978

C<sub>2</sub>N-NiMn\*CO

C	N	Ni	Mn	O
49	24	1	1	1

Cartesian

-1.403913856	4.712496758	8.994689941
-0.681131721	3.486345768	9.028854370
1.493429184	4.759994030	9.079056740
0.781974554	3.513005257	9.053063393
-0.686336756	5.992139816	9.011754990
5.637451172	2.333385944	8.996075630
2.753135681	2.358863831	9.033102036
3.482810974	3.589164972	9.033732414
4.927615166	3.565531731	9.019008636
3.462340832	1.083313584	9.008711815
0.742002010	5.999964714	9.111078262
4.888449669	1.074162841	8.984268188
6.970910072	4.681758881	9.017910004
7.645080090	3.436542749	8.997371674

9.825715065	4.684741974	8.985744476
9.110457420	3.444166183	8.986410141
7.683163643	5.917593956	9.017064095
13.992540359	2.306308508	9.000395775
11.090428352	2.305141211	8.972009659
11.803463936	3.541696787	8.971721649
13.269109726	3.543815136	8.975753784
11.821840286	1.035254359	8.976779938
9.098606110	5.957064152	8.995391846
13.255111694	1.027818441	8.999910355
-5.629990578	11.930701256	8.966825485
-4.909595490	10.693784714	8.935631752
-2.734052181	11.932674408	8.912015915
-3.447379589	10.696624756	8.910180092
-4.893768311	13.205948830	8.969346046
1.373901844	9.569286346	9.096570015
-1.472483158	9.553564072	8.923212051
-0.755844593	10.795724869	8.923986435
0.705090046	10.807066917	8.977913857
-0.750998020	8.283374786	8.977716446
-3.462534428	13.200112343	8.940024376
0.655358791	8.323536873	9.096822739
2.722095013	11.897383690	9.011123657
3.429452419	10.657024384	9.109674454
5.603466511	11.864989281	9.049139977
4.878857613	10.625824928	9.076499939
3.472186089	13.158465385	8.994113922
9.766304970	9.525190353	8.977428436
6.885735989	9.485762596	9.029610634
7.587197304	10.732622147	9.028043747
9.046153069	10.755779266	9.002825737
7.627378464	8.245215416	9.015011787
4.895740509	13.145755768	9.025848389
9.049584389	8.247089386	8.990766525
3.958337784	7.245137691	11.461950302
6.982867241	2.274389267	8.988696098
5.605792046	4.747096539	9.037206650
-1.413392782	7.119001865	8.960003853
2.847670794	4.782171726	9.044909477
1.419493675	2.340778589	9.032256126
1.393487930	7.187466621	9.225179672
-1.309522748	2.300544262	9.027090073
13.898597717	4.723506451	8.967240334
6.943036079	7.066835880	9.034343719



11.161053658	4.715076447	8.977193832
9.753051758	2.273380518	8.977733612
9.773496628	7.111609459	8.984448433
2.726856232	9.499539375	9.224603653
1.382401943	11.963009834	8.959824562
-5.570732117	14.358620644	9.002555847
-1.397265911	11.966295242	8.909387589
-2.807198048	9.522726059	8.907030106
-2.752932549	14.333733559	8.949545860
11.102487564	9.512537003	8.942957878
9.673112869	11.940715790	8.998271942
2.794466019	14.311122894	8.968391418
6.937323570	11.897253990	9.027107239
5.535221577	9.441450119	9.042119980
5.608828545	14.282705307	9.024551392
3.036862850	7.783529758	10.123541832
4.894031525	6.700044155	9.218376160
4.502636909	6.923536777	12.452453613

C<sub>2</sub>N- NiMn \*CHO

C	N	Ni	Mn	O	H
49	24	1	1	1	1

Cartesian

-1.405044675	4.690650463	9.101375580
-0.685574055	3.461213827	9.132678032
1.487414360	4.738075733	9.211571693
0.776617289	3.490813017	9.154836655
-0.690537453	5.971518040	9.154961586
5.631644249	2.325604439	8.908668518
2.751754999	2.343819141	9.050202370
3.477902651	3.578558922	9.071585655
4.928230762	3.559623480	9.005435944
3.458930016	1.069969296	8.970930099
0.735986710	5.985309124	9.278891563
4.883358479	1.064882398	8.905697823
6.986692905	4.659984589	8.946144104
7.649772167	3.411554813	8.866871834
9.833810806	4.658730984	8.837964058
9.116631508	3.418371201	8.846730232
7.700826645	5.888239384	8.943174362
13.990244865	2.279677868	9.057293892
11.093250275	2.274662971	8.919936180
11.807800293	3.511189461	8.919881821
13.271398544	3.517227650	8.999657631

11.820525169	1.002801776	8.991432190
9.111001968	5.936745167	8.847035408
13.252932549	1.002167702	9.049841881
-5.628650665	11.916679382	8.899740219
-4.909179688	10.680469513	8.867033958
-2.732263565	11.918683052	8.900460243
-3.447819471	10.684533119	8.896626472
-4.892561913	13.192445755	8.910180092
1.354633808	9.546978951	9.275256157
-1.480128765	9.537006378	9.019224167
-0.759521484	10.776300430	9.017640114
0.702012539	10.785450935	9.114749908
-0.764208794	8.263574600	9.118116379
-3.460795403	13.188570023	8.882351875
0.636739254	8.312499046	9.272213936
2.724733353	11.861833572	9.137573242
3.431176186	10.620551109	9.262025833
5.605712891	11.843517303	9.113651276
4.883459568	10.601110458	9.168822289
3.473203182	13.124399185	9.079704285
9.766297340	9.509958267	8.865989685
6.892391682	9.469766617	9.021167755
7.592722893	10.717144966	9.003041267
9.047683716	10.741541862	8.932643890
7.633144855	8.227908134	8.973648071
4.896882534	13.120840073	9.104094505
9.050617218	8.228268623	8.867465973
4.601475239	7.635101318	11.215151787
6.978599548	2.259387732	8.850185394
5.620793343	4.734660149	9.046800613
-1.422826767	7.100239277	9.092304230
2.835041761	4.759748936	9.147762299
1.418861866	2.325071096	9.083231926
1.379802704	7.176211834	9.412829399
-1.311502337	2.275239468	9.118314743
13.897576332	4.698562145	9.028997421
6.960000992	7.040277004	9.070343971
11.168100357	4.684944153	8.866134644
9.756654739	2.246821880	8.874666214
9.779977798	7.092601776	8.822861671
2.713977814	9.469796181	9.437598228
1.381870747	11.937186241	9.090143204
-5.571637630	14.343474388	8.960579872
-1.395875931	11.948266983	8.951921463

-2.811989307	9.508920670	8.950553894
-2.755477428	14.324539185	8.866835594
11.102569580	9.498905182	8.837045670
9.674776077	11.926737785	8.937018394
2.793959618	14.277791977	9.013139725
6.936225891	11.877396584	9.032094002
5.547335148	9.428740501	9.080621719
5.608038902	14.257818222	9.097398758
3.074210644	7.765589237	10.153062820
5.120340347	6.613335609	9.666611671
3.913372278	6.476377487	11.280546188
4.944439411	8.156763077	12.118860245

C<sub>2</sub>N- NiMn \*COOH

C	N	Ni	Mn	O	H
49	24	1	1	2	1
Cartesian					
-1.467087030			4.740986347		8.924814224
-0.748423100			3.511189461		8.978940010
1.426063061			4.776782036		9.065124512
0.712378740			3.530110598		9.035586357
-0.744717598			6.019649506		8.927549362
5.571174622			2.362697124		9.001565933
2.685420036			2.377871513		9.056916237
3.413381577			3.609757900		9.100079536
4.864283562			3.592537165		9.095526695
3.398943424			1.105534554		9.012437820
0.680317879			6.024693012		9.018305779
4.825534344			1.103531480		8.965836525
6.906255245			4.713159561		9.073548317
7.577663422			3.469038725		8.976761818
9.758148193			4.718563557		8.930303574
9.044281006			3.478780270		8.922690392
7.616820335			5.949383736		9.088416100
13.922436714			2.341873884		8.923337936
11.023952484			2.341023684		8.870940208
11.736406326			3.577117920		8.878139496
13.202232361			3.579092026		8.887626648
11.754806519			1.071151018		8.874234200
9.029724121			5.991951942		8.995409966
13.185457230			1.065141797		8.920295715
-5.684427738			11.956624985		8.959518433
-4.970148563			10.717447281		8.907965660
-2.792550087			11.958859444		8.827055931

-3.504770041	10.721669197	8.842661858
-4.949503899	13.229971886	8.949078560
1.323807716	9.595557213	8.923913956
-1.526987076	9.580555916	8.804051399
-0.812787056	10.822960854	8.786844254
0.652707100	10.836205482	8.823599815
-0.801632643	8.307728767	8.848367691
-3.520457745	13.229423523	8.883719444
0.609107971	8.348164558	8.923086166
2.662714958	11.932156563	8.902818680
3.369373798	10.697675705	9.026046753
5.546631813	11.911636353	9.049302101
4.823188782	10.672875404	9.089946747
3.410110950	13.195284843	8.904833794
9.701369286	9.556532860	9.005094528
6.823750973	9.528129578	9.143604279
7.528549671	10.774484634	9.089838028
8.988452911	10.791417122	9.042875290
7.562116146	8.278964996	9.139175415
4.834390163	13.186393738	8.976455688
8.981403351	8.281976700	9.041813850
3.473840714	7.285602093	11.637539864
6.919536591	2.309031963	8.950248718
5.541720390	4.770484924	9.156455994
-1.469002724	7.148543358	8.852058411
2.772825480	4.795458317	9.112877846
1.352776408	2.360074282	9.036503792
1.351289749	7.206027031	9.049446106
15.257775307	2.328803539	8.970443726
13.836223602	4.756492138	8.881992340
6.880603313	7.100527763	9.197351456
11.093053818	4.750684738	8.900910378
9.685976028	2.308599710	8.886384010
9.704399109	7.143269062	8.984268188
2.677700996	9.533347130	9.094697952
1.322440147	11.992998123	8.820323944
-5.629436493	14.380178452	9.007397652
-1.457011223	11.991873741	8.789004326
-2.862300873	9.550091743	8.821709633
-2.814199924	14.363073349	8.895095825
11.039087296	9.540291786	8.933994293
9.619132996	11.971814156	9.023526192
2.730278015	14.345002174	8.856683731
6.881247044	11.938121796	9.054756165

5.475167274	9.495201111	9.151128769
5.542977333	14.325143814	8.972694397
2.907562256	7.849660397	10.004508018
4.929900646	6.658814907	9.799361229
4.582822800	6.638193607	11.784059525
2.761625767	7.500866890	12.767688751
3.262754440	7.098466873	13.517117500

C<sub>2</sub>N-NiCr\*CO

C	N	Ni	Cr	O
49	24	1	1	1

Cartesian

-1.404221654	4.715652466	8.992835999
-0.679168582	3.491331816	9.023940086
1.495184660	4.772112846	9.079397202
0.783995867	3.524605989	9.050831795
-0.690172195	5.996333122	9.015786171
5.634630680	2.348358631	8.996166229
2.753651142	2.370911121	9.031661987
3.486496449	3.602523565	9.027954102
4.924744129	3.581743717	9.013787270
3.458205700	1.093818784	9.012023926
0.738016367	6.009317398	9.116729736
4.882750511	1.086858511	8.986302376
6.988689423	4.681917667	9.024911880
7.648191452	3.432075500	9.004770279
9.830715179	4.682104588	8.995679855
9.114044189	3.441010237	8.994294167
7.694469929	5.903255463	9.026136398
13.997365952	2.302763462	8.993807793
11.093624115	2.301509857	8.973072052
11.807083130	3.537359238	8.973828316
13.272619247	3.540097237	8.973449707
11.824561119	1.031320214	8.973683357
9.106492043	5.956545353	9.007667542
13.258665085	1.022731543	8.993268013
-5.641480446	11.936422348	8.976852417
-4.921376705	10.698742867	8.947026253
-2.744901657	11.940370560	8.924310684
-3.458536386	10.704449654	8.923625946
-4.904009819	13.214667320	8.978471756
1.359567165	9.572788239	9.117072105
-1.484214306	9.560279846	8.941752434
-0.767160416	10.802095413	8.942525864

0.695755005	10.812082291	8.996490479
-0.761905670	8.287914276	8.994870186
-3.471911430	13.210099220	8.948574066
0.643170357	8.332571983	9.116567612
2.716670036	11.894963264	9.017495155
3.419577122	10.651360512	9.116963387
5.594064236	11.854901314	9.047142029
4.869656086	10.614988327	9.078065872
3.468434334	13.154070854	8.993160248
9.755098343	9.524512291	8.985870361
6.878647327	9.475530624	9.026782990
7.578303814	10.726208687	9.028241158
9.036602020	10.754828453	9.008693695
7.616247177	8.240661621	9.014562607
4.891282082	13.138751984	9.021348000
9.039310455	8.242175102	8.998002052
4.061247349	7.190910339	11.324951172
6.980347157	2.275671721	8.993466377
5.613487244	4.772732735	9.036197662
-1.421587706	7.123281956	8.969958305
2.850590706	4.797173500	9.041579247
1.422097445	2.353013277	9.030708313
1.385301113	7.196919441	9.235440254
-1.303565860	2.302763462	9.018557549
13.898189545	4.721503258	8.966429710
6.928826809	7.049168587	9.037260056
11.165470123	4.711112976	8.983763695
9.756288528	2.270339727	8.981567383
9.774643898	7.112935066	8.997012138
2.714201450	9.497075081	9.234720230
1.374973297	11.965415955	8.972208023
-5.577486992	14.369196892	9.008910179
-1.407857895	11.972448349	8.924165726
-2.818055868	9.530234337	8.922725677
-2.761168957	14.344051361	8.953289986
11.092134476	9.516255379	8.953020096
9.661390305	11.942055702	9.005508423
2.794359207	14.309091568	8.967240334
6.927589417	11.888117790	9.025650024
5.526136398	9.428710938	9.041130066
5.608097076	14.274087906	9.016056061
3.108148098	7.734562874	9.988451958
4.983837605	6.655688286	9.226386070
4.521081924	6.931275368	12.376314163

C<sub>2</sub>N- NiCr \*CHO

C	N	Ni	Cr	O	H
49	24	1	1	1	1

## Cartesian

-1.455387115	4.659307480	9.074592590
-0.721623063	3.433732748	9.108269691
1.426621675	4.731461048	9.183131218
0.739402771	3.479270220	9.131741524
-0.760897875	5.954700947	9.120402336
5.607240200	2.414013147	9.007956505
2.746587276	2.389342070	9.069479942
3.451094151	3.645395041	9.077291489
4.908692837	3.671967983	9.031266212
3.464012623	1.118864417	9.029250145
0.660518169	5.962813854	9.253386497
4.881967545	1.132712960	9.010134697
6.968878269	4.731763840	8.958563805
7.628622055	3.469254732	8.963064194
9.837679863	4.653442383	8.897760391
9.096323013	3.429712296	8.948087692
7.737224579	5.924251556	8.895996094
13.966634750	2.225061893	9.062279701
11.051710129	2.229918242	8.999981880
11.780945778	3.457351685	8.969364166
13.240407944	3.457092285	9.014490128
11.787539482	0.949036002	9.047628403
9.148158073	5.946198940	8.854902267
13.228300095	0.941974759	9.065322876
-5.609216690	11.962763786	8.931077957
-4.876892090	10.740086555	8.893278122
-2.696306229	11.969580650	8.981477737
-3.425657511	10.743069649	8.938692093
-4.870940208	13.239353180	8.973323822
1.352671146	9.493169785	9.262458801
-1.492008686	9.544932365	9.034938812
-0.747574329	10.771833420	9.067356110
0.707978725	10.740677834	9.146537781
-0.807122707	8.252017975	9.109062195
-3.431935310	13.246802330	8.980398178
0.595765591	8.276947975	9.271260262
2.739227772	11.791625023	9.157211304
3.451852322	10.531393051	9.225629807
5.599391937	11.761866570	9.070631981

4.889484406	10.502081871	9.118404388
3.468528748	13.063355446	9.109007835
9.831100464	9.536113739	8.841653824
6.973060608	9.451666832	8.938223839
7.621267796	10.712058067	8.942202568
9.081678391	10.757047653	8.899488449
7.742365837	8.265635490	8.866260529
4.884012699	13.050040245	9.092934608
9.150287628	8.241411209	8.821782112
4.661234379	7.397615910	11.087262154
6.946617126	2.328760386	8.989020348
5.601936340	4.857899189	9.017135620
-1.479759216	7.092500687	9.069804192
2.767076254	4.800948620	9.116370201
1.414585233	2.331930399	9.075275421
1.306921959	7.135746956	9.417491913
15.305377007	2.239241838	9.103949547
13.851559639	4.646957397	9.021473885
7.035035610	7.095973969	8.897184372
11.170740128	4.645300388	8.909478188
9.711179733	2.238204241	8.990099907
9.854032516	7.093394279	8.810009956
2.714570522	9.375133514	9.357624054
1.408770084	11.882122993	9.131850243
-5.556172371	14.386519432	9.005508423
-1.360558510	11.965343475	9.036144257
-2.818097591	9.551633835	8.962433815
-2.742758751	14.394502640	8.992584229
-5.479150295	9.547497749	8.838306427
9.691506386	11.952893257	8.934840202
2.776755333	14.214269638	9.076211929
6.931350708	11.852408409	8.997083664
5.602390289	9.309319496	9.032976151
5.587183952	14.197077751	9.079416275
3.042556763	7.664383411	10.124855995
5.152599812	7.188964844	9.179316521
3.783765793	6.480009079	11.399399757
5.107676506	8.031190872	11.879028320

C<sub>2</sub>N- NiCr \*COOH

C	N	Ni	Cr	O	H
49	24	1	1	2	1

Cartesian

-1.477503538	4.742571831	8.913257599
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-0.755087256	3.514835596	8.971380234
1.416054010	4.786941528	9.045522690
0.703310013	3.540716648	9.028043747
-0.761565208	6.021652222	8.913023949
5.559576988	2.381257772	9.029088020
2.676492214	2.390913010	9.065897942
3.408855438	3.625753403	9.087768555
4.851670742	3.613922358	9.087947845
3.386596203	1.117927670	9.040356636
0.663635969	6.032114506	8.999928474
4.812072754	1.119469643	9.003834724
6.916164398	4.716315746	9.063179970
7.573087692	3.465724230	9.005255699
9.756450653	4.715018749	8.966177940
9.040370941	3.474860668	8.963675499
7.620830536	5.934972763	9.067644119
13.919775009	2.335072041	8.933777809
11.018379211	2.334740639	8.908614159
11.731288910	3.569552422	8.909873962
13.196492195	3.572347879	8.902080536
11.748716354	1.064233899	8.902691841
9.031562805	5.990929127	9.010835648
13.182004929	1.056481004	8.937521935
-5.703804970	11.964941025	8.991647720
-4.988826275	10.725330353	8.940150261
-2.809721947	11.969061852	8.878662109
-3.523697853	10.732578278	8.881956100
-4.967300415	13.240707397	8.987345695
1.302068233	9.595714569	8.946539879
-1.548418999	9.588251114	8.839907646
-0.831706047	10.828841209	8.838018417
0.635186195	10.839173317	8.866476059
-0.825144768	8.311993599	8.866007805
-3.536191463	13.241802216	8.933994293
0.585837364	8.355182648	8.938278198
2.651043415	11.927357674	8.923193932
3.353874207	10.688208580	9.025667191
5.530542374	11.900077820	9.055655479
4.808038712	10.658853531	9.078263283
3.399678230	13.187214851	8.923500061
9.684146881	9.556360245	9.016992569
6.812843800	9.516068459	9.114030838
7.514389038	10.769181252	9.089208603
8.971879959	10.791244507	9.055350304

7.545361042	8.275448799	9.105155945
4.823749065	13.175484657	8.989235878
8.966237068	8.277207375	9.042407990
3.637542248	7.254878998	11.483136177
6.909053326	2.310646296	8.995878220
5.539232731	4.803066730	9.127854347
-1.488712788	7.153630733	8.855172157
2.763972282	4.811598301	9.077903748
1.347069144	2.371112823	9.042407990
1.326072693	7.213534832	9.043523788
15.255395889	2.328630686	8.970678329
13.825092316	4.751390934	8.881757736
6.857059002	7.085079193	9.139554024
11.090566635	4.744358540	8.935542107
9.680353165	2.304017305	8.931528091
9.701720238	7.143672943	9.004985809
2.659232140	9.525276184	9.078497887
1.307424068	11.992320061	8.859653473
-5.644095898	14.392541885	9.035820007
-1.473310471	11.999007225	8.847053528
-2.882418156	9.559745789	8.852219582
-2.829243183	14.375697136	8.946450233
11.023037910	9.545927048	8.956511497
9.600120544	11.974825859	9.045053482
2.722706795	14.340188980	8.883972168
6.865864754	11.929144859	9.066887856
5.461706638	9.478456497	9.112554550
5.535664558	14.314235687	8.983530045
2.998300076	7.782853127	9.859824181
4.970467567	6.659161091	9.623268127
4.751582146	6.615453720	11.604689598
2.954162598	7.494930267	12.622104645
3.465666771	7.111018181	13.373226166

C<sub>2</sub>N-CoFe\*CO

C	N	Fe	Co	O
49	24	1	1	1

Cartesian

-1.411859274	4.714643955	8.998434067
-0.696906090	3.481647968	9.002555847
1.467196703	4.751650333	8.999261856
0.764178514	3.501750708	9.006066322
-0.692559958	5.996030331	9.004121780
5.628015995	2.351658821	9.034002304

2.745839119	2.366285324	9.011394501
3.466145992	3.605002403	8.999279976
4.916132927	3.592104673	9.029357910
3.456566572	1.091066480	9.016937256
0.734089851	5.993638039	9.017999649
4.881053448	1.085071564	9.017189980
6.970376968	4.684843063	9.116225243
7.636950970	3.440765142	9.093689919
9.820207596	4.688229561	9.079073906
9.103519440	3.449007988	9.079974174
7.686400414	5.920000553	9.116441727
13.976931572	2.310055256	9.006695747
11.079995155	2.307216406	9.029934883
11.794445038	3.543742895	9.029844284
13.260314941	3.547950983	9.010601997
11.809610367	1.034966111	9.009324074
9.096866608	5.963563442	9.092105865
13.240327835	1.033827662	9.005598068
-5.631346703	11.932387352	9.016325951
-4.911060333	10.694649696	9.014220238
-2.730682850	11.934908867	9.008711815
-3.445041656	10.698338509	9.011232376
-4.893277168	13.210977554	9.015552521
1.375258446	9.556388855	9.049571991
-1.468963623	9.552396774	9.015498161
-0.751875877	10.792684555	9.013409615
0.711413383	10.800149918	9.020177841
-0.746530056	8.279815674	9.023003578
-3.461012363	13.206784248	9.011322021
0.662289143	8.325367928	9.050778389
2.717435837	11.892599106	9.001565933
3.432115078	10.656678200	9.016236305
5.604014874	11.880811691	9.003816605
4.875005245	10.644976616	8.997245789
3.465779781	13.157659531	8.995896339
9.759034157	9.529541969	9.017585754
6.870685101	9.492924690	8.997336388
7.580898762	10.737046242	9.009863853
9.040393829	10.760016441	9.016254425
7.608491898	8.245273590	9.028259277
4.890441418	13.156116486	9.000018120
9.037829399	8.248486519	9.032489777
4.195198536	7.108309269	10.967634201
6.968748093	2.284173965	9.058842659

5.603237152	4.767717838	9.093420029
-1.422402859	7.122128963	9.009359360
2.815581322	4.783828735	8.971110344
1.410225630	2.338789940	9.003492355
1.418897152	7.177148819	9.072197914
-1.325804710	2.298599005	9.002465248
13.889929771	4.727051735	9.001170158
6.934309006	7.063795090	9.098352432
11.154405594	4.716848850	9.051605225
9.743692398	2.277746916	9.052380562
9.765667915	7.120154858	9.058553696
2.748263359	9.471798897	9.070704460
1.377709866	11.963067055	9.005615234
-5.572295189	14.362338066	9.016703606
-1.394087791	11.964277267	9.006786346
-2.804444313	9.525190353	9.011412621
-2.757458687	14.344858170	9.011861801
11.096154213	9.515692711	9.014616013
9.671764374	11.944001198	9.015768051
2.784616470	14.309855461	8.999279976
6.934253693	11.905741692	9.000827789
5.525029182	9.463080406	8.967275620
5.599553108	14.292864799	9.000504494
3.294340611	7.617823124	9.346985817
5.109459877	6.591114521	9.423072815
4.196496010	7.107877254	12.154589653

C<sub>2</sub>N- CoFe \*CHO

C	N	Fe	Co	O	H
49	24	1	1	1	1

Cartesian

-1.459155917	4.654883385	9.057312012
-0.731340408	3.425230742	9.087641716
1.414758444	4.714024067	9.172584534
0.731998920	3.461314678	9.117396355
-0.758767605	5.946631432	9.107046127
5.608222485	2.387670755	9.043740273
2.741961479	2.375133514	9.080135345
3.442225933	3.630235195	9.110322952
4.909608841	3.643896341	9.072756767
3.465543509	1.103848577	9.038357735
0.657382250	5.945161343	9.216917992
4.885745049	1.110895276	9.037151337
6.944252014	4.723895550	8.987363815

7.618963242	3.464830875	8.983386040
9.817319870	4.653975487	8.879418373
9.085681915	3.427363396	8.948807716
7.705634594	5.938128948	8.926019669
13.951858521	2.230998993	9.043235779
11.042509079	2.230984688	8.988840103
11.766685486	3.462107182	8.945531845
13.229850769	3.463418484	8.992584229
11.777571678	0.950304091	9.037961960
9.120044708	5.945752144	8.843507767
13.216327667	0.949309766	9.052740097
-5.596362591	11.952201843	8.921051979
-4.870310783	10.728427887	8.885106087
-2.691147804	11.953382492	9.009431839
-3.417395115	10.728788376	8.951292038
-4.861529350	13.225994110	8.973666191
1.361533165	9.478053093	9.240390778
-1.484296322	9.534023285	9.065177917
-0.742765427	10.760045052	9.104166031
0.719626904	10.730820656	9.163475990
-0.797121525	8.240546227	9.126468658
-3.425262451	13.229855537	9.002034187
0.608228207	8.270895004	9.255258560
2.745086193	11.787070274	9.138653755
3.459406376	10.537560463	9.177102089
5.611754417	11.785442352	9.068526268
4.899359226	10.529937744	9.094373703
3.468986034	13.063111305	9.095237732
9.833080292	9.533692360	8.821331978
6.985873222	9.473628998	8.935793877
7.629503727	10.728427887	8.942669868
9.091686249	10.759627342	8.888363838
7.740927219	8.270635605	8.893367767
4.887365818	13.061612129	9.084311485
9.145862579	8.239941597	8.810550690
4.606704235	7.472982407	11.130858421
6.946018219	2.320027590	9.008424759
5.590465069	4.813586712	9.039905548
-1.477595806	7.088696480	9.081126213
2.758474112	4.784866333	9.151830673
1.407197714	2.315358400	9.075096130
1.323596001	7.116782665	9.370637894
15.290467262	2.236330986	9.081954002
13.846293449	4.649911880	9.001224518

7.024694920	7.112531662	9.001115799
11.152709961	4.647188187	8.878986359
9.701761246	2.238319635	8.991197586
9.836378098	7.087889671	8.794458389
2.737966537	9.360031128	9.290628433
1.406890392	11.873679161	9.138132095
-5.551305294	14.371056557	9.000486374
-1.354709625	11.950947762	9.075582504
-2.810143471	9.538346291	8.979029655
-2.736168861	14.375826836	9.026622772
-5.476720810	9.539571762	8.819964409
9.704271317	11.949750900	8.922528267
2.772155762	14.211430550	9.066078186
6.945810318	11.872698784	8.994689941
5.610384941	9.347839355	8.987040520
5.583338737	14.212237358	9.070667267
3.142763138	7.562443256	9.876689911
5.217146397	7.457045078	9.342450142
3.759287119	6.541369438	11.430881500
5.095511913	8.059492111	11.932937622

C<sub>2</sub>N- CoFe \*COOH

C	N	Fe	Co	O	H
49	24	1	1	2	1

Cartesian

-1.360792279	4.715249538	9.082781792
-0.652985573	3.482671261	9.101699829
1.536884546	4.735856056	9.186300278
0.806385279	3.496462107	9.147888184
-0.623438597	5.982657433	9.092483521
5.653718472	2.266650677	8.992763519
2.757937193	2.310862303	9.108324051
3.503112555	3.531407595	9.127764702
4.941261292	3.489674807	9.072954178
3.461468697	1.030153036	9.049895287
0.808751822	5.999373913	9.160865784
4.889491558	1.014517546	8.983008385
6.979322433	4.620297909	9.058967590
7.655737877	3.385284662	8.987976074
9.818776131	4.673617363	9.023741722
9.120907784	3.423876047	8.973629951
7.657114983	5.872906685	9.093510628
14.010584831	2.324739695	9.007704735
11.118516922	2.325863838	8.932554245

11.821018219	3.566021681	8.988227844
13.293251038	3.569696426	9.011808395
11.845908165	1.059939623	8.899218559
9.067989349	5.933229446	9.073007584
13.273281097	1.048223853	8.952857971
-5.647502899	11.875090599	9.020195961
-4.931666851	10.629556656	8.997282028
-2.756764412	11.874168396	8.896572113
-3.459383249	10.631963730	8.941356659
-4.909649849	13.151577950	9.004697800
1.389601231	9.573509216	8.936729431
-1.456399918	9.523893356	8.914752007
-0.760170460	10.771947861	8.847612381
0.707536221	10.809055328	8.836073875
-0.703299522	8.264684677	8.980649948
-3.483224392	13.141879082	8.937899590
0.714038849	8.320466995	9.022697449
2.709206581	11.937834740	8.836434364
3.420622826	10.717879295	8.931365967
5.603897572	11.891331673	8.984429359
4.860543728	10.674719810	9.008225441
3.472959518	13.188165665	8.853318214
9.722137451	9.484191895	9.077256203
6.822305679	9.458728790	9.126162529
7.552605152	10.704261780	9.085247993
9.015104294	10.716553688	9.078102112
7.552142620	8.202834129	9.147743225
4.902013779	13.169331551	8.926865578
8.985963821	8.214622498	9.110952377
4.690330505	6.992736816	11.429874420
7.000989437	2.215450048	8.955072403
5.614920616	4.667564869	9.131472588
-1.358098984	7.108396053	9.026639938
2.887548923	4.733651638	9.185562134
1.428546309	2.313312054	9.123894691
1.479831696	7.189887524	9.161856651
-1.293973207	2.304651260	9.057042122
-2.701906204	4.740769863	9.041921616
6.877269268	7.010216713	9.159731865
11.155786514	4.727252960	9.027287483
9.783436775	2.269460917	8.924274445
9.725133896	7.093927383	9.086183548
2.749984741	9.540955544	8.995535851
1.358932018	11.977318764	8.785458565

-5.577577591	14.309667587	9.057149887
-1.422540665	11.927789688	8.837676048
-2.793277025	9.470285416	8.949240685
-2.765335083	14.268611908	8.926650047
11.063209534	9.458972931	9.030941963
9.656007767	11.894746780	9.054000854
2.807877541	14.345160484	8.839566231
6.936283112	11.884298325	9.029016495
5.467347622	9.470761299	9.104022980
5.620976448	14.300372124	8.966267586
3.436303616	7.859690189	9.728027344
5.074112892	6.396903515	9.703727722
5.501711845	6.679609299	12.462570190
3.697023869	7.773586750	11.696219444
5.157725334	7.137086868	13.267782211

C<sub>2</sub>N-CoMn\*CO

C	N	Co	Mn	O
49	24	1	1	1

Cartesian

-1.397307634	4.711343765	8.973594666
-0.676489115	3.482944965	8.995302200
1.494161129	4.758120537	9.035316467
0.784212589	3.510396957	9.020538330
-0.681552649	5.992413521	8.993771553
5.641469955	2.336023092	9.019619942
2.757395029	2.360391378	9.031193733
3.487004042	3.592104673	9.033605576
4.931666851	3.569408178	9.042065620
3.464869976	1.084754586	9.024641991
0.747201681	5.999661922	9.053459167
4.890529633	1.076526165	9.011898041
6.990686417	4.675865173	9.049175262
7.655488014	3.427939653	9.016488075
9.836414337	4.679756165	8.997318268
9.119808197	3.438315392	8.996471405
7.699961185	5.904667377	9.049770355
13.998813629	2.301351309	8.975753784
11.098582268	2.299550056	8.969597816
11.812532425	3.536134243	8.970029831
13.277179718	3.539549351	8.964630127
11.827713966	1.029374838	8.964845657
9.113065720	5.953086853	9.017981529
13.260810852	1.023394346	8.975952148



-5.630756378	11.931047440	9.010530472
-4.910686016	10.693885803	8.996093750
-2.735608101	11.933784485	8.983962059
-3.448594093	10.698468208	8.984645844
-4.894226074	13.207260132	9.010512352
1.366647243	9.566173553	9.079668045
-1.475345135	9.555265427	8.991990089
-0.758607388	10.797080994	8.990298271
0.704882145	10.809213638	9.009287834
-0.753934383	8.281775475	9.013031960
-3.462892056	13.202230453	8.995553970
0.653520107	8.330382347	9.081665993
2.723767281	11.891518593	8.989146233
3.431881905	10.650596619	9.048527718
5.605620861	11.863101006	9.016794205
4.880263329	10.624398232	9.030221939
3.474982262	13.152240753	8.971343994
9.766372681	9.523143768	9.011502266
6.886359215	9.481050491	9.030779839
7.588071346	10.728946686	9.028638840
9.046577454	10.753746986	9.022878647
7.628344059	8.241295815	9.041255951
4.899160385	13.142052650	8.993124008
9.051332474	8.243140221	9.019331932
3.870105267	7.295704365	11.249423981
6.987385750	2.270570517	9.011322021
5.620601654	4.749286652	9.080783844
-1.414998293	7.119477272	8.984321594
2.845981598	4.780860424	9.019313812
1.424818277	2.340605736	9.015840530
1.404146194	7.189642429	9.148860931
-1.302991748	2.296350956	8.991179466
13.904823303	4.720163345	8.957825661
6.951256275	7.054500103	9.080748558
11.170988083	4.709283352	8.982162476
9.761879921	2.268091679	8.980974197
9.781175613	7.110442162	9.012618065
2.730034828	9.486800194	9.145458221
1.380988598	11.962779045	8.979335785
-5.569749832	14.360695839	9.023885727
-1.399121284	11.967432976	8.980613708
-2.809003115	9.524325371	8.983116150
-2.752124786	14.335043907	8.996345520
11.103108406	9.512264252	8.996940613

9.672089577	11.939491272	9.022806168
2.798743248	14.306194305	8.956979752
6.939004421	11.893017769	9.012762070
5.536369324	9.442112923	9.014831543
5.613688469	14.277805328	8.990262032
3.163709164	7.705972195	9.708137512
5.008314133	6.640240192	9.397134781
4.093653679	7.163429737	12.401208878

C<sub>2</sub>N- CoMn \*CHO

C	N	Co	Mn	O	H
49	24	1	1	1	1

Cartesian

-1.443173647	4.659883499	9.069120407
-0.714584470	3.432897091	9.100872040
1.438619137	4.725235939	9.168660164
0.748404980	3.473621130	9.122112274
-0.741695881	5.955133438	9.111348152
5.618139744	2.388160467	9.020232201
2.751861811	2.375767469	9.064062119
3.455937386	3.627324343	9.071262360
4.921156883	3.644213676	9.031949997
3.470651627	1.103473902	9.028997421
0.679712057	5.962108135	9.224100113
4.891027927	1.113186598	9.021114349
6.965335369	4.718275547	8.965548515
7.633639336	3.457942486	8.972406387
9.834226608	4.652101994	8.879976273
9.102064133	3.424322844	8.947296143
7.725785732	5.925361156	8.914841652
13.970727921	2.231460094	9.058877945
11.060445786	2.232569695	8.998056412
11.784147263	3.463303328	8.957196236
13.247030258	3.464210987	9.007649422
11.794069290	0.953402400	9.047555923
9.135820389	5.941688538	8.838990211
13.232616425	0.946773529	9.064277649
-5.601154327	11.952749252	8.925191879
-4.874279022	10.729278564	8.886707306
-2.694983006	11.955846786	8.999478340
-3.421388626	10.730978966	8.948375702
-4.864965916	13.226008415	8.974386215
1.358828545	9.494235992	9.233370781
-1.485877514	9.538837433	9.052542686

-0.744055271	10.766861916	9.087048531
0.716298580	10.742117882	9.150192261
-0.796198368	8.247247696	9.111707687
-3.428466320	13.231455803	8.994167328
0.608361244	8.279829979	9.241793633
2.741815567	11.792849541	9.145241737
3.456170082	10.538785934	9.188424110
5.607511044	11.775845528	9.063161850
4.895491600	10.521996498	9.088217735
3.473761082	13.067261696	9.101034164
9.831025124	9.531718254	8.816058159
6.977104187	9.459708214	8.917451859
7.625618458	10.717432976	8.932769775
9.088850021	10.755290031	8.885087967
7.737083435	8.264496803	8.873729706
4.891550541	13.056697845	9.087065697
9.144239426	8.237996101	8.799444199
4.541493893	7.446121693	11.192273140
6.959163666	2.314810753	8.995517731
5.603659630	4.818572998	8.997174263
-1.466979742	7.088955879	9.077705383
2.779290199	4.783828735	9.116225243
1.418529034	2.324177742	9.074772835
1.333487034	7.140689850	9.374112129
15.308578491	2.241331339	9.098945618
13.863157272	4.651626587	9.016325951
7.033130646	7.097342491	8.985779762
11.169490814	4.648009777	8.885663986
9.718866348	2.236907482	8.993448257
9.844289780	7.090468884	8.791866302
2.729181290	9.365189552	9.318204880
1.409160614	11.886662483	9.139122009
-5.550647736	14.374155045	9.000900269
-1.359078407	11.956265450	9.059328079
-2.811973572	9.541257858	8.975700378
-2.735578537	14.374918938	9.011951447
-5.478484631	9.538994789	8.817605972
9.698329926	11.947503090	8.925444603
2.783170700	14.216935158	9.074069977
6.944313049	11.859152794	8.985744476
5.600400925	9.336311340	8.965116501
5.593314171	14.206228256	9.078425407
3.056932926	7.675595284	10.031489372
5.139884949	7.298341274	9.330642700

3.590702057	6.586834431	11.466593742
5.020534992	8.016721725	12.010571480

C<sub>2</sub>N- CoMn \*COOH

C	N	Co	Mn	O	H
49	24	1	1	2	1

Cartesian

-1.463467479	4.727627754	8.886347771
-0.744570851	3.497370005	8.942111969
1.422011375	4.770484924	9.010817528
0.714375734	3.520974398	9.001709938
-0.747321367	6.007501602	8.884727478
5.574744225	2.360232830	9.059778214
2.691493511	2.379889011	9.072341919
3.417608023	3.614887714	9.102240562
4.868601799	3.594021559	9.123821259
3.402237892	1.106226325	9.059687614
0.676474333	6.011377811	8.945856094
4.828396797	1.101225853	9.037313461
6.922787189	4.701443672	9.105983734
7.588487625	3.454181194	9.029394150
9.772342682	4.700492859	8.971991539
9.055455208	3.461502075	8.974853516
7.635922909	5.931168556	9.111797333
13.930765152	2.320358753	8.913707733
11.031507492	2.319090605	8.910342216
11.745541573	3.554032087	8.902673721
13.210536957	3.557505131	8.884799957
11.761354446	1.047935605	8.903736115
9.048692703	5.976907730	9.030546188
13.193744659	1.043900609	8.923427582
-5.687988281	11.953138351	9.026945114
-4.969107628	10.715329170	8.986878395
-2.791459560	11.954435349	8.943138123
-3.505369425	10.720229149	8.940132141
-4.951683044	13.228443146	9.025110245
1.311760902	9.577802658	8.911727905
-1.533318281	9.573768616	8.884962082
-0.814891338	10.813925743	8.892395973
0.651518822	10.824028015	8.891783714
-0.812439919	8.296705246	8.873928070
-3.519717693	13.225576401	8.987093925
0.597618103	8.346190453	8.901576042
2.666959286	11.908782959	8.922006607

3.375764370	10.673667908	8.980542183
5.549727440	11.890942574	9.035783768
4.822730541	10.651216507	9.048510551
3.414854527	13.170354843	8.923031807
9.706993103	9.545552254	9.043830872
6.826547146	9.508156776	9.129581451
7.530372143	10.755130768	9.095651627
8.988204956	10.777956963	9.072125435
7.572168350	8.264064789	9.142470360
4.839365482	13.165325165	8.973053932
8.992527962	8.268157005	9.067841530
3.458961010	7.408207417	11.365578651
6.923480034	2.298858404	9.020520210
5.555597782	4.768409729	9.181457520
-1.478919983	7.139493942	8.858214378
2.769663811	4.798080921	9.070991516
1.358924866	2.355794430	9.032760620
1.347288609	7.196646214	8.968841553
15.267219543	2.312620401	8.945261955
13.838446617	4.737167835	8.861021996
6.897418499	7.082730293	9.202409744
11.105883598	4.728665352	8.931311607
9.694296837	2.289923668	8.941428185
9.719259262	7.129867554	9.023759842
2.682944298	9.498242378	8.989704132
1.321484566	11.979379654	8.889408112
-5.628962517	14.380510330	9.057222366
-1.455039501	11.984768867	8.914518356
-2.866768360	9.546071053	8.903790474
-2.812453270	14.358634949	8.996525764
11.044553757	9.535666466	8.997714043
9.615315437	11.962692261	9.065573692
2.735678673	14.323199272	8.894142151
6.880873203	11.919143677	9.060390472
5.477364063	9.471856117	9.107675552
5.550099373	14.302404404	8.962253571
3.055117130	7.739117146	9.589949608
4.965383530	6.658858299	9.726515770
4.531010628	6.790700912	11.712834358
2.626927853	7.804080009	12.351131439
3.020612240	7.529991150	13.213296890

C<sub>2</sub>N-CoCr\*CO

C N Co Cr O

49	24	1	1	1
Cartesian				
-1.401060224		4.709427357		8.976222038
-0.677462697		3.482872725		8.987633705
1.497713804		4.754099846		9.000180244
0.784645081		3.509013653		8.999675751
-0.682085037		5.990885735		8.985834122
5.638599396		2.341167688		9.028403282
2.755506516		2.358157873		9.014867783
3.488301992		3.588934422		9.010296822
4.928812504		3.572304726		9.030203819
3.464970112		1.081728458		9.020483017
0.746619463		5.995800018		9.016812325
4.890295982		1.079177737		9.020843506
6.985934734		4.680952072		9.052271843
7.648041725		3.432911396		9.039113998
9.830565453		4.681816578		9.028818130
9.115133286		3.441716194		9.028710365
7.691649914		5.905027866		9.052380562
13.996076584		2.304161549		8.988714218
11.094463348		2.303513050		9.002862930
11.807092667		3.538439989		9.003474236
13.272387505		3.540442944		8.989361763
11.825267792		1.033784389		8.987759590
9.103555679		5.956243038		9.039258003
13.257616043		1.024806738		8.988300323
-5.627577782		11.928626060		9.019656181
-4.911143303		10.689980507		9.016865730
-2.732762814		11.931623459		9.010601997
-3.446015120		10.695644379		9.013013840
-4.891106606		13.204479218		9.019313812
1.378793716		9.563234329		9.064529419
-1.470893860		9.552858353		9.017388344
-0.754879951		10.794025421		9.014165878
0.710905552		10.805611610		9.018522263
-0.746846199		8.278172493		9.023813248
-3.460463047		13.203152657		9.014616013
0.662979603		8.321807861		9.067212105
2.724249363		11.894055367		8.980092049
3.434377193		10.654776573		9.012078285
5.607243061		11.864152908		8.997570038
4.885197639		10.624730110		8.996598244
3.474890709		13.157270432		8.972873688
9.762637138		9.521054268		9.020915985

6.888264179	9.480920792	9.008262634
7.588362694	10.730719566	9.012798309
9.048323631	10.754265785	9.018846512
7.621929169	8.240647316	9.029196739
4.899003029	13.143651962	8.986140251
9.043304443	8.242146492	9.027935982
3.857532978	7.310475349	11.244546890
6.986553669	2.273106575	9.034200668
5.609193802	4.764259338	9.060101509
-1.411404133	7.117949963	8.995446205
2.847529411	4.779649734	8.986013412
1.425467610	2.337723494	9.001242638
1.410752296	7.177940845	9.109709740
-1.306477666	2.296884060	8.988929749
13.902658463	4.720422745	8.978724480
6.929875374	7.055162907	9.059705734
11.164889336	4.712957859	9.015749931
9.756454468	2.271175861	9.014885902
9.776674271	7.109188080	9.034416199
2.743188858	9.488832474	9.106577873
1.383350849	11.961423874	8.988696098
-5.567968845	14.358677864	9.020735741
-1.396566868	11.963729858	9.006929398
-2.804718256	9.522841454	9.012618065
-2.751010418	14.335908890	9.016163826
11.101478577	9.509583473	9.018432617
9.674226761	11.937978745	9.019638062
2.797852516	14.308572769	8.975250244
6.941849232	11.893565178	8.999225616
5.536909580	9.442444801	8.982414246
5.611931801	14.281192780	8.988317490
3.143740654	7.720556259	9.722807884
4.969743252	6.657042503	9.265266418
4.201047421	7.113367558	12.356856346

C<sub>2</sub>N- CoCr\*CHO

C	N	Co	Cr	O	H
49	24	1	1	1	1

Cartesian

-1.451343894	4.656483173	9.070181847
-0.720741034	3.430418491	9.100817680
1.429558992	4.725451946	9.160956383
0.742315054	3.473361731	9.121985435
-0.751080513	5.952971935	9.109908104

5.608447075	2.404314756	9.014525414
2.748126268	2.381430626	9.068220139
3.450927973	3.635048389	9.076626778
4.911588669	3.661419868	9.037026405
3.467107773	1.109555125	9.029196739
0.670735121	5.959182739	9.217692375
4.885910988	1.124037743	9.017981529
6.963112354	4.730567455	8.971938133
7.626001835	3.466185331	8.973972321
9.831656456	4.653269291	8.911727905
9.095224380	3.427521944	8.960058212
7.726119041	5.926917553	8.908632278
13.965785980	2.225897551	9.057618141
11.051860809	2.228304386	9.008658409
11.778017044	3.457928181	8.974871635
13.240748405	3.458230734	9.014309883
11.787247658	0.946859956	9.055475235
9.137583733	5.945060253	8.870346069
13.227067947	0.939870834	9.061883926
-5.603043556	11.956711769	8.928792000
-4.875227928	10.732563972	8.898623466
-2.693527222	11.960588455	9.001728058
-3.421962976	10.734941483	8.951904297
-4.865831375	13.231484413	8.973378181
1.356307507	9.486785889	9.246311188
-1.487708092	9.538375854	9.053405762
-0.743979931	10.765089035	9.095724106
0.714701653	10.735864639	9.168498993
-0.801023960	8.245316505	9.112535477
-3.428200245	13.239353180	8.992746353
0.604276180	8.273734093	9.248147964
2.741915226	11.783741951	9.170028687
3.455696583	10.527040482	9.212021828
5.602536678	11.764431953	9.060659409
4.893644333	10.504185677	9.104886055
3.471214771	13.059595108	9.117792130
9.830409050	9.531920433	8.843904495
6.978285789	9.453396797	8.929512024
7.624719620	10.715127945	8.935919762
9.086503983	10.756470680	8.895311356
7.738430977	8.264064789	8.859672546
4.887581825	13.047951698	9.086977005
9.146228790	8.238097191	8.825345993
4.620989799	7.473285675	11.092320442



6.949587345	2.325431347	8.998667717
5.596712589	4.845304489	9.030528069
-1.473610401	7.087356091	9.075510025
2.770046949	4.790962219	9.108324051
1.415176153	2.325431347	9.076571465
1.328462124	7.134003639	9.371393204
15.303704262	2.237411737	9.095219612
13.855245590	4.646741390	9.020358086
7.019154072	7.099245071	8.892503738
11.166371346	4.644594193	8.918999672
9.710537910	2.237411737	9.000467300
9.848466873	7.090036392	8.821512222
2.726602077	9.352508545	9.317214012
1.410142422	11.879630089	9.158508301
-5.552678108	14.378939629	9.000918388
-1.358179092	11.956640244	9.065609932
-2.814103365	9.544802666	8.974979401
-2.737991333	14.385611534	9.008621216
-5.478800774	9.541934967	8.845649719
9.696775436	11.949420929	8.927171707
2.779227257	14.209154129	9.092988014
6.938006878	11.852120399	8.995716095
5.608090401	9.316943169	9.030528069
5.588032722	14.198893547	9.069660187
3.076992989	7.651313305	9.995867729
5.120625019	7.240828514	9.190925598
3.715324879	6.578289032	11.420891762
5.077756405	8.110505104	11.873717308

C<sub>2</sub>N- CoCr\*COOH

C	N	Co	Cr	O	H
49	24	1	1	2	1

Cartesian

-1.447909594	4.737570763	8.921195984
-0.724204063	3.512010813	8.986517906
1.442219973	4.794795513	9.046080589
0.733286142	3.544362783	9.045215607
-0.737096310	6.018871307	8.917218208
5.586974144	2.363489628	9.053892136
2.706335306	2.398190260	9.105821609
3.442283869	3.633563995	9.142938614
4.885007858	3.597191811	9.160938263
3.406297684	1.118273497	9.074610710
0.688570976	6.029563904	8.964431763

4.830759048	1.108085275	9.033209801
6.968738079	4.682782173	9.111834526
7.612890244	3.433444738	8.999442101
9.791620255	4.696270466	8.927136421
9.077768326	3.451875687	8.929853439
7.663645267	5.904249668	9.092231750
13.956098557	2.322592497	8.945910454
11.057682037	2.320531845	8.890307426
11.767671585	3.554954529	8.883431435
13.231893539	3.559018135	8.894969940
11.785664558	1.051768780	8.910665512
9.068504333	5.972080231	8.991000175
13.217772484	1.042373180	8.953056335
-5.704919815	11.957937241	9.028458595
-4.983717442	10.718960762	8.987957954
-2.804987907	11.959391594	8.960525513
-3.517798662	10.724724770	8.956439972
-4.965477467	13.237435341	9.030726433
1.302317142	9.593957901	8.915669441
-1.540964127	9.583149910	8.914752007
-0.824101448	10.825469017	8.920853615
0.643905640	10.840642929	8.914391518
-0.816009521	8.307238579	8.901756287
-3.532513142	13.231166840	8.992008209
0.593891144	8.363741875	8.910918236
2.662025452	11.921997070	8.942130089
3.367393970	10.683957100	8.980757713
5.542838573	11.882699013	9.059958458
4.810043812	10.646014214	9.057905197
3.419763565	13.177213669	8.947259903
9.692874908	9.541185379	9.026226044
6.811289310	9.485013962	9.128502846
7.516753197	10.738832474	9.100889206
8.973743439	10.770234108	9.067824364
7.558930874	8.250533104	9.130716324
4.844108105	13.161982536	9.005832672
8.980355263	8.260159492	9.042156219
3.386613369	7.373219013	11.221055984
6.937383175	2.284606218	8.993519783
5.600083351	4.765887737	9.268847466
-1.475275993	7.147102833	8.894592285
2.794664145	4.825850010	9.106451035
1.376970172	2.378202915	9.070847511
1.351838589	7.219659805	8.957736015

15.291804314	2.322635651	8.992782593
13.854661942	4.740842342	8.877869606
6.889299393	7.048317909	9.193895340
11.124844551	4.728305340	8.892756462
9.720687866	2.284419060	8.901989937
9.725198746	7.131654263	8.976564407
2.673634052	9.510332108	8.959626198
1.315926552	11.995606422	8.915652275
-5.633039474	14.395669937	9.069766998
-1.468509197	11.993487358	8.940761566
-2.874830008	9.552396774	8.930448532
-2.819026470	14.360134125	8.988767624
11.032007217	9.538059235	8.984951973
9.598467827	11.958872795	9.066690445
2.750494957	14.333790779	8.904726028
6.873368263	11.903753281	9.082151413
5.454194069	9.455327988	9.111383438
5.564558983	14.295746803	9.002862930
3.127175808	7.728409290	9.420623779
5.112431049	6.557927132	9.864792824
4.280706406	6.551744938	11.664522171
2.571290016	7.929120541	12.137616158
2.820785522	7.578352451	13.025447845

C<sub>2</sub>N-FeMn\*CO

C	N	Fe	Mn	O
49	24	1	1	1

Cartesian

-1.398913383	4.708014965	8.982234001
-0.677296162	3.479385614	9.003258705
1.490849972	4.751376629	9.005832672
0.783114672	3.503508806	9.017873764
-0.681827068	5.988882542	8.989470482
5.641237259	2.334870338	9.025019646
2.759134054	2.359743118	9.037619591
3.487519979	3.592594862	9.035424232
4.933921337	3.567750931	9.047052383
3.467865229	1.082996488	9.029465675
0.743541241	5.989228725	9.005130768
4.893424988	1.076065063	9.016794205
6.991518021	4.675749779	9.042156219
7.655678272	3.428444147	9.014273643
9.837862015	4.678142071	8.999513626
9.121856689	3.437738895	8.999099731

7.700693130	5.904379368	9.042119980
13.997498512	2.301380157	8.999640465
11.099988937	2.299420357	8.988444328
11.812832832	3.534376144	8.989055634
13.276098251	3.537676096	8.987471581
11.828645706	1.030556560	8.986463547
9.112915993	5.952827454	9.014760017
13.260104179	1.024042845	8.998559952
-5.625489712	11.928899765	9.011843681
-4.906476021	10.691234589	9.002483368
-2.729026794	11.930282593	9.001943588
-3.442054272	10.694952011	9.003456116
-4.889300823	13.204262733	9.012204170
1.376139641	9.559934616	9.063233376
-1.468322754	9.550883293	9.030851364
-0.751435280	10.792613029	9.028458595
0.713992596	10.804732323	9.035136223
-0.745988846	8.275679588	9.038808823
-3.458017349	13.200444221	9.001476288
0.663088322	8.324762344	9.065015793
2.726603985	11.892801285	8.984645844
3.438879490	10.658306122	9.000882149
5.611228466	11.867194176	9.012528419
4.884597778	10.630263329	9.001133919
3.477103710	13.154474258	8.978633881
9.768726349	9.521226883	9.015534401
6.886575222	9.480503082	9.032004356
7.589902401	10.727880478	9.033246994
9.049962997	10.752378464	9.026333809
7.631256104	8.240286827	9.045180321
4.901822567	13.144069672	8.999028206
9.052721977	8.244106293	9.023435593
3.756454945	7.362626553	11.209230423
6.990313530	2.271262169	9.015011787
5.621375084	4.746188641	9.079901695
-1.413791895	7.116984367	9.010044098
2.841223240	4.780427933	9.002754211
1.426507592	2.335922241	9.027324677
1.416501522	7.173315048	9.084941864
-1.304980040	2.293857813	9.008243561
13.904479980	4.718678951	8.976041794
6.954475880	7.055667400	9.079200745
11.171586037	4.709052563	8.992584229
9.762037277	2.267270327	8.991594315

9.782406807	7.107646465	9.015048027
2.750069141	9.483428001	9.082368851
1.383592606	11.962389946	9.004859924
-5.565090179	14.358937263	9.025848389
-1.392714977	11.962736130	9.009863853
-2.802247524	9.521327972	9.013715744
-2.748822689	14.332781792	9.001115799
11.107061386	9.511096954	9.001728058
9.676207542	11.936824799	9.023237228
2.799807549	14.306425095	8.973810196
6.944029808	11.893766403	9.021617889
5.534772396	9.446263313	8.998991966
5.614886284	14.280371666	9.005255699
3.177943707	7.696879864	9.584154129
4.990867615	6.649852276	9.361889839
4.012392521	7.214227200	12.354426384

C<sub>2</sub>N- FeMn\*CHO

C	N	Fe	Mn	O	H
49	24	1	1	1	1

Cartesian

-1.465154290	4.648499489	9.048995972
-0.732837796	3.419985056	9.070991516
1.407436609	4.716157436	9.163062096
0.728679180	3.460521936	9.103949547
-0.770224333	5.943043232	9.087803841
5.602830887	2.404963255	9.050742149
2.744149208	2.384975672	9.080316544
3.441742897	3.644155741	9.123696327
4.904533386	3.664042234	9.084563255
3.468230486	1.115247250	9.038933754
0.646949053	5.942135334	9.187325478
4.886509895	1.126804590	9.045935631
6.948844910	4.735798359	8.980848312
7.617856503	3.473289728	8.985312462
9.821089745	4.651424885	8.913599968
9.083967209	3.427680254	8.961011887
7.714703560	5.938503742	8.906795502
13.952239990	2.218375444	9.027990341
11.036751747	2.219340801	8.994078636
11.765162468	3.449209690	8.963873863
13.227128983	3.449858189	8.996399879
11.773354530	0.936570883	9.034955978
9.130105019	5.945968151	8.875692368

13.215220451	0.935345948	9.036773682
-5.592252731	11.962347031	8.933291435
-4.864236832	10.738745689	8.916407585
-2.681322098	11.964118958	9.024893761
-3.411646366	10.740504265	8.974133492
-4.856229782	13.235894203	8.977536201
1.360034943	9.465084076	9.218592644
-1.483689308	9.534527779	9.062315941
-0.736999512	10.757926941	9.105228424
0.723712444	10.718643188	9.164106369
-0.803361654	8.237260818	9.102167130
-3.417042732	13.242825508	9.013518333
0.603809834	8.262955666	9.211122513
2.748438358	11.770110130	9.161405563
3.464324474	10.513393402	9.197046280
5.609841824	11.770110130	9.065520287
4.897155285	10.509748459	9.115595818
3.470217705	13.047173500	9.105299950
9.842481613	9.535709381	8.862354279
7.000990391	9.464852333	8.960058212
7.637549400	10.725300789	8.953074455
9.097625732	10.762393951	8.905427933
7.752200127	8.270880699	8.880822182
4.886857986	13.045487404	9.077976227
9.160188675	8.241612434	8.844461441
4.601287365	7.508389473	11.091258049
6.941275597	2.332478285	9.019853592
5.590281487	4.837220192	9.057024002
-1.487354994	7.085828781	9.062981606
2.750860691	4.797303200	9.166878700
1.410342693	2.318125248	9.068688393
1.319627285	7.110225677	9.315252304
15.290760040	2.228044987	9.057546616
13.840620041	4.637864113	9.005057335
7.023821354	7.114044666	8.894483566
11.155547142	4.637806892	8.918261528
9.695454597	2.233794689	8.994582176
9.849582672	7.086923599	8.834292412
2.740064144	9.327751160	9.272142410
1.415376663	11.862294197	9.155591965
-5.546380043	14.380885124	8.996310234
-1.344243526	11.953484535	9.085211754
-2.810243130	9.547483444	8.993393898
-2.732042789	14.390640259	9.039527893

-5.466886520	9.547929764	8.868599892
9.708037376	11.955040932	8.927856445
2.771689415	14.196155548	9.073997498
6.943315506	11.861601830	9.004913330
5.627466679	9.328515053	9.069120407
5.581576347	14.198518753	9.050489426
3.135599613	7.540813446	9.830214500
5.149323940	7.420298100	9.239831924
3.771017313	6.574225426	11.437470436
5.056880474	8.168738365	11.852945328

C<sub>2</sub>N- FeMn\*COOH

C	N	Fe	Mn	O	H
49	24	1	1	2	1
Cartesian					
-1.518651962			4.689022064		8.859077454
-0.776934028			3.466761827		8.908506393
1.358148575			4.775413036		8.937053680
0.684923887			3.514662504		8.957790375
-0.829620361			5.983954430		8.839925766
5.551239014			2.431291342		9.094644547
2.693505526			2.440845490		9.068850517
3.401215553			3.699189901		9.078425407
4.851518631			3.685283661		9.124631882
3.407320023			1.162268996		9.079974174
0.586313486			5.977325916		8.870526314
4.825449944			1.160539746		9.079631805
6.931388855			4.741735935		9.144486427
7.580515862			3.482426167		9.090756416
9.785272598			4.675418377		9.043109894
9.045886993			3.448359728		9.053009987
7.683903694			5.941212654		9.142866135
13.912788391			2.255180120		8.923751831
10.998946190			2.250554323		8.988462448
11.725909233			3.478693724		8.962326050
13.182916641			3.481878519		8.911007881
11.733775139			0.972582877		8.975987434
9.095035553			5.970480442		9.085554123
13.174253464			0.974312127		8.947566032
-5.671699524			11.996629715		9.047267914
-4.944416523			10.768418312		9.024966240
-2.757907391			11.996441841		9.023903847
-3.486692667			10.771371841		8.996129990
-4.933671951			13.276127815		9.057240486

1.301953793	9.502220154	8.973648071
-1.548485041	9.571850777	8.941607475
-0.805023670	10.796287537	8.997426033
0.663051605	10.761514664	9.009216309
-0.862433434	8.276832581	8.892323494
-3.493094921	13.275522232	9.049194336
0.545387268	8.308261871	8.922798157
2.687678814	11.806928635	9.017352104
3.391716003	10.553729057	9.014147758
5.547150612	11.816007614	9.006606102
4.839116096	10.555660248	9.040103912
3.415846348	13.084885597	8.998038292
9.758216858	9.561274529	9.057042122
6.890635490	9.484538078	9.094949722
7.560324669	10.742506981	9.053748131
9.019802094	10.787238121	9.056861877
7.656555176	8.275578499	9.121985435
4.832978725	13.089035034	8.978724480
9.069468498	8.268128395	9.082980156
3.445406914	7.494454384	11.106557846
6.894118309	2.344439030	9.083951950
5.560221672	4.854642868	9.191789627
-1.550261736	7.124838352	8.847720146
2.714259624	4.877439976	8.993483543
1.361270905	2.371386766	9.013715744
1.269998550	7.148745537	8.929602623
15.252528191	2.270311117	8.926343918
13.788578033	4.673357964	8.864981651
6.966422558	7.104000568	9.174870491
11.115420341	4.668429375	8.992134094
9.658689499	2.257442474	9.027143478
9.785851479	7.120500565	9.066366196
2.685060501	9.366241455	8.976437569
1.348476410	11.902946472	9.026405334
2.704573631	0.017263846	9.069966316
-1.417849541	11.987737656	9.028367996
-2.878816366	9.582471848	8.945136070
5.518320560	0.008934544	9.061326027
11.091476440	9.576535225	9.032832146
9.628482819	11.982910156	9.055944443
2.723401070	14.235583305	8.997714043
6.880058765	11.884356499	9.014400482
5.534631729	9.390018463	9.099431992
5.535691261	14.234848022	8.949888229



3.089584827	7.475980282	9.272195816
5.059100151	6.903131485	9.522467613
4.638192654	7.247716904	11.497914314
2.521980762	7.837829590	12.022451401
2.954594612	7.849011898	12.908663750

C<sub>2</sub>N-FeCr\*CO

C	N	Fe	Cr	O
49	24	1	1	1

Cartesian

-1.392864943	4.711804867	8.988138199
-0.661455631	3.490510464	9.008927345
1.504652023	4.784275532	9.033803940
0.799961567	3.530989647	9.028134346
-0.688699722	5.997788429	8.999549866
5.651678085	2.337853193	9.018936157
2.770980835	2.386460066	9.033803940
3.508110762	3.617769957	9.035136223
4.947307587	3.573414326	9.035316467
3.467249393	1.102450728	9.024372101
0.737200499	6.008510113	9.039167404
4.891453266	1.085129261	9.012671471
7.028616428	4.659826279	9.050561905
7.676229477	3.409710646	9.026333809
9.860358238	4.666959286	9.013229370
9.142730713	3.423861504	9.013338089
7.732975006	5.880169868	9.050417900
14.022758484	2.289534569	8.996399879
11.120456696	2.289102316	8.991827965
11.831851959	3.521262407	8.991846085
13.294351578	3.523957491	8.986104012
11.849394798	1.021160841	8.985239983
9.139463425	5.944282055	9.026298523
13.282650948	1.007787824	8.995409966
-5.651772022	11.941104889	9.016272545
-4.926693916	10.705357552	9.006336212
-2.752214909	11.942172050	8.999405861
-3.464002371	10.709794998	9.001745224
-4.912471771	13.221137047	9.015912056
1.340314388	9.576909065	9.075132370
-1.493183136	9.564199448	9.012042046
-0.774856091	10.807786942	9.009036064
0.690522194	10.822384834	9.021654129
-0.773503304	8.287510872	9.026280403

-3.479690552	13.211007118	9.004139900
0.630115509	8.347286224	9.077129364
2.715788364	11.893781662	8.993448257
3.419194221	10.653636932	9.034578323
5.595912933	11.838618279	9.022086143
4.863099575	10.601586342	9.028836250
3.477028847	13.146965981	8.983116150
9.759858131	9.518632889	9.011988640
6.875286579	9.450139999	9.031860352
7.572888851	10.704146385	9.029861450
9.032899857	10.743430138	9.021852493
7.633194447	8.225775719	9.033480644
4.900227070	13.124500275	9.003906250
9.055311203	8.233657837	9.017423630
3.769633293	7.355594158	11.155607224
7.000189781	2.257701874	9.016739845
5.651983261	4.750151157	9.070560455
-1.430098534	7.122143269	9.000395775
2.865573883	4.819552898	9.022500992
1.440925002	2.364296675	9.024281502
1.388471127	7.203591824	9.121464729
-1.279088974	2.296912909	9.007811546
13.911102295	4.709485054	8.977193832
6.966357708	7.027220726	9.069911957
11.193067551	4.696573257	9.000611305
9.783262253	2.254805326	9.000900269
9.799013138	7.105859280	9.016110420
2.709983349	9.492074966	9.118673325
1.371428490	11.973687172	8.993393898
-5.576904774	14.382397652	9.025506020
-1.415645123	11.976454735	8.997083664
-2.825659752	9.535046577	9.002340317
-2.761518002	14.337191582	9.001890182
11.096803665	9.520276070	9.003545761
9.649916649	11.935787201	9.023777962
2.810956001	14.304811478	8.974349976
6.926774979	11.866991997	9.018846512
5.513282776	9.405525208	9.018522263
5.625144958	14.256146431	9.004932404
3.177860260	7.696447849	9.525329590
5.077171326	6.599861622	9.296478271
3.995561600	7.224818707	12.307769775

C<sub>2</sub>N- FeCr\*CHO

C	N	Fe	Cr	O	H
49	24	1	1	1	1
Cartesian					
-1.454263926				4.655430794	9.065303802
-0.723344922				3.428472996	9.090522766
1.421546936				4.723996162	9.145889282
0.738271713				3.470883369	9.113435745
-0.755489826				5.951501846	9.114246368
5.607556343				2.415338993	9.039186478
2.748367310				2.387094021	9.072576523
3.450345755				3.644299984	9.089136124
4.910839081				3.674245119	9.062064171
3.467681170				1.117005467	9.034110069
0.664054394				5.952885151	9.193626404
4.886002541				1.134024262	9.033300400
6.967131615				4.738680840	8.984142303
7.626109600				3.473232031	8.982126236
9.832878113				4.653975487	8.895438194
9.095407486				3.429452896	8.950086594
7.730827332				5.932566643	8.931852341
13.964630127				2.222885847	9.033335686
11.049871445				2.225926638	8.978148460
11.776834488				3.454786539	8.945783615
13.239442825				3.455017328	8.991558075
11.785408974				0.944078743	9.019098282
9.140853882				5.947005749	8.870561600
13.226768494				0.936815798	9.032346725
-5.599257946				11.961568832	8.923049927
-4.870211124				10.738947868	8.895618439
-2.688934803				11.967822075	9.016056061
-3.416505575				10.741541862	8.963928223
-4.864000320				13.237997055	8.970804214
1.362522602				9.482073784	9.242424011
-1.484238625				9.542626381	9.096570015
-0.742324829				10.768388748	9.129708290
0.718636513				10.736138344	9.182790756
-0.796930313				8.245892525	9.153107643
-3.424771786				13.247393608	8.999549866
0.612696171				8.272667885	9.255311966
2.747797489				11.785428047	9.131958008
3.462118149				10.534505844	9.160956383
5.605789661				11.760642052	9.046854019
4.899019718				10.502196312	9.085428238
3.472038746				13.057735443	9.079614639

9.837489128	9.534008980	8.852705956
6.983027935	9.448670387	8.966735840
7.625553131	10.711294174	8.950337410
9.091786385	10.756139755	8.901810646
7.746360302	8.265520096	8.920169830
4.888805389	13.044276237	9.061794281
9.152884483	8.239249229	8.851338387
4.588202477	7.438973904	11.142810822
6.948588371	2.333530188	9.013175964
5.598176003	4.859830379	9.041562080
-1.475366354	7.092443466	9.109476089
2.763282061	4.797519207	9.114713669
1.415516973	2.325993538	9.078534126
1.335725784	7.121768951	9.335556030
15.302754402	2.235249996	9.077004433
13.852267265	4.644291878	9.009503365
7.025052071	7.104245663	8.970983505
11.167486191	4.643239498	8.893079758
9.707901001	2.237570286	8.980361938
9.854557037	7.092256069	8.828568459
2.736418724	9.362682343	9.262439728
1.411374092	11.874672890	9.148283958
-5.551263809	14.385192871	8.997444153
-1.353353977	11.961251259	9.089729309
-2.809694529	9.550683022	9.004482269
-2.736968040	14.394819260	9.023292542
-5.472062111	9.545884132	8.845541954
9.698504448	11.950226784	8.924453735
2.777779579	14.207107544	9.048851967
6.943881512	11.851601601	8.990298271
5.606092930	9.301812172	9.039329529
5.588356972	14.195997238	9.046115875
3.150965214	7.594492912	9.849978447
5.093087196	7.214918613	9.245088577
3.644780397	6.582021236	11.439431190
5.011514187	8.099237442	11.923254013

C<sub>2</sub>N- FeCr\*COOH

C	N	Fe	Cr	O	H
49	24	1	1	2	1

Cartesian

-1.319767952	4.739559650	9.091781616
-0.606653452	3.516406298	9.096012115
1.600147009	4.779981136	9.144377708

0.858923674	3.535730839	9.124919891
-0.579593658	6.007385731	9.110861778
5.681806564	2.235869884	8.974205971
2.784992933	2.318182945	9.085986137
3.549836874	3.521032095	9.080369949
4.966795921	3.449108839	9.020249367
3.472999811	1.028394938	9.045413971
0.863695145	6.020845413	9.144215584
4.903178215	0.996374607	8.986392021
6.999689102	4.604187012	9.013715744
7.677927971	3.368179321	8.968121529
9.829400063	4.680923462	9.021005630
9.143953323	3.424567699	8.970587730
7.641473770	5.853769302	9.059453964
14.052309036	2.350376129	9.025704384
11.155113220	2.351874828	8.954010010
11.849755287	3.595476866	9.007524490
13.327437401	3.597321510	9.033191681
11.883421898	1.089437962	8.931635857
9.057622910	5.931643963	9.058338165
13.310612679	1.068701267	8.979840279
-5.662302971	11.865219116	9.043308258
-4.947032928	10.613258362	9.038375854
-2.771922112	11.862957001	8.962074280
-3.468060255	10.615752220	9.008802414
-4.923136234	13.146317482	9.027143478
1.388127804	9.617186546	9.002465248
-1.446133614	9.532568932	9.009234428
-0.760287762	10.790393829	8.942436218
0.701445103	10.847473145	8.921339989
-0.681053162	8.286357880	9.061397552
-3.497867107	13.127554893	8.976185799
0.728963852	8.356003761	9.079631805
2.702774525	11.976959229	8.885268211
3.417386532	10.753459930	8.954532623
5.603182793	11.897787094	8.999981880
4.848597050	10.686594963	9.009954453
3.484257698	13.219466209	8.895959854
9.695280075	9.472173691	9.080297470
6.797013283	9.446652412	9.096462250
7.536397934	10.689591408	9.074016571
8.996591568	10.704953194	9.075203896
7.509712219	8.186550140	9.109980583
4.913469791	13.185832024	8.957717896

8.946121216	8.207229614	9.095957756
4.591875076	6.915726662	11.344265938
7.034619331	2.191153765	8.945460320
5.630271912	4.641812801	9.045162201
-1.325884581	7.115082264	9.088811874
2.974722862	4.765729427	9.126846313
1.456292272	2.340994835	9.111348152
1.528335094	7.229199409	9.165204048
-1.250952244	2.335014582	9.059976578
-2.662004948	4.765902042	9.063504219
6.824996948	6.979479313	9.106163979
11.167990685	4.750526428	9.037008286
9.820608139	2.279605865	8.934966087
9.701030731	7.091520786	9.083915710
2.746364117	9.582846642	9.029124260
1.358323574	12.021458626	8.863253593
-5.579291344	14.313903809	9.060534477
-1.439812660	11.934764862	8.918729782
-2.786604404	9.464406013	9.030258179
-2.766075611	14.244791031	8.952425957
11.040529251	9.444879532	9.059562683
9.640701294	11.883736610	9.059543610
2.833941460	14.381201744	8.881307602
6.932582378	11.878520966	9.036234856
5.436248302	9.466899872	9.075437546
5.644994736	14.312204361	8.990262032
3.375428200	7.834024906	9.522846222
4.818438530	6.358153343	9.393533707
5.263829708	6.421271801	12.392009735
3.758946419	7.850265980	11.535570145
4.978439331	6.901733875	13.208364487

C<sub>2</sub>N-MnCr\*CO

C	N	Cr	Mn	O
49	24	1	1	1

Cartesian

-1.282029867	4.769591331	9.108449936
-0.582576632	3.545371294	9.125820160
1.640854836	4.817953110	9.185778618
0.886752844	3.568975925	9.169145584
-0.525673628	6.036336899	9.096876144
5.692856789	2.188199759	8.995734215
2.791748524	2.319191456	9.121500015
3.563806534	3.505079508	9.132966042

4.982006073	3.404666662	9.061650276
3.457833052	1.015843272	9.063467026
0.925734758	6.068386078	9.119411469
4.889001846	0.960895836	8.992403984
7.001564026	4.557424545	9.093132019
7.693295479	3.331965446	9.015462875
9.828060150	4.682580471	9.097956657
9.158164978	3.415892601	9.014976501
7.626557350	5.828277111	9.180990219
14.075994492	2.373533964	9.031698227
11.186238289	2.381113768	8.953866005
11.870429039	3.628894806	9.039258003
13.355216980	3.628866196	9.053063393
11.911616325	1.123663068	8.893926620
9.036890030	5.913775444	9.170495987
13.333666801	1.088083506	8.958815575
-5.720541000	11.841384888	9.066905975
-4.991926193	10.588992119	9.057095528
-2.826416969	11.837623596	8.905409813
-3.507986307	10.588962555	8.978382111
-4.976631641	13.128391266	9.035712242
1.357301235	9.660951614	8.809793472
-1.462257862	9.536949158	8.916678429
-0.796071529	10.805078506	8.818019867
0.666642189	10.886511803	8.757450104
-0.665370464	8.304125786	8.967383385
-3.553217888	13.095751762	8.954261780
0.742440701	8.394105911	8.936964035
2.664118290	12.035408020	8.745353699
3.380386353	10.821808815	8.793882370
5.564328194	11.892973900	8.957843781
4.783559322	10.713095665	8.923248291
3.467217445	13.260882378	8.803080559
9.645195007	9.453151703	9.163097382
6.702067852	9.401317596	9.139896393
7.457651615	10.642252922	9.114642143
8.932390213	10.669748306	9.133740425
7.437680721	8.163263321	9.223631859
4.897288322	13.201005936	8.901144028
8.893239975	8.191175461	9.213461876
3.921921730	7.580240250	11.005685806
7.043256760	2.152360678	8.965278625
5.648651123	4.577642441	9.104976654
-1.291898727	7.128469944	9.046314240

3.021837950	4.766608715	9.204425812
1.459228516	2.368821621	9.157355309
1.593985081	7.294090271	9.045504570
-1.225627303	2.364094734	9.077507973
-2.628094196	4.795501232	9.082295418
6.798624516	6.932270050	9.257652283
11.169944763	4.771032333	9.108233452
9.852889061	2.288309813	8.942760468
9.653358459	7.094575882	9.213119507
2.715279102	9.641728401	8.810729980
1.315799713	12.071161270	8.718083382
-5.612047195	14.309797287	9.085445404
-1.496420860	11.933352470	8.811630249
-2.801987171	9.446291924	8.981712341
-2.804212570	14.203289032	8.936621666
10.990220070	9.424171448	9.115901947
9.580181122	11.851169586	9.097632408
11.161538124	0.020837663	8.802071571
6.891890526	11.851155281	9.049032211
5.306351662	9.429965019	9.043955803
5.648106575	14.314682007	8.964035988
3.603587627	7.972453117	9.228690147
4.823366165	6.234885693	9.619254112
4.017909050	7.508576870	12.189293861

C<sub>2</sub>N- MnCr\*CHO

C	N	Cr	Mn	O	H
49	24	1	1	1	1

Cartesian

-1.460296154	4.674409389	9.016397476
-0.725217462	3.447163343	9.069282532
1.406520844	4.748148441	9.170045853
0.733088017	3.490380764	9.122598648
-0.769509315	5.966647625	9.051713943
5.607015133	2.432472944	9.079919815
2.746203899	2.415137053	9.125063896
3.453265190	3.675498724	9.159606934
4.906029701	3.684851170	9.113975525
3.463803768	1.144558430	9.077274323
0.639286041	5.960940838	9.164502144
4.882282734	1.153867602	9.070542336
6.984951973	4.744675636	8.980937958
7.630277634	3.483103514	8.991306305
9.844575882	4.665100574	8.852975845



9.099692345	3.444771290	8.940473557
7.747058868	5.933762550	8.885645866
13.965502739	2.241547585	9.016434669
11.051477432	2.240927935	8.970983505
11.782259941	3.465162277	8.914770126
13.240549088	3.469903231	8.957159996
11.785551071	0.959743083	9.019170761
9.157109261	5.961214542	8.810100555
13.226735115	0.961544335	9.027197838
-5.609225273	11.984941483	8.929637909
-4.880536079	10.759194374	8.877852440
-2.696664333	11.987089157	9.002340317
-3.424002171	10.761875153	8.935254097
-4.871389389	13.263100624	8.990657806
1.356465816	9.491469383	9.218879700
-1.489705086	9.561893463	9.028169632
-0.747733116	10.786170959	9.082260132
0.718753338	10.751816750	9.151758194
-0.804476738	8.264670372	9.072504044
-3.431295395	13.267222404	9.011843681
0.602112770	8.298347473	9.198395729
2.749020100	11.797431946	9.139769554
3.453474522	10.547057152	9.182430267
5.608059883	11.801610947	9.056628227
4.899651051	10.539232254	9.094032288
3.472537994	13.072838783	9.084294319
9.822796822	9.554616928	8.809776306
6.952701569	9.472779274	8.926542282
7.621217251	10.732953072	8.941517830
9.081403732	10.778015137	8.890865326
7.724828243	8.268748283	8.844893456
4.890684128	13.076008797	9.064691544
9.135662079	8.261758804	8.778960228
4.638912678	7.057065487	11.314908028
6.950069904	2.342781544	9.041507721
5.605888367	4.874428272	9.071856499
-1.487388849	7.116033077	9.017747879
2.757782221	4.838373184	9.195624352
1.414110780	2.347854376	9.111672401
1.313428402	7.133873940	9.300869942
15.303196907	2.252932072	9.065520287
13.847008705	4.660719872	8.955018044
7.041083813	7.100109577	8.916983604
11.174932480	4.653802395	8.841258049

9.710720062	2.253119230	8.984844208
9.847126007	7.110139370	8.755290031
2.741452217	9.363792419	9.283284187
1.404668331	11.889718056	9.137988091
-5.555690289	14.410181046	9.030275345
-1.358246803	11.978111267	9.066096306
-2.817083120	9.571029663	8.946864128
5.577042103	0.003372070	9.045053482
-5.483901501	9.569819450	8.804088593
9.691381454	11.971929550	8.935883522
2.777637482	14.223752022	9.055097580
6.939212799	11.873058319	8.994024277
5.597255707	9.367927551	9.007344246
5.589927673	14.223190308	9.044712067
3.144878387	7.466584206	9.898253441
5.166809082	6.894341469	9.438227654
3.442238331	6.752267838	11.719493866
5.353767872	7.394690514	12.097980499

C<sub>2</sub>N- MnCr\*COOH

C	N	Cr	Mn	O	H
49	24	1	1	2	1

Cartesian

-1.442508340	4.664725780	8.982378006
-0.711223245	3.435317993	9.042551994
1.423901320	4.725826740	9.114137650
0.748288631	3.468548775	9.096660614
-0.743542433	5.950464249	8.984951973
5.620294094	2.402499199	9.097919464
2.757061720	2.386878014	9.129546165
3.465662479	3.646043539	9.156797409
4.912695408	3.648896933	9.131039619
3.479628325	1.116947770	9.090324402
0.667440891	5.940765858	9.060390472
4.899655342	1.124614239	9.082079887
6.981699467	4.729991436	9.025613785
7.635643005	3.471819878	9.027917862
9.842163086	4.661007881	8.903772354
9.104093552	3.438301086	8.976149559
7.730876923	5.929108143	8.939988136
13.971184731	2.244732380	9.004409790
11.059472084	2.242440939	8.980992317
11.787849426	3.470407724	8.933274269
13.248544693	3.474702120	8.954010010

11.794219971	0.961501062	9.013500214
9.145628929	5.953375340	8.874414444
13.233780861	0.967870533	9.017603874
-5.583991051	11.956078529	8.960579872
-4.860002518	10.725589752	8.912159920
-2.671912193	11.957273483	8.994167328
-3.399017096	10.729177475	8.939087868
-4.847145081	13.234078407	9.009287834
1.408073902	9.467619896	9.108827591
-1.453230858	9.537770271	8.974619865
-0.715467930	10.760895729	9.026586533
0.753596306	10.726886749	9.076536179
-0.757852077	8.245330811	8.987201691
-3.407316685	13.238083839	9.017784119
0.655310154	8.270564079	9.065718651
2.768530846	11.795630455	9.096407890
3.475613594	10.548194885	9.129978180
5.632894516	11.818774223	9.062388420
4.923744678	10.560818672	9.089009285
3.488462925	13.074422836	9.064620018
9.829511642	9.535810471	8.871191978
6.959066391	9.478067398	8.971595764
7.639521599	10.733414650	8.980721474
9.098276138	10.765275955	8.937917709
7.714353085	8.257119179	8.905896187
4.908630371	13.086168289	9.058104515
9.127849579	8.249726295	8.849177361
4.568951130	7.061863899	11.471490860
6.963938713	2.325561047	9.065177917
5.601895332	4.841572285	9.109385490
-1.452237368	7.101983070	8.948933601
2.777167559	4.819034100	9.161064148
1.423653960	2.322044849	9.111834526
1.365528107	7.103611469	9.118097305
15.309061050	2.246576786	9.047159195
13.862608910	4.660849571	8.938907623
7.019628048	7.094763279	8.965188026
11.173834801	4.656972885	8.883972168
9.719622612	2.248306274	9.002916336
9.836959839	7.097458363	8.826893806
2.789525032	9.352609634	9.168498993
1.424403667	11.873692513	9.082746506
-5.535381317	14.379011154	9.050489426
-1.331814289	11.950832367	9.031193733

-2.784335613	9.541977882	8.926181793
-2.722241879	14.386489868	9.051300049
-5.474799156	9.540134430	8.859365463
9.717922211	11.953945160	8.972189903
2.789211273	14.223478317	9.039852142
6.964986801	11.880898476	9.020267487
5.611091137	9.394284248	9.034541130
5.602824211	14.233881950	9.036954880
3.279962540	7.334007740	9.646182060
5.136319160	6.805730820	9.540612221
5.426789284	7.115067959	12.499992371
3.324734211	7.212886333	11.705904007
4.915232658	7.281423569	13.329917908