Supporting Information

Metallocene-Coupled Cumulene: A Quest for Chiral Single Molecule Magnet

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Table S1: Bond angles (in degree) of C_n chain of [Ni]-C_n-[Ni] [UB3LYP/6-311++g(d,p)].

Sys	∠C1 - C2 - C3	C2 - C3 - C4	C3 - C4 - C5	C4 - C5 - C6	C5 - C6 - C7	C6 - C7 - C8	C7 - C8 - C9
C_3	179.24						
C_5	179.60	179.88	179.60				
C_7	179.24	179.88	179.87	179.87	179.29		
C_9	179.14	179.79	179.66	179.77	179.73	179.75	179.14
C_4	178.59	178.59					
C_6	179.30	179.94	179.94	179.30			
C_8	179.39	179.86	179.94	179.94	179.89	179.39	

Table S2: Bond angles (in degree) of C_n carbon chain of [Cr]-C_n-[Cr] [UB3LYP/6-311++g(d,p)].

Sys	∠C1 – C2 – C3	C2 – C3 – C4	C3 – C4 – C5	C4 – C5 – C6	C5 – C6 – C7	C6 – C7 – C8	C7 – C8 – C9
C_3	179.04						
C_5	179.40	179.93	179.41				
C_7	179.42	179.83	179.66	179.87	179.37		
C_9	179.36	179.68	179.52	179.62	179.63	179.93	179.30
C_4	178.59	178.59					
C_6	179.35	179.95	179.95	179.39			
C_8	179.37	179.90	179.73	179.85	179.95	179.38	

Table S3: Bond angles (in degree) of C_n carbon chain of [Cr]-C_n-[Ni] [UB3LYP/6-311++g(d,p)]. Numbering is done considering chromocene unit at the left end.

Sys	$\angle C1-C2-C3$	$C2-C3-C4$	$C3-C4-C5$	$C4-C5-C6$	$C5-C6-C$	$C6-C7-C8$	$C7-C8-C9$
C_3	179.12						
C_5	179.55	179.93	179.36				
C_7	179.41	179.94	179.74	179.86	179.42		
C_9	179.31	179.94	179.64	179.69	179.69	179.71	179.32
C_4	178.77	178.61					
C_6	179.41	179.89	179.89	179.12			
C_8	179.37	179.81	179.69	179.91	179.85	179.14	

Table S4: Bond lengths (in Å) of C_n chain of [Ni]-C_n-[Ni] systems [UMN12SX/6-311++g(d,p)]. C-L and C-R represents bond lengths of nickelocene unit with end carbon atom of the coupler at the left end and nickelocene unit with end carbon atom of the coupler at the right end respectively.

Sys	C1-C2	C2-C3	C3-C4	C4-C5	C5-C6	C6-C7	C7-C8	C8-C9	Average bond length	C-L	C-R
C_3	1.309	1.309							1.309	1.460	1.460
C_5	1.321	1.272	1.272	1.321					1.296	1.447	1.447
C_7	1.327	1.265	1.280	1.280	1.265	1.327			1.291	1.440	1.440
C_9	1.332	1.261	1.285	1.272	1.272	1.285	1.261	1.331	1.287	1.436	1.436
C_4	1.330	1.254	1.330						1.305	1.443	1.443
C_6	1.331	1.256	1.296	1.256	1.331				1.294	1.440	1.440
C_8	1.333	1.256	1.293	1.259	1.293	1.256	1.333		1.289	1.437	1.437

Table S5: Bond lengths (in Å) of C_n chain of [Cr]-C_n-[Cr] complexes [UMN12SX/6-311++g(d,p)]. C-L and C-R represents bond lengths of chromocene unit with end carbon atom of the coupler at the left end and chromocene unit with end carbon atom of the coupler at the right end respectively.

Sys	C1-C2	C2-C3	C3-C4	C4-C5	C5-C6	C6-C7	C7-C8	C8-C9	Average bond length	C-L	C-R
C_3	1.308	1.308							1.308	1.463	1.463
C_5	1.319	1.272	1.272	1.319					1.296	1.453	1.453
C_7	1.324	1.266	1.279	1.279	1.266	1.324			1.290	1.447	1.447
C_9	1.328	1.263	1.284	1.273	1.273	1.284	1.263	1.328	1.287	1.443	1.443
C_4	1.328	1.255	1.328						1.304	1.450	1.450
C_6	1.329	1.257	1.294	1.257	1.329				1.293	1.445	1.445
C_8	1.331	1.258	1.292	1.260	1.292	1.258	1.331		1.289	1.443	1.443

Table S6: Bond lengths (in Å) of C_n chain of [Cr]-C_n-[Ni] [UMN12SX/6-311++g(d,p)]. Numbering is done considering chromocene unit at the left end. C-L and C-R represents bond

lengths of chromocene unit with end carbon atom of the coupler at the left end and nickelocene unit with end carbon atom of the coupler at the right end respectively.

Sys	C1-C2	C2-C3	C3-C4	C4-C5	C5-C6	C6-C7	C7-C8	C8-C9	Average bond length	C-L	C-R
C_3	1.311	1.312							1.311	1.468	1.463
C_5	1.323	1.275	1.273	1.325					1.299	1.456	1.452
C_7	1.329	1.268	1.283	1.283	1.270	1.330			1.294	1.450	1.445
C_9	1.334	1.264	1.288	1.276	1.276	1.288	1.264	1.334	1.291	1.445	1.441
C_4	1.339	1.252	1.340						1.310	1.444	1.439
C_6	1.348	1.250	1.312	1.250	1.349				1.302	1.435	1.429
C_8	1.357	1.245	1.317	1.247	1.317	1.245	1.357		1.298	1.427	1.421

Table S7: Bond angles (in degree) of C_n chain of [Ni]-C_n-[Ni] complexes [UMN12SX/6-311++g(d,p)].

Sys	$\angle C1 - C2 - C3$	$C2 - C3 - C4$	$C3 - C4 - C5$	$C4 - C5 - C6$	$C5 - C6 - C7$	$C6 - C7 - C8$	$C7 - C8 - C9$
C_3	177.99						
C_5	179.51	179.88	179.84				
C_7	179.38	179.69	179.45	179.80	179.40		
C_9	179.42	179.65	179.31	179.45	179.46	179.72	179.37
C_4	179.00	179.00					
C_6	179.49	179.79	179.79	179.49			
C_8	179.50	179.56	179.57	179.43	179.71	179.48	

Table S8: Bond angles (in degree) of C_n chain of [Cr]-C_n-[Cr] [UMN12SX/6-311++g(d,p)].

Sys	$\angle C1 - C2 - C3$	$C2 - C3 - C4$	$C3 - C4 - C5$	$C4 - C5 - C6$	$C5 - C6 - C7$	$C6 - C7 - C8$	$C7 - C8 - C9$
C_3	177.62						
C_5	179.52	179.87	179.20				
C_7	179.12	179.65	179.30	179.56	179.30		
C_9	179.00	179.55	179.02	179.36	179.21	179.63	179.11
C_4	176.55	176.56					
C_6	179.44	179.76	179.76	179.45			
C_8	179.31	179.56	179.92	179.85	179.54	179.29	

Table S9: Bond angles (in degree) of C_n chain of [Cr]-C_n-[Ni] [UMN12SX/6-311++g(d,p)]. Numbering is done considering chromocene unit at the left end.

Sys	$\angle C1$ - $C2$ - $C3$	$C2$ - $C3$ - $C4$	$C3$ - $C4$ - $C5$	$C4$ - $C5$ - $C6$	$C5$ - $C6$ - $C7$	$C6$ - $C7$ - $C8$	$C7$ - $C8$ - $C9$
C_3	177.55						
C_5	179.34	179.82	179.77				
C_7	179.34	179.63	179.35	179.78	179.34		
C_9	179.21	179.54	179.29	179.39	179.29	179.69	179.29
C_4	176.45	174.73					
C_6	179.50	179.71	179.87	179.65			
C_8	179.01	179.39	179.52	179.36	179.71	179.44	

Table S10: Spin-density distribution on Ni and each atom of the coupler of [Ni]-C_n-[Ni] [UMN12SX/6-311++g(d,p)].

sys	Ni1	Ni2	C1	C2	C3	C4	C5	C6	C7	C8	C9	Average Spin-density on each atom of coupler
C_3	1.142	1.142	−0.027	0.083	−0.027							0.046
C_5	1.133	1.133	−0.054	0.135	−0.105	0.135	−0.054					0.097
C_7	1.126	1.126	−0.087	0.176	−0.131	0.195	−0.131	0.176	−0.087			0.140
C_9	1.118	1.118	−0.108	0.200	−0.196	0.259	−0.151	0.259	−0.196	0.201	−0.108	0.186
C_4	−1.132	1.132	0.135	−0.112	0.112	−0.135						0.124
C_6	−1.121	1.121	0.147	−0.128	0.197	−0.197	0.128	−0.147				0.157
C_8	−1.115	1.115	0.180	−0.160	0.206	−0.171	0.172	−0.206	0.161	−0.180		0.180

Table S11: Spin-density distribution on Cr and each atom of the coupler of [Cr]-C_n-[Cr] [UMN12SX/6-311++g(d,p)].

sys	Cr1	Cr2	C1	C2	C3	C4	C5	C6	C7	C8	C9	Average Spin-density on each atom of coupler
C_3	2.479	2.479	0.034	−0.011	0.034							0.026
C_5	2.561	2.561	0.039	−0.042	0.047	−0.038	0.039					0.051
C_7	2.605	2.605	0.067	−0.082	0.100	−0.145	0.097	−0.082	0.067			0.091
C_9	2.651	2.651	0.089	−0.124	0.141	−0.172	0.100	−0.170	0.138	−0.125	0.089	0.128
C_4	2.459	−2.459	0.034	−0.027	0.027	−0.034						0.031
C_6	2.639	−2.639	0.089	−0.056	0.107	−0.107	0.056	−0.088				0.084
C_8	2.691	−2.691	0.139	−0.116	0.156	−0.127	0.127	−0.156	0.117	−0.139		0.135

Table S12: Spin-density distribution on Cr, Ni and each atom of the coupler of [Cr]-C_n-[Ni] [UMN12SX/6-311++g(d,p)]. Numbering is done considering chromocene unit at the left end.

sys	Cr1	Ni2	C1	C2	C3	C4	C5	C6	C7	C8	C9	Average

												Spin-density on each atom of coupler
C_3	−2.535	1.135	−0.013	0.029	−0.052							0.031
C_5	−2.564	1.130	−0.042	0.076	−0.075	0.094	−0.043					0.066
C_7	−2.604	1.124	−0.069	0.119	−0.132	0.194	−0.121	0.120	−0.071			0.118
C_9	−2.654	1.120	−0.092	0.158	−0.170	0.219	−0.125	0.204	−0.158	0.161	−0.099	0.154
C_4	2.632	1.124	0.129	−0.058	0.103	−0.140						0.108
C_6	2.737	1.118	0.159	−0.117	0.204	−0.191	0.126	−0.160				0.160
C_8	2.826	1.104	0.210	−0.179	0.246	−0.191	0.186	−0.226	0.176	−0.214		0.204

Table S13: $< S^2 >_{HS}$ and $< S^2 >_{BS}$ of the complexes calculated in UB3LYP/6-311++g(d,p) level of theory.

system	[Ni]-C_n-[Ni]		[Cr]-C_n-[Cr]		[Cr]-C_n-[Ni]	
	$< S^2 >_{HS}$	$< S^2 >_{BS}$	$< S^2 >_{HS}$	$< S^2 >_{BS}$	$< S^2 >_{HS}$	$< S^2 >_{BS}$
C_3	6.0200	2.0185	6.0714	2.0713	6.0445	2.0448
C_5	6.0356	2.0255	6.1114	2.1041	6.0644	2.0740
C_7	6.0792	2.0405	6.2106	2.1661	6.1031	2.1480
C_9	6.1725	2.0680	6.4318	2.2781	6.1688	2.2973
C_4	6.0195	2.0221	6.1017	2.1354	6.1549	2.0601
C_6	6.0218	2.0694	6.1246	2.2598	6.3378	2.0846
C_8	6.0246	2.1350	6.1622	2.4589	6.5247	2.1982

Table S14: $< S^2 >_{HS}$ and $< S^2 >_{BS}$ of the complexes calculated in UMN12SX/6-311++g(d,p) level of theory.

system	[Ni]-C_n-[Ni]		[Cr]-C_n-[Cr]		[Cr]-C_n-[Ni]	
	$< S^2 >_{HS}$	$< S^2 >_{BS}$	$< S^2 >_{HS}$	$< S^2 >_{BS}$	$< S^2 >_{HS}$	$< S^2 >_{BS}$
C_3	6.0173	2.0160	6.0839	2.0838	6.0500	2.0501
C_5	6.0275	2.0200	6.1051	2.1017	6.0605	2.0659
C_7	6.0521	2.0271	6.1460	2.1297	6.0770	2.0978
C_9	6.1000	2.0378	6.2160	2.1664	6.0997	2.1561
C_4	6.0180	2.0106	6.0992	2.1008	6.0877	2.0588
C_6	6.0206	2.0373	6.1232	2.1723	6.1678	2.0726
C_8	6.0235	2.0763	6.1480	2.2766	6.3010	2.0943

Table S15: SOMO4 (α) – LUMO (α) energy gaps in electron volt calculated in UB3LYP/6-31g(d,p) level of theory.

C_n	[Ni]-C_n-[Ni]	[Cr]-C_n-[Cr]	[Cr]-C_n-[Ni]
C_3	4.58	4.39	4.37
C_5	3.50	3.19	3.45
C_7	2.90	3.33	2.83
C_9	2.54	2.92	2.41
C_4	2.82	3.19	3.03
C_6	2.29	2.70	2.57
C_8	1.95	2.37	2.28

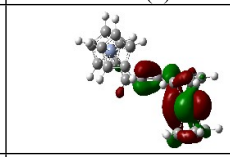
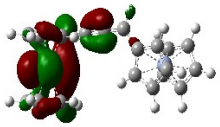
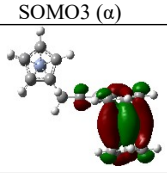
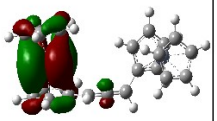
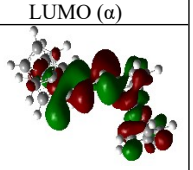
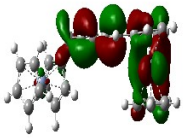
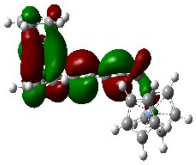
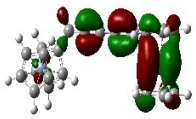
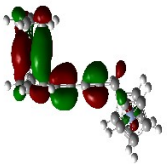
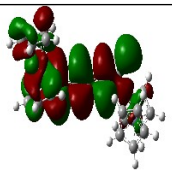
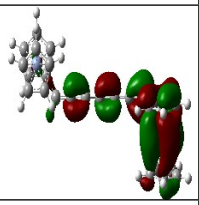
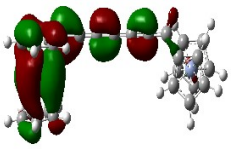
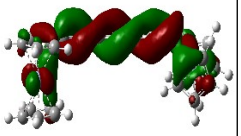
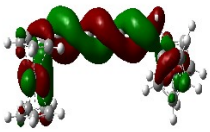
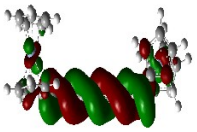
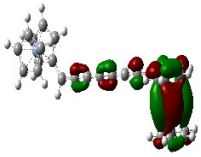
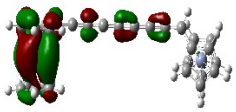
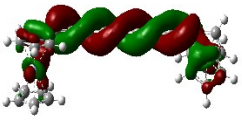
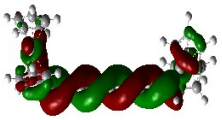
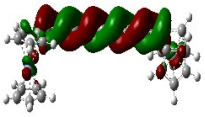
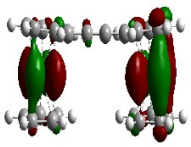
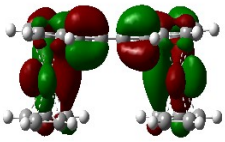
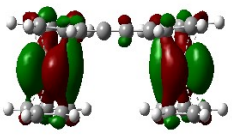
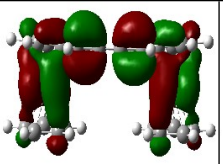
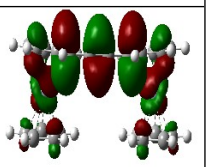
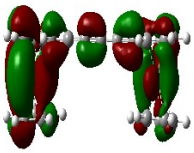
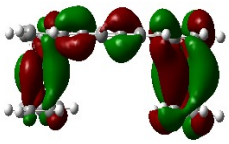
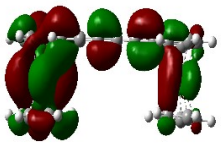
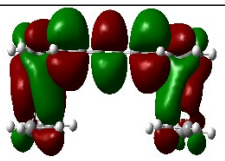
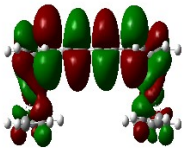
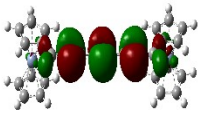
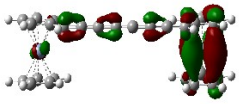
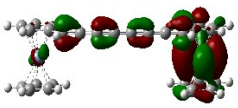
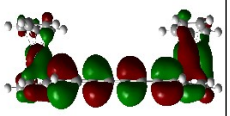
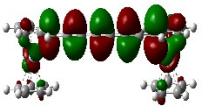
C_n	SOMO1 (α)	SOMO2 (α)	SOMO3 (α)	SOMO4 (α)	LUMO (α)
C_3					
C_5					
C_7					
C_9					
C_4					
C_6					
C_8					

Figure S1: The frontier molecular orbitals of [Cr]-C_n-[Cr] complexes in their high-spin state (quintet) [UB3LYP/6-311++g(d,p)]. The order of energy of the MOs is $E_{SOMO1} < E_{SOMO2} < E_{SOMO3} < E_{SOMO4} < E_{LUMO}$

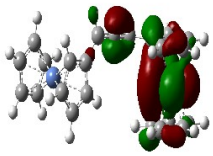
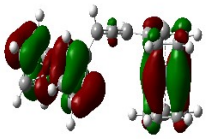
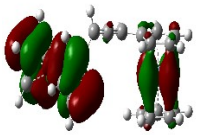
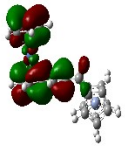
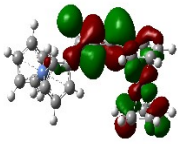
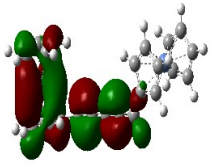
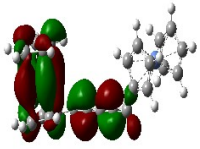
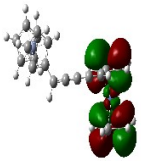
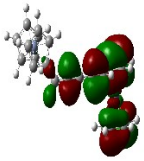
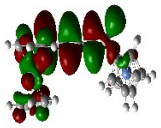
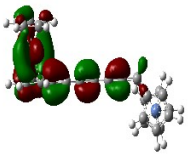
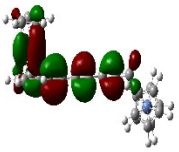
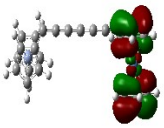
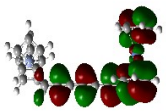
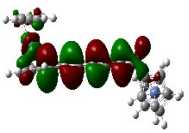
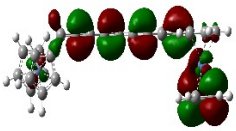
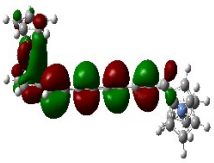
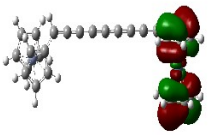
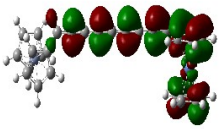
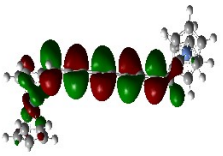
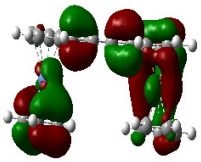
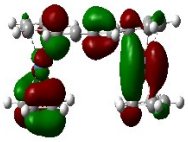
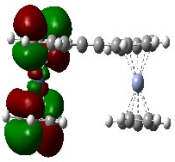
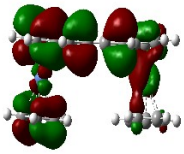
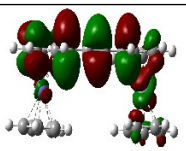
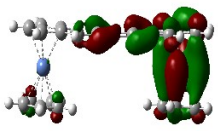
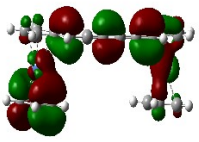
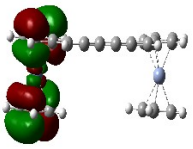
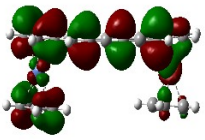
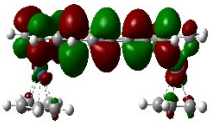
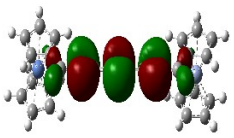
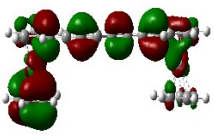
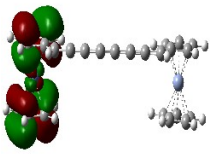
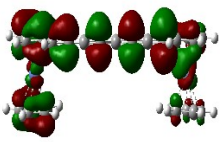
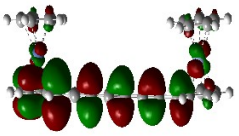
C_n	SOMO1 (α)	SOMO2 (α)	SOMO3 (α)	SOMO4 (α)	LUMO (α)
C_3					
C_5					
C_7					
C_9					
C_4					
C_6					
C_8					

Figure S2: The frontier molecular orbitals of [Cr]-C_n-[Ni] complexes in their high-spin state (quintet) [UB3LYP/6-311++g(d,p)]. The order of energy of the MOs is $E_{SOMO1} < E_{SOMO2} < E_{SOMO3} < E_{SOMO4} < E_{LUMO}$

Optimized coordinate of the complexes in UB3LYP/6-311++g(d,p)

[Ni]-C_3-[Ni]

C	-3.62335586	-1.82622808	-1.15366182
C	-2.45946602	-1.73502939	-0.32985610
C	-2.90687259	-1.61693042	1.02175683
C	-4.32442045	-1.65945017	1.02869246
C	-4.77035700	-1.78743390	-0.31916034
H	-3.62221353	-1.91818611	-2.23040402
H	-2.26615535	-1.51904183	1.88547407
H	-4.95587334	-1.60042970	1.90284414
H	-5.79759127	-1.84594054	-0.64670565
C	-5.01831373	1.97657632	-0.19570380
C	-4.15184362	2.08953578	0.92624257
C	-4.21473346	1.90665908	-1.36652367
H	-6.09718153	1.93962059	-0.16340559
C	-2.81182713	2.09002922	0.44963302
H	-4.45696528	2.15377744	1.96018579
C	-2.85043509	1.97638521	-0.96802257
H	-4.57586726	1.81054383	-2.37975918
H	-1.92185828	2.15424816	1.05794505
H	-1.99479090	1.94342186	-1.62605945
C	4.46967166	1.05804216	-1.80338838
C	5.55245388	1.01998792	-0.88220001
C	5.78407566	-0.33847346	-0.53174589
C	4.84388535	-1.14070847	-1.23639433
C	4.03136476	-0.27731888	-2.02268422
H	4.04807679	1.94587966	-2.25094923
H	6.09653456	1.87396241	-0.50661425
H	6.53623402	-0.69755507	0.15500198

H	4.75792184	-2.21577042	-1.18115781
H	3.21945524	-0.58264264	-2.66574161
C	1.84480592	-0.62644808	1.11153698
C	2.94035094	-0.66607945	2.02787185
C	1.64056313	0.74257702	0.75775118
C	3.38894932	0.66136630	2.25248797
H	3.34766454	-1.56042422	2.47736140
C	2.58189077	1.53334258	1.46546300
H	0.89221094	1.10413932	0.06842369
H	4.19797844	0.95774600	2.90331683
H	2.67488572	2.60801275	1.41187864
C	-1.08076402	-1.78171771	-0.81858031
C	0.00416587	-1.77957944	-0.08039898
C	1.08734173	-1.79459977	0.66004431
H	1.46650633	-2.76144584	0.99333284
H	-0.96551360	-1.83885206	-1.90164995
Ni	3.72131501	0.20891547	0.11829463
Ni	-3.73296638	0.14472418	-0.09051878

[Ni]-C_4-[Ni]

C	-4.27435700	-1.86657522	-0.31014074
C	-2.84459073	-1.78085127	-0.26588447
C	-2.49296782	-1.35810199	1.05639467
C	-3.68101579	-1.21697162	1.81330591
C	-4.78703194	-1.53086249	0.96638440
H	-4.85556755	-2.15268788	-1.17497708
H	-1.48693170	-1.19145936	1.41033832
H	-3.74120385	-0.92261474	2.85064359
H	-5.82859826	-1.51759411	1.25072933
C	-4.25150987	2.36048372	0.81942289
C	-2.91473497	2.30955121	0.33677632
C	-5.11877248	2.00045092	-0.24878487
H	-4.55449492	2.61896551	1.82327572
C	-2.95466222	1.91573948	-1.02952935
H	-2.02456438	2.52346143	0.90936874

C	-4.31798242	1.72556266	-1.39133736
H	-6.19570449	1.93756979	-0.19838536
H	-2.10097129	1.77599056	-1.67573880
H	-4.67971011	1.42086452	-2.36216911
C	2.91444372	2.30947721	0.33626657
C	4.25096489	2.36053289	0.81960411
C	5.11880986	2.00056453	-0.24815008
C	4.31863880	1.72559347	-1.39111123
C	2.95511583	1.91565368	-1.03001421
H	2.02395711	2.52333215	0.90838786
H	4.55340548	2.61905073	1.82361192
H	6.19571984	1.93775773	-0.19718398
H	4.68089647	1.42089693	-2.36174608
H	2.10177180	1.77582645	-1.67666517
C	2.84460098	-1.78081605	-0.26591293
C	4.27437235	-1.86647398	-0.31019511
C	2.49297857	-1.35817783	1.05640396
C	4.78704954	-1.53082772	0.96634866
H	4.85558366	-2.15249991	-1.17505926
C	3.68103263	-1.21704748	1.81330712
H	1.48693836	-1.19162442	1.41037743
H	5.82861995	-1.51752066	1.25067619
H	3.74122147	-0.92275786	2.85066375
C	-1.96142024	-2.08634673	-1.37057076
C	0.62779068	-2.06962770	-1.34222613
C	1.96142157	-2.08631252	-1.37059518
H	2.44315607	-2.36934830	-2.30493842
H	-2.44316043	-2.36940590	-2.30490419
Ni	3.77817735	0.26647861	0.18819899
Ni	-3.77827292	0.26651957	0.18817386
C	-0.62778851	-2.06964245	-1.34221975

[Ni]-C_5-[Ni]

C	-4.90143238	-1.68268778	-1.13606239
C	-3.62243961	-1.65022965	-0.49282656

C	-3.86202629	-1.55282385	0.91514451
C	-5.26056672	-1.55372105	1.13088668
C	-5.90688156	-1.63240246	-0.14092524
H	-5.06289432	-1.74488145	-2.20268274
H	-3.09723179	-1.50016319	1.67555051
H	-5.75413677	-1.50415383	2.09017225
H	-6.97285695	-1.65466548	-0.31144570
C	-5.55592343	2.17291371	0.87194591
C	-4.13391220	2.18445082	0.88387831
C	-5.98411048	2.09928528	-0.48238334
H	-6.19805732	2.20520866	1.73966914
C	-3.68203517	2.11575219	-0.46326473
H	-3.50613465	2.22630387	1.76151862
C	-4.82658474	2.06421677	-1.30786685
H	-7.00823150	2.06671326	-0.82357374
H	-2.65207219	2.09654209	-0.78696936
H	-4.81708682	2.00386197	-2.38607058
C	4.75502742	0.82499720	-2.10988554
C	5.91032852	1.41959112	-1.53174358
C	6.74148473	0.37652369	-1.03764142
C	6.09938042	-0.86299231	-1.30950999
C	4.87019046	-0.58615713	-1.97163621
H	3.92937590	1.35177949	-2.56472913
H	6.11630378	2.47797183	-1.47064337
H	7.68950736	0.50381748	-0.53629924
H	6.47568323	-1.84254318	-1.05432028
H	4.14778616	-1.31730917	-2.30264074
C	3.16407830	-0.61771513	1.38598357
C	4.43383485	-0.66940423	2.04595816
C	2.87809607	0.76179896	1.13226212
C	4.90613681	0.65397251	2.21755314
H	4.93581146	-1.57167459	2.36461261
C	3.93927307	1.54072501	1.65183017
H	1.99413896	1.13421412	0.63650906

H	5.83033591	0.94306249	2.69522080
H	4.00696139	2.61824319	1.62577888
C	-2.34441654	-1.71821412	-1.17609752
C	1.15091502	-1.74727423	0.49126803
C	2.34561016	-1.77139868	1.06351787
H	2.76221288	-2.74244250	1.33260027
H	-2.38731048	-1.77727261	-2.26399318
Ni	4.78991567	0.30067158	0.04850752
Ni	-4.79752685	0.26379815	-0.01499805
C	0.00037467	-1.73824255	-0.05561547
C	-1.15089989	-1.72725824	-0.60085784

[Ni]-C_6-[Ni]

C	-5.53514031	-1.74669985	-0.07027005
C	-4.10183496	-1.70782673	-0.04815331
C	-3.71698161	-1.17475195	1.22553101
C	-4.88852563	-0.92160737	1.97604322
C	-6.01730969	-1.27423015	1.17265123
H	-6.13729597	-2.09125998	-0.89862360
H	-2.70037339	-1.01201586	1.55069197
H	-4.92531008	-0.53086705	2.98214959
H	-7.05363591	-1.19760799	1.46597294
C	-5.37864720	2.56125925	0.65887809
C	-4.03563822	2.43004872	0.20982137
C	-6.23746139	2.13069006	-0.39024475
H	-5.69159432	2.91738474	1.62922832
C	-4.06305024	1.91559597	-1.11602561
H	-3.14936003	2.66802559	0.77899469
C	-5.42506938	1.73163989	-1.48706444
H	-7.31652038	2.10323791	-0.35633881
H	-3.20227223	1.69413987	-1.72922678
H	-5.77836822	1.35154778	-2.43410831
C	4.03654284	2.43043370	0.21085209
C	5.38009768	2.56101996	0.65845590
C	6.23757644	2.13010049	-0.39161199

C	5.42381433	1.73145428	-1.48756228
C	4.06228173	1.91601769	-1.11504099
H	3.15099740	2.66877996	0.78101096
H	5.69426852	2.91694931	1.62848257
H	7.31665897	2.10214530	-0.35888316
H	5.77589945	1.35123097	-2.43500534
H	3.20073603	1.69497067	-1.72731073
C	4.10178130	-1.70780619	-0.04806357
C	5.53508808	-1.74674548	-0.07011360
C	3.71689263	-1.17464619	1.22557315
C	6.01721925	-1.27422509	1.17280641
H	6.13725830	-2.09140153	-0.89841656
C	4.88841510	-0.92150790	1.97612375
H	2.70027931	-1.01184845	1.55068700
H	7.05353770	-1.19763713	1.46616536
H	4.92517473	-0.53070085	2.98220516
C	-3.24235342	-2.14160082	-1.12400253
C	1.90756730	-2.13615234	-1.10954780
C	3.24232129	-2.14162523	-1.12391797
H	3.73815795	-2.51386211	-2.01935497
H	-3.73816888	-2.51375846	-2.01948438
Ni	4.95782804	0.40848278	0.22511472
Ni	-4.95782125	0.40853069	0.22517986
C	0.64941258	-2.13749059	-1.11000740
C	-0.64944371	-2.13749185	-1.11002622
C	-1.90759800	-2.13615722	-1.10959776

[Ni]-C_7-[Ni]

C	6.18949799	-1.59279873	1.06080232
C	4.85133279	-1.57239974	0.54538972
C	4.95286514	-1.46436487	-0.88052127
C	6.32156290	-1.45148867	-1.23037820
C	7.09073224	-1.52919662	-0.02564612
H	6.45456758	-1.65729755	2.10631928
H	4.11713141	-1.41639682	-1.56249528

H	6.71975978	-1.39634025	-2.23270121
H	8.16844103	-1.54411511	0.03907436
C	6.74574334	2.26588984	-0.92080260
C	5.32432202	2.27658825	-0.96201167
C	7.14605291	2.19164306	0.44217909
H	7.40568939	2.29929481	-1.77503154
C	4.84453226	2.20584673	0.37530062
H	4.71477596	2.31849014	-1.85241040
C	5.97170959	2.15470483	1.24350184
H	8.16295971	2.16007113	0.80437031
H	3.80815513	2.18619258	0.67784315
H	5.93966632	2.09461035	2.32126770
C	-5.78434189	1.05306642	2.13136608
C	-7.06105852	1.45588692	1.65165603
C	-7.78853849	0.28518671	1.30002178
C	-6.96057337	-0.84136169	1.56084858
C	-5.72024154	-0.36684837	2.07394719
H	-4.99638537	1.70969396	2.46912070
H	-7.41341654	2.47280417	1.56179701
H	-8.79027378	0.25719297	0.89751078
H	-7.22431098	-1.87549061	1.39585351
H	-4.87674438	-0.97663578	2.36148562
C	-4.49309052	-0.53073609	-1.50324599
C	-5.83203029	-0.57195361	-2.01528997
C	-4.17703763	0.84737720	-1.26654998
C	-6.31483976	0.75202971	-2.11859856
H	-6.36966262	-1.46966787	-2.28470811
C	-5.28559504	1.63227341	-1.65516705
H	-3.24123274	1.21249547	-0.87058591
H	-7.28485409	1.04926078	-2.48819281
H	-5.34602459	2.70971898	-1.61358898
C	3.65247984	-1.65635095	1.34473147
C	-2.39798791	-1.66524660	-0.83692887
C	-3.65052473	-1.68290476	-1.28902565

H	-4.08925580	-2.65123248	-1.53041079
H	3.79727081	-1.73240808	2.42252207
Ni	-5.96500057	0.39062982	0.01826442
Ni	5.97036241	0.35830036	-0.04610095
C	-1.20586326	-1.66520648	-0.40840178
C	0.00123829	-1.66297075	0.02696534
C	1.20929960	-1.66156970	0.45974667
C	2.40262296	-1.65847640	0.88484157

[Ni]-C_8-[Ni]

C	-6.80952894	-1.63088913	0.08832584
C	-5.37509198	-1.60433143	0.10739814
C	-4.98365065	-0.99266880	1.34418832
C	-6.15129033	-0.68084716	2.07623625
C	-7.28511894	-1.07443810	1.29718067
H	-7.41568465	-2.02273727	-0.71569393
H	-3.96528076	-0.81881441	1.65793421
H	-6.18365740	-0.22636846	3.05533259
H	-8.32022531	-0.96975004	1.58604754
C	-6.62379746	2.71217090	0.54289252
C	-5.27813393	2.54641496	0.11372878
C	-7.47709725	2.22130660	-0.48428505
H	-6.94220595	3.12997315	1.48649550
C	-5.29823628	1.94969282	-1.17728739
H	-4.39483662	2.81483710	0.67389569
C	-6.65858054	1.75005057	-1.54729786
H	-8.55651899	2.20184837	-0.45747487
H	-4.43384442	1.68656559	-1.76857114
H	-7.00659417	1.31358025	-2.47171653
C	5.27813247	2.54641663	0.11373083
C	6.62379889	2.71217223	0.54288572
C	7.47709175	2.22130625	-0.48429678
C	6.65856784	1.75004939	-1.54730370
C	5.29822612	1.94969300	-1.17728470
H	4.39483894	2.81484000	0.67390312

H	6.94221373	3.12997550	1.48648612
H	8.55651364	2.20184742	-0.45749355
H	7.00657523	1.31357769	-2.47172412
H	4.43383032	1.68656549	-1.76856256
C	5.37509600	-1.60433172	0.10740267
C	6.80953290	-1.63088674	0.08832953
C	4.98365423	-0.99266783	1.34419206
C	7.28512260	-1.07443262	1.29718320
H	7.41568888	-2.02273510	-0.71568998
C	6.15129388	-0.68084271	2.07623873
H	3.96528417	-0.81881491	1.65793834
H	8.32022896	-0.96974189	1.58604910
H	6.18366068	-0.22636211	3.05533419
C	-4.52181172	-2.11395060	-0.93643965
C	3.18591227	-2.11265154	-0.92553291
C	4.52181600	-2.11395304	-0.93643485
H	5.02049034	-2.54420555	-1.80410655
H	-5.02048538	-2.54420253	-1.80411195
Ni	6.21255540	0.53600213	0.24660621
Ni	-6.21255673	0.53600084	0.24660716
C	1.92710402	-2.11538680	-0.92816257
C	0.63123435	-2.11664458	-0.92879620
C	-0.63123003	-2.11664385	-0.92879732
C	-1.92709978	-2.11538481	-0.92816509
C	-3.18590793	-2.11264878	-0.92553679

[Ni]-C_9-[Ni]

C	7.46700129	-1.48695267	1.03133007
C	6.09732891	-1.48328921	0.60024514
C	6.11042499	-1.39939698	-0.83262319
C	7.45284485	-1.38950975	-1.26637945
C	8.29714260	-1.44183722	-0.10867477
H	7.79682408	-1.53055717	2.05932204
H	5.23378043	-1.36710712	-1.46209971
H	7.78838794	-1.35473614	-2.29226068

H	9.37681611	-1.45413471	-0.11179106
C	7.96826815	2.32573085	-1.02014758
C	6.54721376	2.33857994	-1.07177336
C	8.35882281	2.28064748	0.34710772
H	8.63436652	2.33933423	-1.87013835
C	6.05768194	2.29739408	0.26320933
H	5.94414887	2.36225305	-1.96723941
C	7.17878226	2.26318547	1.14057482
H	9.37306245	2.25525680	0.71714791
H	5.01920071	2.28756925	0.55894846
H	7.13869433	2.22755623	2.21914326
C	-6.83658741	1.22246079	2.13188331
C	-8.15418214	1.58900914	1.74234059
C	-8.88745495	0.39577067	1.49231156
C	-8.02206356	-0.70842125	1.72507979
C	-6.75259333	-0.19754598	2.11915749
H	-6.03549947	1.90218314	2.38153955
H	-8.53007854	2.59679670	1.64530215
H	-9.91771247	0.33878229	1.17358340
H	-8.28046775	-1.75160048	1.61929752
H	-5.87873499	-0.78425128	2.36032640
C	-5.82507859	-0.50389400	-1.54518952
C	-7.20414112	-0.55064931	-1.94243148
C	-5.48799528	0.88003115	-1.36786617
C	-7.68896638	0.77082786	-2.03969274
H	-7.76477880	-1.45223739	-2.14310784
C	-6.62085370	1.65899248	-1.68449822
H	-4.52163972	1.25055908	-1.06020000
H	-8.68446082	1.06418965	-2.33765407
H	-6.67447105	2.73746536	-1.66863018
C	4.95526025	-1.55836704	1.47002698
C	-3.68594932	-1.62298042	-1.01363867
C	-4.97293455	-1.64904549	-1.37492844
H	-5.42554575	-2.62203498	-1.56556253

H	5.16334041	-1.61761015	2.53825757
Ni	-7.17388885	0.47758794	0.06743664
Ni	7.18219942	0.44174974	-0.10648831
C	-2.47122549	-1.61711115	-0.66944213
C	-1.23065122	-1.60658610	-0.31931042
C	-0.00511329	-1.59792618	0.03434805
C	1.22182467	-1.58985620	0.38313311
C	2.46035631	-1.57831443	0.74039036
C	3.67484946	-1.56913508	1.08533491

[Cr]-C_3-[Cr]

C	-2.96822200	-0.79989100	2.01727200
C	-1.87876000	-0.70293600	1.10689400
C	-1.70616100	0.68351900	0.79033500
C	-2.68190600	1.43447100	1.52633500
C	-3.46364800	0.50253200	2.28177700
H	-3.36898500	-1.72366200	2.41122300
H	-0.94034900	1.08460100	0.14411700
H	-2.77700800	2.50940400	1.54644700
H	-4.28601200	0.74409700	2.93864700
C	-4.86687200	1.40533500	-1.18922700
C	-3.93168400	0.65174000	-1.97555600
C	-5.76039300	0.47233100	-0.57263300
H	-4.91984600	2.48089600	-1.11697100
C	-4.25895900	-0.72880700	-1.83674100
H	-3.13898000	1.05706600	-2.58601300
C	-5.38014400	-0.83488500	-0.97757200
H	-6.58056400	0.71684000	0.08602100
H	-3.72317900	-1.55514200	-2.28070700
H	-5.83869200	-1.75681900	-0.64978900
C	4.48448400	1.89493200	0.86699000
C	4.98015900	1.90065800	-0.47572600
C	3.87137700	2.02318600	-1.35431800
C	2.68976200	2.09120800	-0.57590800
C	3.05529300	2.01286700	0.80012500

H	5.08090600	1.85986500	1.76580500
H	6.01571800	1.82232100	-0.77205800
H	3.91661100	2.01899100	-2.43395800
H	1.68341500	2.15978200	-0.96236400
H	2.37827000	2.06096300	1.63955200
C	2.43833600	-1.69471600	-0.37972300
C	3.59776400	-1.81114400	-1.19620100
C	2.87858200	-1.53520700	0.97285400
C	4.74963700	-1.74390900	-0.36974900
H	3.59322700	-1.90500700	-2.27335200
C	4.31182000	-1.57649900	0.98407900
H	2.23176200	-1.44239200	1.83217300
H	5.77347500	-1.81291900	-0.70598100
H	4.94358600	-1.53997800	1.85838100
C	-1.10863700	-1.84301700	0.59743300
C	-0.02343100	-1.77538500	-0.13523600
C	1.05774000	-1.72789500	-0.87537100
H	0.94280900	-1.73594700	-1.95967100
H	-1.47840700	-2.82908400	0.87981400
Cr	-3.69376200	0.17927400	0.12317200
Cr	3.69273800	0.15385900	-0.10409400

[Cr]-C_4-[Cr]

C	2.48327400	-1.25201500	1.05374900
C	2.84361700	-1.73648100	-0.25539400
C	4.26854100	-1.87548700	-0.27031200
C	4.77786600	-1.51839800	0.99842100
C	3.68463400	-1.12909500	1.82631500
H	1.47567700	-1.08782700	1.40275300
H	4.85476800	-2.18101500	-1.12583300
H	5.82129600	-1.50739300	1.27825100
H	3.74956800	-0.82692500	2.86064800
C	4.93746900	2.11353700	0.00722400
C	4.41644600	1.83004700	-1.27977700
C	3.84362800	2.29155900	0.90335100

H	5.98477300	2.15654500	0.26883000
C	2.99867700	1.82782400	-1.19889700
H	4.99974000	1.60932300	-2.16220100
C	2.63274100	2.11582900	0.15363700
H	3.91573600	2.54370300	1.95049300
H	2.31759900	1.63055300	-2.01332600
H	1.62745000	2.22286500	0.53102500
C	-4.94731800	2.09715300	0.00982300
C	-3.86225900	2.27517300	0.91873900
C	-2.64344700	2.12303000	0.17590800
C	-2.99499700	1.85081200	-1.18266300
C	-4.41089400	1.83827300	-1.27657700
H	-5.99740500	2.12879200	0.26138300
H	-3.94543400	2.51671300	1.96749600
H	-1.64220900	2.23357600	0.56303400
H	-2.30488400	1.66762600	-1.99287500
H	-4.98315900	1.62236900	-2.16740400
C	-2.83810300	-1.74201300	-0.26280100
C	-2.48198400	-1.25858000	1.04692700
C	-4.26211900	-1.87899100	-0.28405800
C	-3.68594800	-1.13308400	1.81559700
H	-1.47530900	-1.09484800	1.39886300
C	-4.77730900	-1.52021300	0.98221500
H	-4.84470100	-2.18232000	-1.14288600
H	-3.75367700	-0.83482400	2.85083300
H	-5.82173700	-1.51050500	1.25808000
C	1.96528500	-2.03103700	-1.37185000
C	0.63254700	-2.01617000	-1.34487400
C	-0.62363700	-2.01701300	-1.34666700
C	-1.95622700	-2.03389100	-1.37750600
H	-2.44025000	-2.30946100	-2.31281700
H	2.45233000	-2.30654300	-2.30563700
Cr	-3.70433600	0.25303300	0.16543700
Cr	3.70462500	0.25467500	0.16740100

[Cr]-C_5-[Cr]

C	-4.40612700	-0.57137800	2.09994100
C	-3.16805400	-0.54736600	1.37735600
C	-2.90261900	0.83133300	1.04422900
C	-3.96316400	1.62616300	1.58665500
C	-4.87961600	0.75303600	2.23551800
H	-4.89986100	-1.46200500	2.46277100
H	-2.02034500	1.19358300	0.53927400
H	-4.04718300	2.70102700	1.52840900
H	-5.80524400	1.04539600	2.71017800
C	-6.57775300	0.49615200	-1.17308600
C	-5.55991100	1.37358700	-1.63699900
C	-6.11121800	-0.83560600	-1.29983000
H	-7.52845500	0.79476200	-0.75530500
C	-4.44861300	0.57360600	-2.06018700
H	-5.62119200	2.45090500	-1.67427300
C	-4.79704800	-0.79959800	-1.84569900
H	-6.64882400	-1.72363100	-1.00021800
H	-3.53190700	0.93626000	-2.49931600
H	-4.17594700	-1.65508400	-2.06494800
C	5.18428000	2.17384900	0.94088000
C	5.85102800	2.18518300	-0.31330500
C	4.87822700	2.07629300	-1.33786600
C	3.59304000	1.99817800	-0.72771600
C	3.77827000	2.06041100	0.69237400
H	5.65672700	2.24417800	1.90926600
H	6.92083500	2.22432000	-0.46027100
H	5.08100200	2.03001800	-2.39804500
H	2.64785900	1.91763600	-1.24314100
H	2.99702700	2.06142400	1.43696400
C	3.62900700	-1.59176400	-0.43730900
C	4.91980900	-1.71031700	-1.05235000
C	3.85320300	-1.40774100	0.97664000

C	5.91047700	-1.63199200	-0.04748200
H	5.09858700	-1.82626500	-2.11212900
C	5.26562600	-1.44286200	1.20509600
H	3.08158700	-1.33241600	1.72739600
H	6.97805200	-1.66084000	-0.21211300
H	5.75767100	-1.35184600	2.16192600
C	-2.34956500	-1.71227100	1.07230100
C	-1.15006900	-1.69344700	0.51340700
C	0.00377200	-1.68831800	-0.02737100
C	1.15815400	-1.68254800	-0.56687900
C	2.35354200	-1.67066700	-1.13485400
H	2.40836400	-1.73984800	-2.22165000
H	-2.77317900	-2.67802700	1.34943600
Cr	-4.70066600	0.27085100	0.04861900
Cr	4.70218100	0.26493900	-0.03549300

[Cr]-C_6-[Cr]

C	3.68382265	-1.05794090	1.25719652
C	4.09572444	-1.63081764	-0.00520929
C	5.53410948	-1.70905841	0.02934015
C	5.98230594	-1.24749412	1.28926556
C	4.85444703	-0.84228607	2.04688940
H	2.66216747	-0.89653108	1.56528117
H	6.15974092	-2.07232319	-0.77349763
H	7.01424576	-1.16484686	1.59919355
H	4.87975094	-0.43255115	3.04581705
C	4.85824355	2.56686544	0.65835444
C	6.00599360	2.30797905	-0.13250922
C	3.70522954	2.18596297	-0.09516882
H	4.85883013	2.97024551	1.66018466
C	5.58151868	1.76514299	-1.37291077
H	7.03129897	2.45595927	0.17487537
C	4.15630951	1.68739751	-1.36045168
H	2.67764207	2.28389971	0.22010178
H	6.22786371	1.45252311	-2.17992867
H	3.52940059	1.33466888	-2.16531785

C	-6.02608308	2.26466494	-0.06658347
C	-4.92987214	2.45310246	0.82882133
C	-3.72151794	2.20962902	0.09290784
C	-4.08941406	1.87374906	-1.24560394
C	-5.50419985	1.91047634	-1.33702079
H	-7.07300168	2.35678908	0.18300979
H	-4.99815582	2.76209014	1.86077148
H	-2.71436526	2.29743566	0.47076661
H	-3.40992140	1.61107939	-2.04299455
H	-6.08715341	1.66508936	-2.21317583
C	-4.09548168	-1.67592209	-0.07786940
C	-3.71103432	-1.11237550	1.19083210
C	-5.52405897	-1.74393404	-0.09088981
C	-4.90446500	-0.86926610	1.94708269
H	-2.69532647	-0.96978124	1.52653251
C	-6.01742039	-1.26375393	1.14383203
H	-6.12274206	-2.08109542	-0.92569029
H	-4.95343093	-0.49472902	2.95823306
H	-7.05911777	-1.18529085	1.41870853
C	3.25617699	-2.04797011	-1.10566376
C	1.92028626	-2.05403774	-1.10562267
C	0.66261886	-2.05799871	-1.11866732
C	-0.63710058	-2.06273385	-1.13133197
C	-1.89529524	-2.06798856	-1.14262359
C	-3.22950392	-2.07378588	-1.16980994
H	-3.72159914	-2.41862303	-2.07793365
H	3.76915746	-2.39631747	-2.00093250
Cr	4.86455620	0.38899767	0.21863737
Cr	-4.86636120	0.38919702	0.20371604

[Cr]-C_7-[Cr]

C	5.82835900	-0.42714200	-2.04150500
C	4.50367500	-0.42035500	-1.47434300
C	4.19074300	0.95821100	-1.17144300
C	5.29368400	1.76241500	-1.58981400

C	6.29023500	0.90778000	-2.12459700
H	6.36818600	-1.30754000	-2.35985400
H	3.25558200	1.31140600	-0.76452600
H	5.36494400	2.83657300	-1.50252000
H	7.26148000	1.21740200	-2.48320700
C	7.59030300	0.54457800	1.46588700
C	6.52923700	1.39073700	1.87460600
C	7.11400200	-0.79217300	1.44475600
H	8.57964100	0.86783400	1.17538800
C	5.37963300	0.57723800	2.11469800
H	6.57971400	2.46517800	1.97219500
C	5.74390500	-0.78283800	1.84762600
H	7.68725600	-1.66273000	1.16148700
H	4.41744400	0.92150200	2.46208100
H	5.10370300	-1.64539800	1.95391600
C	-6.22010600	2.31891900	-1.00291000
C	-7.02623300	2.27773500	0.16175700
C	-6.17852600	2.10293800	1.28693800
C	-4.82938900	2.03841200	0.82140500
C	-4.85635300	2.17200600	-0.60523800
H	-6.57887800	2.42505600	-2.01611900
H	-8.10554300	2.32480900	0.18452500
H	-6.50108600	2.02343500	2.31469700
H	-3.94683100	1.93240000	1.43376700
H	-3.99783100	2.18588100	-1.25929900
C	-4.85549600	-1.50464900	0.45532900
C	-6.21146200	-1.60525300	0.93346100
C	-4.93450600	-1.32925400	-0.97750500
C	-7.08678900	-1.54030800	-0.17672900
H	-6.50331700	-1.72462000	1.96709800
C	-6.31160300	-1.36762200	-1.35069600
H	-4.08970000	-1.25382000	-1.64497900
H	-8.16622200	-1.56216400	-0.13038500
H	-6.70001200	-1.26731800	-2.35351000

C	3.66796000	-1.58705600	-1.27108300
C	2.40897100	-1.57861100	-0.84203000
C	1.21158100	-1.58197200	-0.42564900
C	0.00011900	-1.58767500	-0.00267900
C	-1.21244000	-1.58639800	0.41725800
C	-2.41032300	-1.58899500	0.83216000
C	-3.66392000	-1.58270900	1.27685500
H	-3.82794900	-1.65516600	2.35222300
H	4.12369300	-2.54905600	-1.50655300
Cr	5.86349000	0.36001300	0.01960900
Cr	-5.86581800	0.34784400	-0.02858900

[Cr]-C_8-[Cr]

C	-6.84021100	-1.52684800	0.21168200
C	-5.39379000	-1.53853100	0.17961000
C	-4.95943000	-0.88853100	1.39817100
C	-6.11399400	-0.56828500	2.17083200
C	-7.26126600	-0.96251800	1.44359600
H	-7.48511700	-1.92301200	-0.55941900
H	-3.93096500	-0.74007900	1.69064600
H	-6.11543500	-0.08067700	3.13476100
H	-8.28614300	-0.81059200	1.75060200
C	-6.01262700	2.76018700	0.48172200
C	-4.89075200	2.28868200	-0.26076900
C	-7.18662800	2.44516900	-0.24434200
H	-5.97659200	3.25042300	1.44356100
C	-5.37969500	1.67924000	-1.45750100
H	-3.85400500	2.38372900	0.02514000
C	-6.80468500	1.77568000	-1.43996700
H	-8.19934700	2.64769500	0.07288000

H	-4.77784700	1.24089500	-2.23896000
H	-7.47623400	1.40781400	-2.20163200
C	5.00137800	2.38113800	-0.01070600
C	6.19678200	2.58054300	0.75589100
C	7.31045000	2.29455500	-0.10046600
C	6.79705900	1.92622900	-1.37701300
C	5.38322800	1.98151400	-1.32036100
H	3.98883700	2.51679000	0.33855600
H	6.24975500	2.93244300	1.77479000
H	8.35423100	2.36215600	0.16736900
H	7.38301700	1.62343700	-2.23271100
H	4.70821200	1.71268100	-2.12010900
C	5.34011400	-1.60657600	0.07974300
C	6.76795100	-1.62107500	0.04871500
C	4.94761400	-0.96939900	1.30333100
C	7.25875300	-1.03010400	1.24200100
H	7.36693400	-2.00141800	-0.76688000
C	6.13099700	-0.62503000	2.03007100
H	3.92819700	-0.81637600	1.62396700
H	8.29822700	-0.91900200	1.51182200
H	6.16776600	-0.18742400	3.01591100
C	-4.57791400	-2.03878100	-0.88941900
C	3.14082900	-2.07545300	-0.95886400
C	4.48084800	-2.07588100	-0.98589100
H	4.97389100	-2.47378200	-1.87122400
H	-5.09858500	-2.44452000	-1.75498900
C	1.88587600	-2.07452400	-0.94704800

C	0.58227200	-2.07475200	-0.93473000
C	-0.67364000	-2.07185600	-0.92223100
C	-1.97932200	-2.06279000	-0.90831900
C	-3.23124000	-2.05606600	-0.89395000
Cr	-6.09349500	0.52443400	0.23993800
Cr	6.10463900	0.51069800	0.21977800

[Cr]-C_9-[Cr]

C	7.19588800	-0.34535600	-1.96683400
C	5.82070600	-0.34585000	-1.52526400
C	5.47722100	1.03340300	-1.25630900
C	6.60433100	1.84287800	-1.58440100
C	7.65097900	0.99544900	-2.02129800
H	7.76649700	-1.22224400	-2.23701300
H	4.50986500	1.38238500	-0.92836100
H	6.66057700	2.91767900	-1.49253400
H	8.64665500	1.31277800	-2.29643800
C	8.66157700	0.64698500	1.64659200
C	7.56098700	1.46587200	1.99834300
C	8.21104800	-0.69892600	1.57146500
H	9.66253500	0.99257000	1.43180100
C	6.41427000	0.63073500	2.14694500
H	7.58304900	2.54005800	2.10975000
C	6.81648600	-0.71774200	1.88403300
H	8.81829100	-1.55621700	1.32095700
H	5.42299800	0.95522500	2.42517400
H	6.18460200	-1.59123500	1.93656100
C	-7.31574700	2.41423500	-1.08385800
C	-8.21745500	2.36228300	0.00679700
C	-7.46608300	2.17666600	1.19919400
C	-6.08209200	2.11702800	0.84607600
C	-5.99218000	2.26272000	-0.57513900
H	-7.58755000	2.52303200	-2.12362100

H	-9.29456800	2.41369600	-0.06140800
H	-7.87225200	2.09575800	2.19664900
H	-5.25227800	2.00700800	1.52748600
H	-5.08269500	2.27233900	-1.15660700
C	-6.10162700	-1.43558200	0.47683600
C	-7.49228600	-1.50128100	0.86166100
C	-6.08242500	-1.27259900	-0.96036600
C	-8.28698500	-1.44142500	-0.31010200
H	-7.85713500	-1.60897000	1.87300100
C	-7.42927900	-1.29824200	-1.42730300
H	-5.19305600	-1.21101800	-1.56893800
H	-9.36714800	-1.44805100	-0.34068200
H	-7.74522200	-1.19997400	-2.45556400
C	4.98328400	-1.51236800	-1.37500800
C	3.69231300	-1.50542800	-1.03097000
C	2.47443700	-1.50932600	-0.69477800
C	-2.46961600	-1.51342600	0.67619000
C	-3.68785700	-1.51561300	1.01108200
C	-4.97337400	-1.50698400	1.37493500
H	-5.20692700	-1.57181800	2.43755600
H	5.45666600	-2.47384400	-1.57345300
C	1.23150400	-1.51466800	-0.35222400
C	0.00210600	-1.51221600	-0.01037100
C	-1.22699100	-1.51804000	0.33251900
Cr	-7.05592700	0.42669800	-0.08152600
Cr	7.05210400	0.43879100	0.07423600

[Cr]-C_3-[Ni]

C	-3.68399000	-1.82907500	-1.17579000
C	-2.52133200	-1.69869000	-0.36639400
C	-2.95512300	-1.52379400	0.98552900
C	-4.38777200	-1.57020400	1.00556500
C	-4.83267800	-1.75578900	-0.34409700
H	-3.68407400	-1.93767500	-2.25153800
H	-2.30395700	-1.41488200	1.83972400

H	-5.01444400	-1.52560300	1.88315200
H	-5.85784600	-1.83606200	-0.67356600
C	-5.09657400	1.87116600	-0.49952400
C	-4.58974500	1.89478100	0.83940500
C	-3.99599600	1.99423100	-1.38908900
H	-6.13347200	1.77632100	-0.78600200
C	-3.16309400	2.03111000	0.75828700
H	-5.17804900	1.86789400	1.74381900
C	-2.80977700	2.09170400	-0.62123600
H	-4.04928600	1.97205700	-2.46812100
H	-2.47989700	2.10032400	1.59127100
H	-1.80738800	2.16563900	-1.01707200
C	4.37831200	1.14970100	-1.76376000
C	5.47613800	1.06017800	-0.86419700
C	5.70798200	-0.31546600	-0.58893500
C	4.75281600	-1.07679900	-1.31836400
C	3.93083800	-0.17095600	-2.04479400
H	3.95303500	2.06102600	-2.15737800
H	6.02996100	1.89164200	-0.45395200
H	6.47012800	-0.71229200	0.06525300
H	4.66344500	-2.15299900	-1.31779700
H	3.10699400	-0.43966600	-2.68901800
C	1.79549200	-0.67557200	1.10278000
C	2.90512200	-0.76710400	1.99822600
C	1.59164800	0.71074300	0.82448400
C	3.36344500	0.54503300	2.28417800
H	3.31551900	-1.68523600	2.39370100
C	2.54768700	1.45988800	1.55711500
H	0.83227500	1.11096800	0.16958000
H	4.18413100	0.80401400	2.93634400
H	2.64390200	2.53559000	1.55907100
C	-1.14258700	-1.72948200	-0.86858300
C	-0.05847200	-1.76263100	-0.13205200
C	1.02634300	-1.81621800	0.60416700

H	1.39681600	-2.79967200	0.89519700
H	-1.03355400	-1.74862100	-1.95345800
Ni	3.65886500	0.20395500	0.12355200
Cr	-3.78894100	0.14816500	-0.11109100

[Cr]-C_4-[Ni]

C	-4.14210846	-1.87185377	-0.43252536
C	-2.71143423	-1.80633220	-0.34579844
C	-2.39695856	-1.42334747	0.99987725
C	-3.60242700	-1.30308040	1.72844873
C	-4.68861909	-1.58040268	0.83828451
H	-4.70083007	-2.12169469	-1.32311994
H	-1.40016710	-1.27748013	1.38765694
H	-3.69007507	-1.05247819	2.77531686
H	-5.73729184	-1.57559460	1.09559389
C	-4.30537649	2.29870454	0.85551239
C	-2.91258837	2.30168320	0.56985469
C	-4.99900367	1.97006022	-0.34147365
H	-4.75671128	2.49976325	1.81588491
C	-2.74367886	1.97428443	-0.80451332
H	-2.12116578	2.50764425	1.27523715
C	-4.03474993	1.77011801	-1.36766894
H	-6.06966305	1.87973286	-0.45044473
H	-1.80304781	1.88879292	-1.32777941
H	-4.24397001	1.50599680	-2.39366891
C	2.68048270	2.12783571	-0.04452936
C	3.82729275	2.43664432	0.74827239
C	4.98296935	2.18522873	-0.03157416
C	4.56927865	1.71780667	-1.30697609
C	3.14132078	1.68132863	-1.32542696
H	1.65031111	2.23731812	0.25825149
H	3.81838031	2.78409311	1.77091119
H	6.00521132	2.28853893	0.30302948
H	5.22304226	1.43283277	-2.11813615
H	2.52083162	1.39209801	-2.15991892

C	2.96328807	-1.70014899	-0.18649035
C	4.40092258	-1.81163232	-0.14709963
C	2.55670342	-1.20906301	1.11170892
C	4.84843232	-1.45646892	1.14819263
H	5.02493694	-2.13444838	-0.96819445
C	3.72401160	-1.08175808	1.92439215
H	1.53767612	-1.04120004	1.42414458
H	5.87893555	-1.42149826	1.47172682
H	3.75010790	-0.74289244	2.94963487
C	-1.80266027	-2.08642033	-1.42601273
C	0.78747750	-2.03397254	-1.32779667
C	2.12681114	-2.02704965	-1.31776990
H	2.64378816	-2.30488547	-2.23437645
H	-2.25445917	-2.36118636	-2.37735024
Ni	-3.67800558	0.24435139	0.19515889
C	-0.46419219	-2.05118455	-1.36183739
Cr	3.78654807	0.27703465	0.18411867

[Cr]-C_5-[Ni]

C	-5.04859800	-1.64847600	-1.14643400
C	-3.76054600	-1.57067200	-0.52110300
C	-3.98875000	-1.44774800	0.89847500
C	-5.40291700	-1.47711700	1.11929000
C	-6.04353600	-1.60346000	-0.14414100
H	-5.22315000	-1.71341200	-2.21129500
H	-3.21994800	-1.41504700	1.65515500
H	-5.89847800	-1.42661400	2.07722800
H	-7.11039900	-1.61452900	-0.31512900
C	-5.31489800	2.12667600	1.02985200
C	-3.90348400	2.02812700	0.80163800
C	-5.95710900	2.21046600	-0.23560500
H	-5.80555600	2.14628500	1.99142400
C	-3.69189900	2.04807000	-0.61547000
H	-3.13608100	1.98759000	1.55939400
C	-4.96385300	2.16150100	-1.24468400

H	-7.02363700	2.25982900	-0.40184400
H	-2.73732400	1.99337100	-1.11692900
H	-5.14548900	2.17327500	-2.30969800
C	4.63326800	0.88693600	-2.07937600
C	5.79801100	1.44311900	-1.48220900
C	6.61573000	0.37062500	-1.03056600
C	5.95587600	-0.84865800	-1.34773600
C	4.72926100	-0.52988300	-1.99549500
H	3.81383700	1.44199300	-2.51127500
H	6.01875600	2.49546900	-1.38134100
H	7.56654100	0.46568100	-0.52735200
H	6.31896000	-1.84232800	-1.13083100
H	3.99573600	-1.23787900	-2.35143600
C	3.03860300	-0.67051800	1.36571400
C	4.30881900	-0.75421700	2.02109400
C	2.76145900	0.71888600	1.16225400
C	4.79062000	0.55937100	2.23889100
H	4.80515200	-1.67063000	2.30652600
C	3.82910600	1.47192700	1.70719700
H	1.87924900	1.11442200	0.68153800
H	5.71790100	0.82492300	2.72422600
H	3.90433500	2.54921000	1.71870500
C	-2.48303600	-1.62929700	-1.21691300
C	1.01525500	-1.75308300	0.43617500
C	2.21159600	-1.80690600	1.00251100
H	2.62388700	-2.78962600	1.23319000
H	-2.53345800	-1.65185400	-2.30585700
Ni	4.66596300	0.28072300	0.05809200
C	-0.13679900	-1.71514100	-0.10517300
C	-1.28999100	-1.67554400	-0.64675700
Cr	-4.81962200	0.27832200	-0.03498100

[Cr]-C_6-[Ni]

C	-5.37622200	-1.77005500	-0.19875300
C	-3.93959400	-1.74910400	-0.14117800

C	-3.58802800	-1.24133100	1.15676200
C	-4.77254600	-1.01600900	1.88851100
C	-5.88689400	-1.34331500	1.04463500
H	-5.95963500	-2.08489000	-1.05206400
H	-2.57922800	-1.08981600	1.51051000
H	-4.83333700	-0.66832000	2.90919600
H	-6.92933800	-1.28388600	1.31990400
C	-5.32686000	2.52335300	0.75111900
C	-3.96516300	2.42336700	0.35510000
C	-6.13541000	2.12359800	-0.34870200
H	-5.68460300	2.83766300	1.72050600
C	-3.92976000	1.95989700	-0.98991100
H	-3.10666600	2.64838500	0.97040800
C	-5.27303400	1.77643400	-1.42487100
H	-7.21456200	2.08319700	-0.36176700
H	-3.04159100	1.77509100	-1.57556800
H	-5.58160200	1.43057900	-2.40028300
C	3.78145600	2.20635800	-0.22002700
C	4.89913600	2.64384500	0.54977700
C	6.07781700	2.35352200	-0.17875100
C	5.70392700	1.73339600	-1.40295200
C	4.27856200	1.64286200	-1.43651500
H	2.74271600	2.29605300	0.06008500
H	4.85709000	3.09565700	1.53002600
H	7.08864000	2.53819200	0.15510700
H	6.38095800	1.39331500	-2.17263800
H	3.68211600	1.23892600	-2.24031000
C	4.25129000	-1.63189600	0.05361800
C	5.69708500	-1.63741600	0.10317200
C	3.80903200	-1.03239800	1.29527100
C	6.10957900	-1.13366400	1.36348900
H	6.34705200	-2.00543900	-0.67758900
C	4.95798400	-0.75931000	2.09490000
H	2.77867200	-0.88900500	1.58328000

H	7.13244800	-1.00575000	1.68781600
H	4.95354400	-0.31561700	3.07983700
C	-3.06255000	-2.16009700	-1.19215700
C	2.09544800	-2.10188400	-1.05937800
C	3.44325100	-2.08639700	-1.04223400
H	3.97075200	-2.45557500	-1.91966800
H	-3.52899400	-2.52169000	-2.10685300
Ni	-4.85079800	0.38721600	0.24001300
C	0.84601500	-2.11299600	-1.08766400
C	-0.46550400	-2.12725200	-1.11722900
C	-1.71468300	-2.13881300	-1.14424100
Cr	4.96924600	0.41969700	0.21787300

[Cr]-C_7-[Ni]

C	6.04349100	-1.73145600	0.84694000
C	4.70547500	-1.63287800	0.34171700
C	4.80597700	-1.35563400	-1.06069000
C	6.17502200	-1.31579100	-1.41053300
C	6.94450100	-1.54675000	-0.22694500
H	6.30928300	-1.92472400	1.87629600
H	3.96966400	-1.21670000	-1.72935100
H	6.57217900	-1.14357600	-2.39992400
H	8.02209300	-1.58020000	-0.16707600
C	6.61421900	2.33702600	-0.65870400
C	5.19240700	2.36130200	-0.67338800
C	7.03650700	2.09436800	0.67777600
H	7.26012600	2.47044300	-1.51390000
C	4.73441400	2.13091500	0.65349600
H	4.56840700	2.51500000	-1.54120100
C	5.87533900	1.96708100	1.48903200
H	8.05901800	2.01230000	1.01546800
H	3.70302200	2.07962000	0.96908000
H	5.86074700	1.77553400	2.55173200
C	-5.56766700	0.26195600	2.17464200
C	-6.69996000	1.12142900	2.03786900

C	-7.76264700	0.36626600	1.48234000
C	-7.30441800	-0.95979900	1.26659300
C	-5.94371000	-1.03528300	1.69521700
H	-4.60929900	0.53337100	2.59044900
H	-6.73730500	2.16961700	2.29574000
H	-8.74024900	0.74737300	1.22407700
H	-7.88324900	-1.76730800	0.84289500
H	-5.31855100	-1.91519500	1.68401600
C	-4.62513600	-0.19123800	-1.50578800
C	-5.93905400	-0.10643300	-2.09153700
C	-4.31041700	1.12674400	-1.00202500
C	-6.39260700	1.22986700	-1.98805100
H	-6.47696900	-0.92737000	-2.54374400
C	-5.40159300	1.99052600	-1.31827400
H	-3.38143200	1.41107000	-0.53189000
H	-7.35564700	1.59546800	-2.31456300
H	-5.46956300	3.04101800	-1.07676700
C	3.50509100	-1.79746800	1.12968200
C	-2.54560800	-1.44404700	-1.02097900
C	-3.79843300	-1.38121100	-1.46049600
H	-4.25553200	-2.29700800	-1.83578100
H	3.65209200	-2.00694700	2.18945600
Ni	5.83851900	0.34080500	-0.01112500
C	-1.35277900	-1.51613700	-0.59718800
C	-0.14613100	-1.59009900	-0.16940100
C	1.06204200	-1.65846300	0.25793500
C	2.25575800	-1.72598400	0.67696600
Cr	-6.00782700	0.37053500	0.06038600

[Cr]-C_8-[Ni]

C	-6.62283100	-1.65895700	-0.03865700
C	-5.18271800	-1.65956100	0.00717100
C	-4.81446800	-1.06059800	1.26417800
C	-5.98757000	-0.77244900	1.98712300
C	-7.11575700	-1.14348200	1.17476600

H	-7.21769900	-2.02391900	-0.86356500
H	-3.80083400	-0.89765800	1.59850800
H	-6.03577700	-0.35768900	2.98311700
H	-8.15461300	-1.05387000	1.45542600
C	-6.54034200	2.68808000	0.64153500
C	-5.17954800	2.55331500	0.25349100
C	-7.35200400	2.22408900	-0.43091000
H	-6.89590100	3.06720400	1.58829100
C	-5.14727700	2.00299600	-1.05855800
H	-4.31928200	2.81083100	0.85336800
C	-6.49219500	1.80217400	-1.48192600
H	-8.43143900	2.19134600	-0.44207000
H	-4.26020600	1.77605700	-1.63091500
H	-6.80308400	1.39722000	-2.43356300
C	4.97403000	2.28946600	-0.34690900
C	6.07088600	2.80230600	0.40490800
C	7.26531000	2.48817000	-0.28710500
C	6.91876900	1.77755500	-1.47093200
C	5.49720400	1.65708200	-1.51452800
H	3.93005900	2.36948600	-0.08315000
H	6.00499200	3.31947300	1.35095800
H	8.26743200	2.72147700	0.04219000
H	7.61142800	1.40102100	-2.20912200
H	4.91902500	1.18152700	-2.29213200
C	5.54824300	-1.54300600	0.22767400
C	6.99514200	-1.47779800	0.27119200
C	5.08631800	-0.85685600	1.41774700
C	7.38779500	-0.86497800	1.49117100
H	7.65981600	-1.88004400	-0.47973200
C	6.22236400	-0.48202000	2.19363800
H	4.05090800	-0.72377400	1.69293600
H	8.40462700	-0.67667600	1.80483800
H	6.19883400	0.03586100	3.14147000
C	-4.32362900	-2.15749900	-1.00917600

C	3.40266100	-2.10485900	-0.84967700
C	4.75956000	-2.08347100	-0.83157800
H	5.29174800	-2.51623300	-1.67585800
H	-4.79584900	-2.58058000	-1.89380800
Ni	-6.07871800	0.52162700	0.26523500
C	2.15774900	-2.11361400	-0.87451800
C	0.84111400	-2.12705100	-0.89955900
C	-0.40575700	-2.13325500	-0.92152500
C	-1.72216800	-2.13952600	-0.94685600
C	-2.96712700	-2.14476100	-0.96762800
Cr	6.20572500	0.55268500	0.23495600

[Cr]-C_9-[Ni]

C	7.30999000	-1.65640500	0.76569900
C	5.93940100	-1.56896600	0.35001300
C	5.94551000	-1.26439700	-1.05159900
C	7.28699400	-1.19994400	-1.48801500
C	8.13564300	-1.44108800	-0.35988900
H	7.64458800	-1.86374200	1.77195600
H	5.06576500	-1.12543200	-1.66194800
H	7.61723100	-1.00661100	-2.49787900
H	9.21514700	-1.46198200	-0.37147700
C	7.80101400	2.43347700	-0.66867300
C	6.37913300	2.45727700	-0.67621800
C	8.22985800	2.17074900	0.66206100
H	8.44277100	2.58063500	-1.52474200
C	5.92750300	2.20588400	0.64896700
H	5.75097000	2.62394700	-1.53861300
C	7.07263700	2.03002700	1.47665300
H	9.25401800	2.08450500	0.99363600
H	4.89772300	2.14984600	0.96897500
H	7.06297600	1.82273800	2.53643700
C	-6.62655500	0.26734900	2.21744100
C	-7.77432900	1.11417500	2.18765400
C	-8.86326800	0.36475400	1.67877800

C	-8.40484600	-0.94781500	1.38647700
C	-7.01710300	-1.01776500	1.72081500
H	-5.64382700	0.54049700	2.57084200
H	-7.80461200	2.15345900	2.48034800
H	-9.86098800	0.74050300	1.50305200
H	-9.00228000	-1.75039300	0.97974400
H	-6.38269700	-1.88714800	1.63832400
C	-5.95804400	-0.06106300	-1.55349000
C	-7.32199100	0.02096800	-2.01943900
C	-5.61935100	1.24841100	-1.04108700
C	-7.77702300	1.35079800	-1.84547600
H	-7.88626700	-0.79338400	-2.45064700
C	-6.74053800	2.10546000	-1.24404800
H	-4.65903900	1.53226900	-0.63827800
H	-8.76704900	1.71424400	-2.08086800
H	-6.79966000	3.14763700	-0.96652000
C	4.79772800	-1.76421500	1.20748500
C	-3.83855000	-1.29883700	-1.24141300
C	-5.12271600	-1.23947900	-1.59634900
H	-5.59370600	-2.15063400	-1.96500300
H	5.01256500	-1.99313200	2.25139400
Ni	7.02973400	0.42859300	-0.04555700
C	-2.62427700	-1.36814100	-0.89756400
C	-1.38649300	-1.43900700	-0.54926500
C	-0.16121700	-1.50249800	-0.19992500
C	1.06477100	-1.57158900	0.14539100
C	2.30231000	-1.63474400	0.49648100
C	3.51811200	-1.69786200	0.83489000
Cr	-7.21841600	0.43202200	0.13328100