

Effect of Heteroatom Incorporation on Electronic Communication in Metal Chalcogenide Nanoclusters

Shana Havenridge¹, Xilai Li², Julia Laskin^{2*} and Cong Liu^{1*}

¹ Chemical Sciences and Engineering Division, Argonne National Laboratory, Lemont, IL 60439, United States.

² James Tarpo Jr. and Margaret Tarpo Department of Chemistry, Purdue University, West Lafayette, IN, 47907, United States.

Supporting Information

Note S1. Synthesis details

All the chemicals including cobalt (II) chloride (CoCl_2 , 97%), iron (II) chloride tetrahydrate ($\text{FeCl}_2 \cdot 4\text{H}_2\text{O}$, 99%), sodium sulfide nonahydrate ($\text{Na}_2\text{S} \cdot 9\text{H}_2\text{O}$), triethylphosphine (PET_3 , 99%) and HPLC grade methanol were purchased from Sigma-Aldrich (St. Louis, MO) and used without further purification.

$\text{Co}_{6-x}\text{Fe}_x\text{S}_8(\text{PET}_3)_6$ ($x=0-6$) NCs were synthesized in an inert atmosphere in a standard nitrogen box (830ABB, Plas Labs, Lansing, MI) using a previously reported procedure, which allowed us to prepare a distribution of $[\text{Co}_{6-x}\text{Fe}_x\text{S}_8(\text{PET}_3)_6]^+$ NC. Specifically, 0.016 g (0.125 mmol) of CoCl_2 and 0.099 g (0.500 mmol) of $\text{FeCl}_2 \cdot 4\text{H}_2\text{O}$ were dissolved in 4 mL of methanol to obtain a 1:4 molar ratio of the two precursors. The solution of FeCl_2 and CoCl_2 was then purged with N_2 for 3 min to remove dissolved oxygen. Next, 120 μL (0.8 mmol) of pure PET_3 was added to the solution. The solution was stirred for 5 min. Subsequently, 0.085 g (0.35 mmol) of $\text{Na}_2\text{S} \cdot 9\text{H}_2\text{O}$ dissolved in 2 mL of methanol was added dropwise to the stirred solution. The mixture was stirred for 60 min at room temperature.

Table S1. Bruker timsTOF Pro2 parameters used in energy-resolved CID experiments.

ESI-MS	Source	End Plate Offset	500 V
		Capillary	4500 V
		Nebulizer	not used
		Dry Gas	4.0 L/min
		Dry Temp	279 C°
	Transfer	Deflection 1 Delta	80 V
		Funnel 1 RF	500 V _{pp}
		isCID Energy	0.0 eV
		Funnel 2 RF	250 V _{pp}
		Multipole RF	200 V _{pp}
	Collision Cell	Collision Energy	10 eV
		Collision EF	1100 V _{pp}
	Quadrupole	Ion Energy	5.0 eV
		Low Mass	150 m/z
	Focus Pre TOF	Transfer Time	65 μs
		Pre Pulse Storage	5 μs

Table S2. Magnetic moment values (calculated using VASP) and the lowest energy spin multiplicity (calculated using ORCA) for each NC.

		VASP	ORCA
L6	Co ₆	1	2
L6	Co ₅ Fe	2	3
L6	Co ₃ Fe ₃	4	3
L6	Fe ₆	7	4
L5	Co ₆	3	4
L5	Co ₅ Fe	4	5
L5	Co ₃ Fe ₃	6	9
L5	Fe ₆	9	6

Table S3. Relative energies for different multiplicities in the fully ligated (L6) NCs at the PBE0-D3/def2TZVP level of theory.

	Charge/Multiplicity	Relative Energy (eV)
Co ₆	1/2	0.00
	1/4	0.66
	1/6	1.08
Co ₅ Fe	1/1	1.36
	1/3	0.00
	1/5	0.34
Co ₃ Fe ₃	1/1	2.50
	1/3	0.00
	1/5	0.03
	1/7	0.07
Fe ₆	1/2	NC
	1/4	0.00
	1/6	0.01
	1/8	0.04
	1/10	0.09

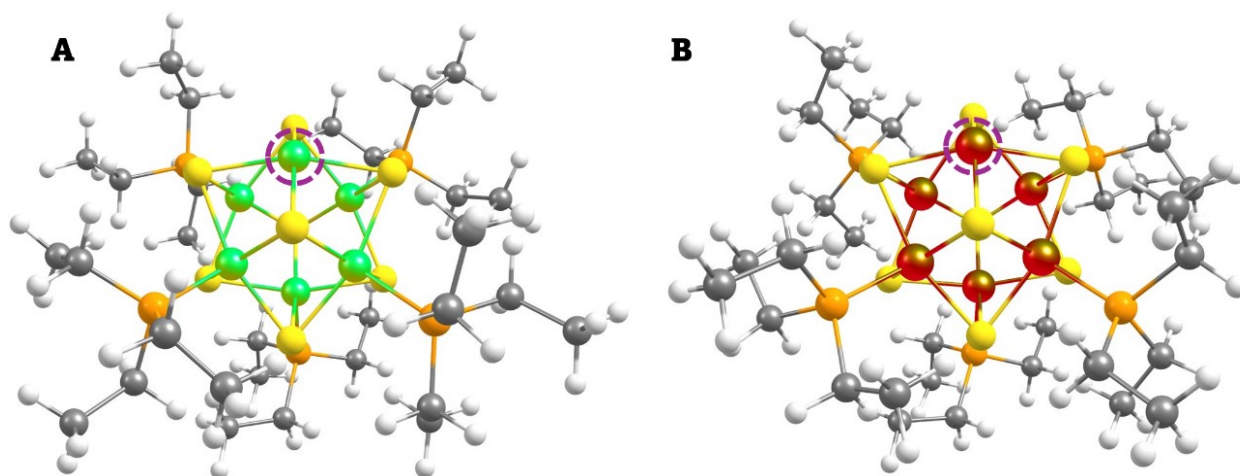


Figure S1. Symmetry isomers of undercoordinated (A) Co₆ and (B) Fe₆ NCs. The circle shows the metal where the ligand was removed. (Color scheme: green = Co, red = Fe, yellow = S, orange = P, grey = C, white = H)

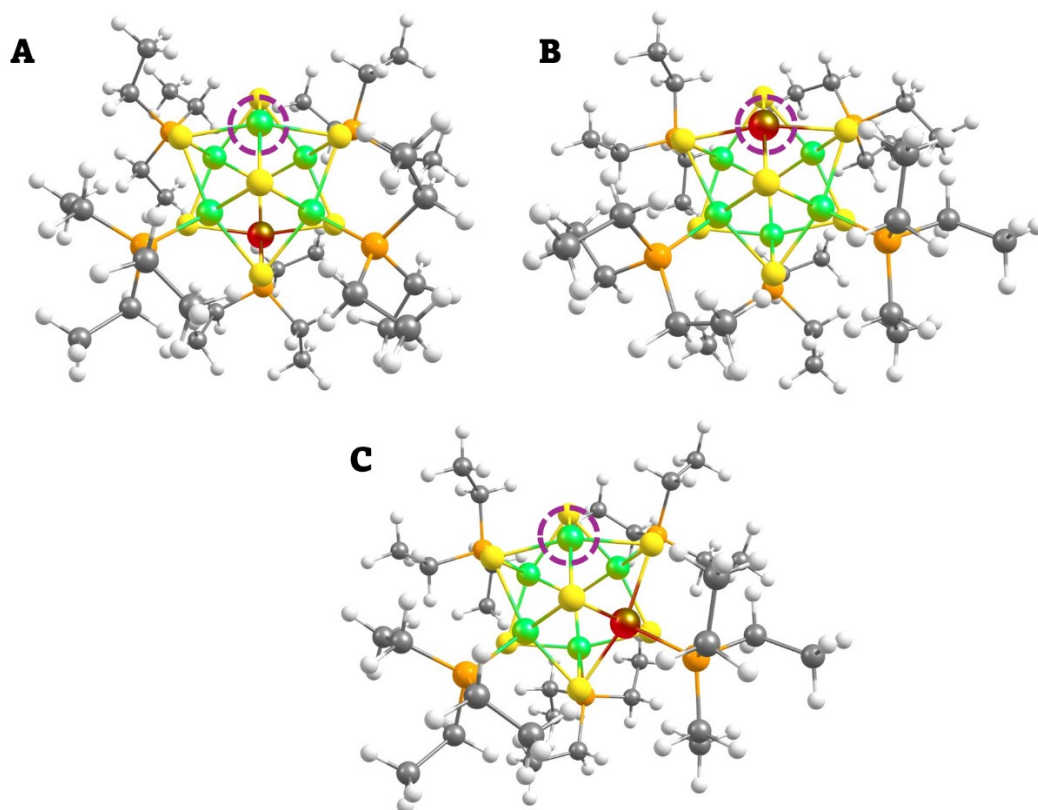


Figure S2. Symmetry isomers of undercoordinated $\text{Co}_5\text{Fe NC}$ (A) Co – trans, (B) Fe, and (C) Co – cis. The circle shows the metal where the ligand was removed. (Color scheme: green = Co, red = Fe, yellow = S, orange = P, grey = C, white = H)

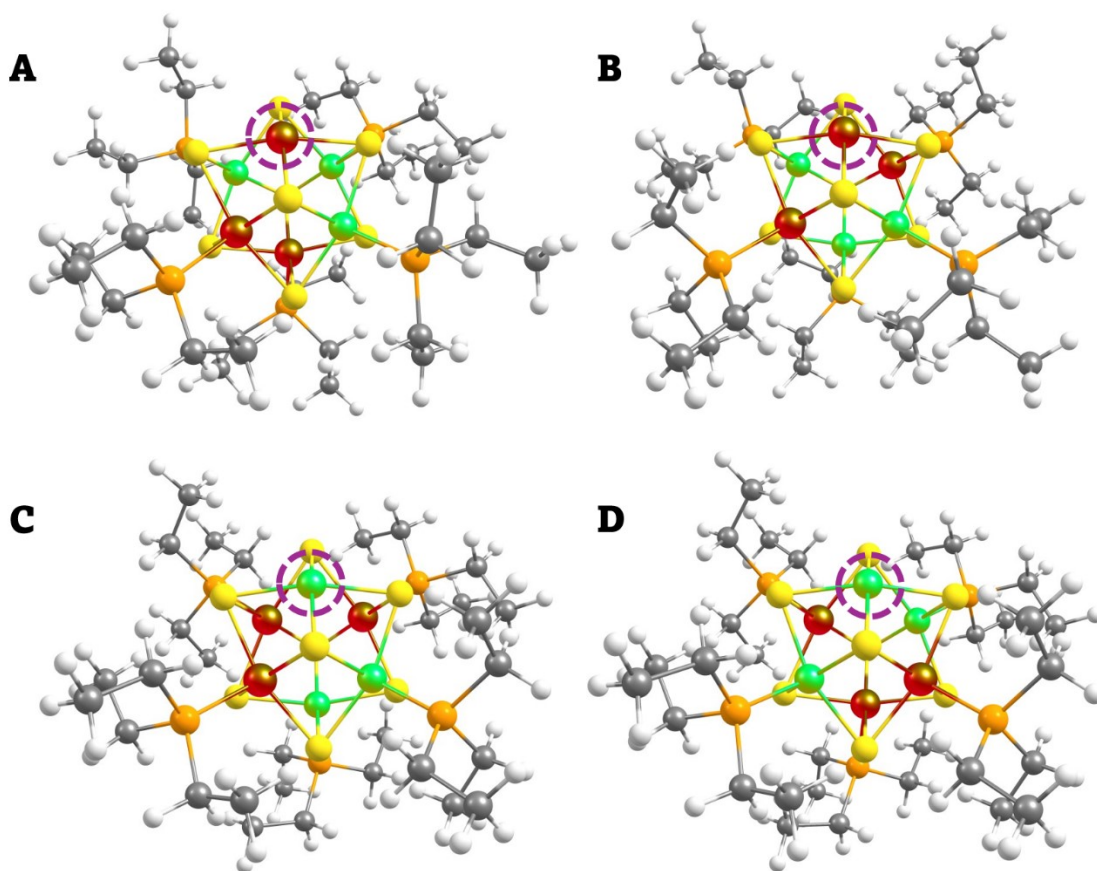


Figure S3. Symmetry isomers of undercoordinated Co_3Fe_3 NC (A) Fe – 1 (B) Fe – 2 (C) Co – 1 (D) Co – 2 . The circle shows the metal where the ligand was removed. (Color scheme: green = Co, red = Fe, yellow = S, orange = P, grey = C, white = H)

Table S4. Relative energies for different multiplicities in the undercoordinated (L5) NCs at the PBE0-D3/def2TZVP level of theory for different symmetry isomers.

NC	Charge/ Multiplicity	Relative Energy (eV)	NC	Charge/ Multiplicity	Relative Energy (eV)
Co₆	1/2	0.01	Co₃Fe₃ (Fe - 1)	1/1	3.83
	1/4	0.00		1/3	0.13
	1/6	0.74		1/5	0.12
NC	Charge/ Multiplicity	Relative Energy (eV)		1/7	0.12
Fe₆	1/2	0.21	1/9	0.06	
	1/4	0.68	1/11	0.08	
	1/6	0.00	Co₃Fe₃	1/1	3.82
	1/8	0.04	(Fe - 2)	1/3	0.14
	1/10	0.10	1/5	0.85	
NC	Charge/ Multiplicity	Relative Energy (eV)		1/7	0.08
Co₅Fe	1/1	2.30	1/9	0.00	
(Fe)	1/3	0.29	1/11	0.38	
	1/5	0.00	Co₃Fe₃	1/3	0.86
	1/7	0.65	(Co - 1)	1/5	0.73
Co₅Fe	1/1	2.59		1/7	0.75
(Co - Cis)	1/3	0.68		1/9	0.50
	1/5	0.23	Co₃Fe₃	1/1	3.95
	1/7	0.71	(Co - 2)	1/3	0.79
Co₅Fe	1/3	0.74		1/5	0.69

(Co - trans)	1/5	0.18	1/7	0.65
	1/7	0.58	1/9	0.66
			1/11	0.63
			1/13	0.74

Table S5. Relative energies of the isomers with the ligand removed from different metals in the undercoordinated (L5) NCs at the PBE0-D3/def2TZVP level of theory starting with the lowest energy isomer from table S2.

NC	Charge/Multiplicity	Metal	Relative Energy (eV)
Co₆	1/4	M1	0.00
		M2	0.11
		M3	0.11
		M4	0.11
		M5	0.11
		M6	0.11
Co₅Fe	1/5	M1	0.23
		M2	0.18
		M3	0.22
		M4	0.23
		M5	0.00
		M6	0.21
Co₃Fe₃	1/9	M1	0.00
		M2	0.50
		M3	0.69
		M4	0.66
		M5	0.06
		M6	0.66
Fe₆	1/6	M1	0.45
		M2	0.00
		M3	0.97
		M4	0.96
		M5	0.44
		M6	0.97
	1/8	M1	0.03
		M2	1.00
		M3	0.17
		M4	0.01
		M5	1.01
		M6	0.11

Table S6. Zero-point energy and Gibbs free energy corrections for the calculation of ligand binding in Co_{6-x}Fe_x (x = 1, 3) NCs at the PBE0-D3/def2TZVP (ORCA – geometry optimizations) and PBE0-D3/CEP-31G (Gaussian - single point calculations) level of theory. All values are shown in Hartree.

(PEt3) (0/1)	Total Energy (ORCA)	-578.7160561			
	ZPE Correction (Gaussian)	0.203149			
	G Correction (Gaussian)	0.170378			
	EZPE	-578.5129071			
	G	-578.5456781			
(PEt3)6 NCs			(PEt3)5 NCs		
Co6 (1/2)	Total Energy (ORCA)	-14953.00157	Co6 (1/4)	Total Energy (ORCA)	-14374.20305
	ZPE Correction (Gaussian)	1.263446		ZPE Correction (Gaussian)	1.057345
	G Correction (Gaussian)	1.163217		G Correction (Gaussian)	0.966758
	EZPE	-14951.73812		EZPE	-14373.1457
	G	-14951.83835		G	-14373.23629
Co5Fe (1/3)	Total Energy (ORCA)	-14833.95307	Co5Fe (1/5)	Total Energy (ORCA)	-14255.16344
	ZPE Correction (Gaussian)	1.263307		ZPE Correction (Gaussian)	1.057452
	G Correction (Gaussian)	1.16344		G Correction (Gaussian)	0.966854
	EZPE	-14832.68977		EZPE	-14254.10599
	G	-14832.78963		G	-14254.19659
Co3Fe3 (1/3)	Total Energy (ORCA)	-14595.81399	Co3Fe3 (1/9)	Total Energy (ORCA)	-14017.04295
	ZPE Correction (Gaussian)	1.262693		ZPE Correction (Gaussian)	1.053611
	G Correction (Gaussian)	1.160122		G Correction (Gaussian)	0.962007
	EZPE	-14594.55129		EZPE	-14015.98934
	G	-14594.65386		G	-14016.08094
Fe6 (1/4)	Total Energy (ORCA)	-14238.60925	Fe6 (1/6)	Total Energy (ORCA)	-13659.83543
	ZPE Correction (Gaussian)	1.260987		ZPE Correction (Gaussian)	1.054838
	G Correction (Gaussian)	1.159024		G Correction (Gaussian)	0.962608
	EZPE	-14237.34826		EZPE	-13658.78059
	G	-14237.45023		G	-13658.87282

Table S7. Ligand binding energy for the ligand removed from Co and Fe in Co_{6-x}Fe_x (x = 1, 3) NCs at the PBE0-D3/def2TZVP level of theory. (C/M = Charge/Multiplicity; ZPE = Zero Point Energy)

	C/M - L6	C/M - L5	ΔE (eV)	ΔE_{ZPE} (eV)	$\Delta G_{298.15}$ (eV)
Co ₅ Fe - Fe	1/3	1/5	2.00	1.93	1.29
Co ₅ Fe - Co	1/3	1/5	2.18	2.09	1.43
Co ₃ Fe ₃ - Fe	1/3	1/9	1.50	1.33	0.74
Co ₃ Fe ₃ - Co	1/3	1/11	2.14	1.92	1.39

Table S8. SOMO-LUMO gaps of L6 and L5 NCs

SOMO-LUMO Gap (eV)		
L6	Co ₆	2.91
L6	Co ₅ Fe	2.77
L6	Co ₃ Fe ₃	2.59
L6	Fe ₆	2.53
L5	Co ₆	2.70
L5	Co ₅ Fe	2.21
L5	Co ₃ Fe ₃	2.23
L5	Fe ₆	2.33

Table S9. POS values calculated at different threshold values for each metal in each NC.

Ligands	L6			L6			L6			L6		
Cluster	Co ₆	(1/2)		Co ₅ Fe	(1/3)		Co ₃ Fe ₃	(1/3)		Fe ₆	(1/4)	
Metal #	Co1			Co1			Fe1			Fe1		
Threshold	0.5	0.65	0.85	0.5	0.65	0.85	0.5	0.65	0.85	0.5	0.65	0.85
POS	-1	1	3	-1	2	3	0	2	2	0	2	2
Metal #	Co2			Co2			Fe2			Fe2		
Threshold	0.5	0.65	0.85	0.5	0.65	0.85	0.5	0.65	0.85	0.5	0.65	0.85
POS	-1	1	3	-1	2	3	-1	1	3	0	1	3
Metal #	Co3			Co3			Co1			Fe3		
Threshold	0.5	0.65	0.85	0.5	0.65	0.85	0.5	0.65	0.85	0.5	0.65	0.85
POS	-1	0	4	-1	2	3	-1	2	3	0	1	3
Metal #	Co4			Co4			Co2			Fe4		
Threshold	0.5	0.65	0.85	0.5	0.65	0.85	0.5	0.65	0.85	0.5	0.65	0.85
POS	-1	2	3	-1	2	3	-1	2	3	0	1	3
Metal #	Co5			Fe1			Fe3			Fe5		
Threshold	0.5	0.65	0.85	0.5	0.65	0.85	0.5	0.65	0.85	0.5	0.65	0.85
POS	-1	2	3	0	2	3	0	1	3	0	1	3
Metal #	Co6			Co5			Co3			Fe6		
Threshold	0.5	0.65	0.85	0.5	0.65	0.85	0.5	0.65	0.85	0.5	0.65	0.85
POS	-1	1	3	-1	2	3	-1	2	3	0	1	3
Ligands	L5			L5			L5			L5		
Cluster	Co ₆	(1/4)		Co ₅ Fe	(1/5)		Co ₃ Fe ₃	(1/9)		Fe ₆	(1/6)	
Metal #	Co1			Co1			Fe1			Fe1		
Threshold	0.5	0.65	0.85	0.5	0.65	0.85	0.5	0.65	0.85	0.5	0.65	0.85
POS	1	2	3	-1	2	3	1	2	3	0	1	3
Metal #	Co2			Co2			Fe2			Fe2		
Threshold	0.5	0.65	0.85	0.5	0.65	0.85	0.5	0.65	0.85	0.5	0.65	0.85
POS	-1	3	3	-1	2	3	2	2	3	2	2	3
Metal #	Co3			Co3			Co1			Fe3		
Threshold	0.5	0.65	0.85	0.5	0.65	0.85	0.5	0.65	0.85	0.5	0.65	0.85
POS	-1	2	3	-1	2	3	-1	2	3	0	1	3
Metal #	Co4			Co4			Co2			Fe4		
Threshold	0.5	0.65	0.85	0.5	0.65	0.85	0.5	0.65	0.85	0.5	0.65	0.85
POS	-1	2	3	-1	2	3	-1	2	3	1	1	3
Metal #	Co5			Fe1			Fe3			Fe5		
Threshold	0.5	0.65	0.85	0.5	0.65	0.85	0.5	0.65	0.85	0.5	0.65	0.85
POS	0	2	3	1	2	3	1	2	3	0	2	3
Metal #	Co6			Co5			Co3			Fe6		
Threshold	0.5	0.65	0.85	0.5	0.65	0.85	0.5	0.65	0.85	0.5	0.65	0.85
POS	-1	2	3	-1	2	3	-1	2	3	0	1	3

Table S10. POS value at ‘0.65’ value threshold for each system at the lowest spin multiplicity from PBE0-D3/def2TZVP level of theory. M1-M6 represent each metal in the TM core. (Color scheme: black = Co atom, red = Fe atom)

L6	Co ₆	Co ₅ Fe	Co ₃ Fe ₃	Fe ₆
M1	1	2	2	2
M2	1	2	1	1
M3	0	2	2	1
M4	2	2	2	1
M5	2	2	1	1
M6	1	2	2	1
L5	Co ₆	Co ₅ Fe	Co ₃ Fe ₃	Fe ₆
M1	2	2	2	1
M2	3	2	2	2
M3	2	2	2	1
M4	2	2	2	1
M5	2	2	2	2
M6	2	2	2	1

Table S11. Total alpha and beta d-orbital occupancy for each metal center in the fully ligated $\text{Co}_{6-x}\text{Fe}_x$ ($x = 0, 1, 3, 6$) NCs at the PBE0-D3/def2TZVP level of theory. M1-M6 represent each metal in the TM core. (Color scheme: green = Co atom, orange = Fe atom)

		L6	1	2	3	4	5	SUM	SUM_ALL
Co ₆	M1	up	0.62	0.66	0.98	0.98	0.99	4.23	
		down	0.64	0.68	0.96	0.98	0.98	4.24	8.47
	M2	up	0.62	0.66	0.98	0.98	0.98	4.22	
		down	0.63	0.67	0.97	0.98	0.98	4.23	8.45
	M3	up	0.66	0.72	0.98	0.98	0.99	4.33	
		down	0.63	0.70	0.82	0.98	0.99	4.12	8.45
	M4	up	0.61	0.65	0.98	0.99	0.98	4.21	
		down	0.63	0.67	0.98	0.98	0.98	4.24	8.45
	M5	up	0.59	0.65	0.99	0.98	0.98	4.19	
		down	0.65	0.72	0.93	0.98	0.99	4.27	8.46
	M6	up	0.62	0.68	0.99	0.98	0.98	4.25	
		down	0.65	0.72	0.89	0.98	0.99	4.23	8.48
Co ₅ Fe	M1	up	0.62	0.64	0.98	0.98	0.98	4.20	
		down	0.62	0.68	0.98	0.99	0.98	4.25	8.45
	M2	up	0.64	0.62	0.98	0.98	0.98	4.20	
		down	0.63	0.68	0.98	0.98	0.98	4.25	8.45
	M3	up	0.62	0.65	0.98	0.98	0.99	4.22	
		down	0.63	0.67	0.97	0.98	0.99	4.24	8.46
	M4	up	0.62	0.64	0.98	0.98	0.98	4.20	
		down	0.63	0.68	0.97	0.98	0.98	4.24	8.44
	M5	up	0.85	0.91	0.98	0.97	0.97	4.68	
		down	0.98	0.60	0.53	0.18	0.18	2.47	7.15
	M6	up	0.64	0.62	0.99	0.98	0.98	4.21	
		down	0.63	0.68	0.98	0.98	0.98	4.25	8.46
Co ₃ Fe ₃	M1	up	0.86	0.91	0.97	0.97	0.97	4.68	
		down	0.98	0.53	0.59	0.18	0.19	2.47	7.15
	M2	up	0.70	0.70	0.97	0.98	0.97	4.32	
		down	0.16	0.51	0.57	0.98	0.97	3.19	7.51
	M3	up	0.61	0.63	0.99	0.98	0.98	4.19	
		down	0.64	0.68	0.97	0.98	0.99	4.26	8.45
	M4	up	0.61	0.64	0.99	0.98	0.98	4.20	
		down	0.64	0.67	0.98	0.98	0.97	4.24	8.44
	M5	up	0.16	0.49	0.54	0.98	0.97	3.14	
		down	0.68	0.74	0.97	0.98	0.98	4.35	7.49
	M6	up	0.62	0.65	0.99	0.98	0.98	4.22	
		down	0.63	0.66	0.98	0.98	0.98	4.23	8.45
Fe ₆	M1	up	0.86	0.91	0.98	0.97	0.97	4.69	

		down	0.98	0.58	0.53	0.18	0.18	2.45	7.14
	M2	up	0.71	0.70	0.97	0.98	0.97	4.33	
		down	0.19	0.49	0.58	0.97	0.96	3.19	7.52
	M3	up	0.16	0.47	0.55	0.97	0.97	3.12	
		down	0.70	0.75	0.98	0.97	0.97	4.37	7.49
	M4	up	0.69	0.70	0.97	0.98	0.97	4.31	
		down	0.19	0.50	0.59	0.97	0.97	3.22	7.53
	M5	up	0.18	0.56	0.49	0.97	0.97	3.17	
		down	0.70	0.73	0.98	0.97	0.97	4.35	7.52
	M6	up	0.69	0.71	0.97	0.97	0.97	4.31	
		down	0.17	0.48	0.58	0.97	0.97	3.17	7.48

Table S12. Total alpha and beta d-orbital occupancy for each metal center in the undercoordinated $\text{Co}_{6-x}\text{Fe}_x$ ($x = 0, 1, 3, 6$) NCs at the PBE0-D3/def2TZVP level of theory. M1-M6 represent each metal in the TM core. (Color scheme: green = Co atom, orange = Fe atom)

		L5	1	2	3	4	5	SUM	SUM_ALL
Co ₆	M1	up	0.84	0.99	0.99	0.99	0.99	4.80	
		down	0.20	0.11	0.56	0.99	0.99	2.85	7.65
	M2	up	0.65	0.63	0.98	0.99	0.99	4.24	
		down	0.65	0.61	0.98	0.98	0.99	4.21	8.45
	M3	up	0.62	0.61	0.99	0.98	0.98	4.18	
		down	0.63	0.71	0.98	0.98	0.98	4.28	8.46
	M4	up	0.62	0.61	0.98	0.99	0.98	4.18	
		down	0.63	0.72	0.98	0.98	0.98	4.29	8.47
	M5	up	0.85	0.94	0.98	0.98	0.99	4.74	
		down	0.19	0.57	0.58	0.99	0.99	3.32	8.06
	M6	up	0.63	0.65	0.99	0.98	0.98	4.23	
		down	0.64	0.68	0.96	0.98	0.98	4.24	8.47
Co ₅ Fe	M1	up	0.64	0.73	0.98	0.98	0.99	4.32	
		down	0.60	0.60	0.97	0.99	0.98	4.14	8.46
	M2	up	0.65	0.73	0.98	0.98	0.98	4.32	
		down	0.61	0.57	0.98	0.98	0.98	4.12	8.44
	M3	up	0.64	0.73	0.98	0.98	0.99	4.32	
		down	0.59	0.60	0.97	0.99	0.99	4.14	8.46
	M4	up	0.64	0.72	0.98	0.99	0.98	4.31	
		down	0.60	0.60	0.97	0.98	0.99	4.14	8.45
	M6	up	0.89	0.98	0.98	0.97	0.97	4.79	
		down	0.62	0.66	0.19	0.17	0.17	1.81	6.60
	M5	up	0.72	0.64	0.98	0.98	0.99	4.31	
		down	0.60	0.60	0.97	0.99	0.99	4.15	8.46
Co ₃ Fe ₃	M1	up	0.83	0.99	0.98	0.97	0.97	4.74	
		down	0.96	0.52	0.12	0.19	0.18	1.97	6.71
	M2	up	0.82	0.98	0.98	0.97	0.97	4.72	
		down	0.98	0.13	0.15	0.48	0.47	2.21	6.93
	M3	up	0.57	0.59	0.98	0.98	0.98	4.10	
		down	0.64	0.75	0.98	0.98	0.98	4.33	8.43
	M4	up	0.57	0.59	0.98	0.98	0.98	4.10	
		down	0.65	0.76	0.98	0.98	0.98	4.35	8.45
	M5	up	0.85	0.98	0.97	0.98	0.97	4.75	
		down	0.94	0.54	0.47	0.14	0.16	2.25	7.00
	M6	up	0.61	0.61	0.98	0.98	0.99	4.17	
		down	0.63	0.71	0.97	0.98	0.99	4.28	8.45
Fe ₆	M1	up	0.71	0.68	0.97	0.98	0.98	4.32	

	down	0.15	0.97	0.95	0.46	0.56	3.09	7.41
M2	up	0.85	0.99	0.97	0.98	0.98	4.77	
	down	0.98	0.49	0.14	0.12	0.12	1.85	6.62
M3	up	0.16	0.47	0.55	0.96	0.98	3.12	
	down	0.75	0.70	0.97	0.97	0.98	4.37	7.49
M4	up	0.96	0.94	0.13	0.50	0.38	2.91	
	down	0.71	0.83	0.97	0.97	0.97	4.45	7.36
M5	up	0.85	0.94	0.97	0.97	0.97	4.70	
	down	0.98	0.57	0.52	0.18	0.20	2.45	7.15
M6	up	0.72	0.68	0.97	0.98	0.98	4.33	
	down	0.16	0.97	0.95	0.55	0.47	3.10	7.43

Table S13. Total d-orbital occupancy between all six metals in each NC system, and the difference between the total orbital occupancy between the fully ligated and undercoordinated NCs. (L6 = fully ligated, L5 = undercoordinated, L6-L5 = occupancy difference)

NC	Sum of All Metals		
	L5	L6	L6-L5
Co ₆	49.56	50.76	1.20
Co ₅ Fe	48.87	49.41	0.54
Co ₃ Fe ₃	45.97	47.49	1.52
Fe ₆	43.46	44.68	1.22

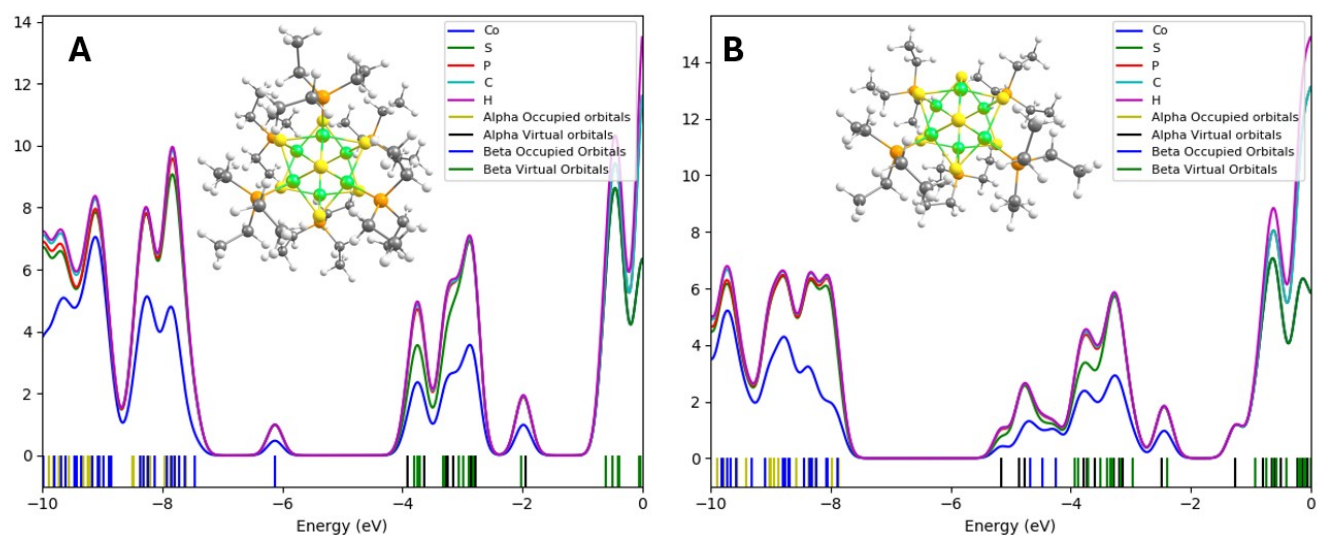


Figure S4. Partial density of States (PDOS) for (A) [Co₆S₈L₆]⁺ and (B) [Co₆S₈L₅]⁺ at the PBE0-D3/CEP-31G level of theory on the optimized geometry. FWHM = 0.30 eV

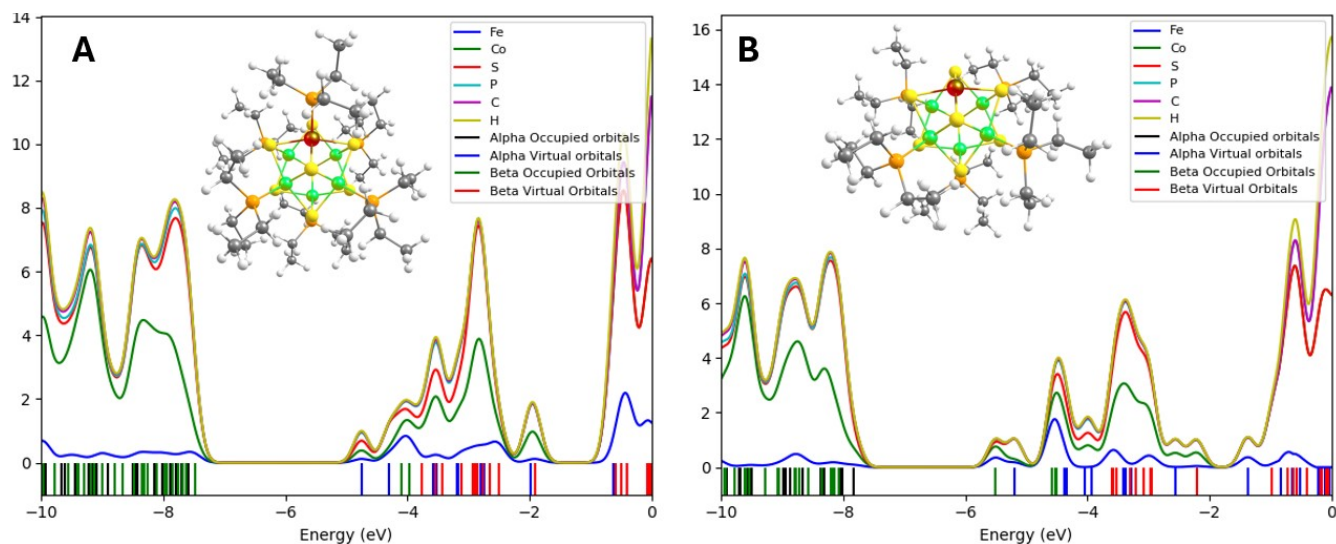


Figure S5. Partial density of States (PDOS) for (A) $[\text{Co}_5\text{FeS}_8\text{L}_6]^+$ and (B) $[\text{Co}_5\text{FeS}_8\text{L}_5]^+$ at the PBE0-D3/CEP-31G level of theory on the optimized geometry. FWHM = 0.30 eV

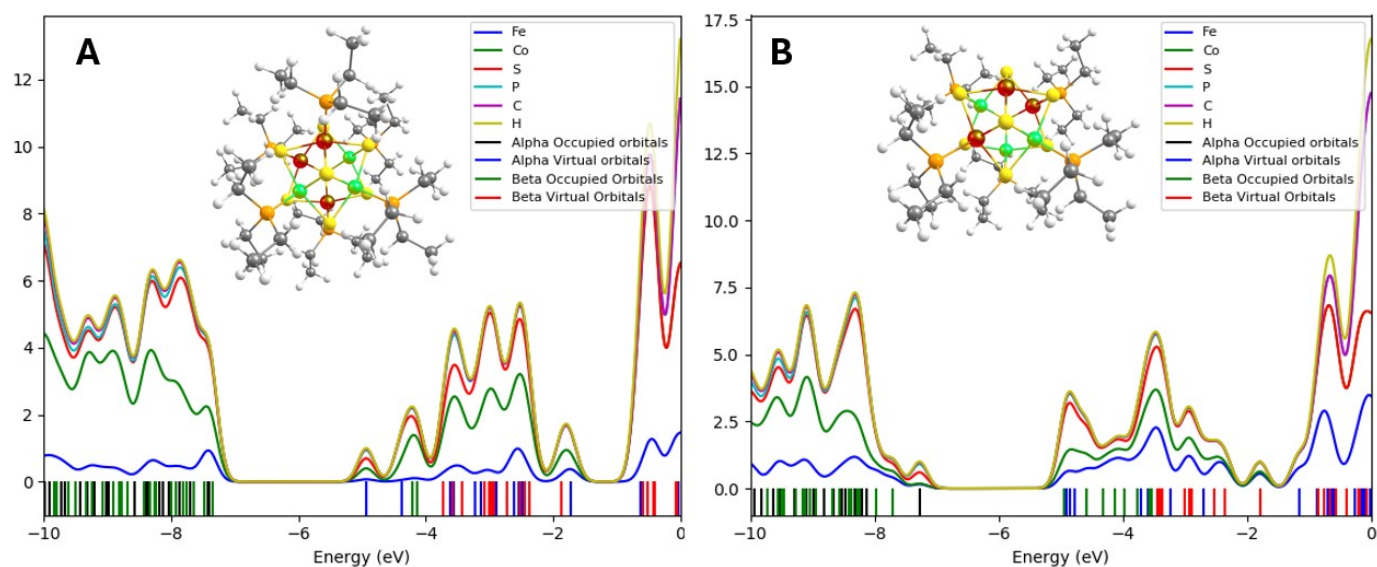


Figure S6. Partial density of States (PDOS) for (A) $[\text{Co}_3\text{Fe}_3\text{S}_8\text{L}_6]^+$ and (B) $[\text{Co}_3\text{Fe}_3\text{S}_8\text{L}_5]^+$ at the PBE0-D3/CEP-31G level of theory on the optimized geometry. FWHM = 0.30 eV

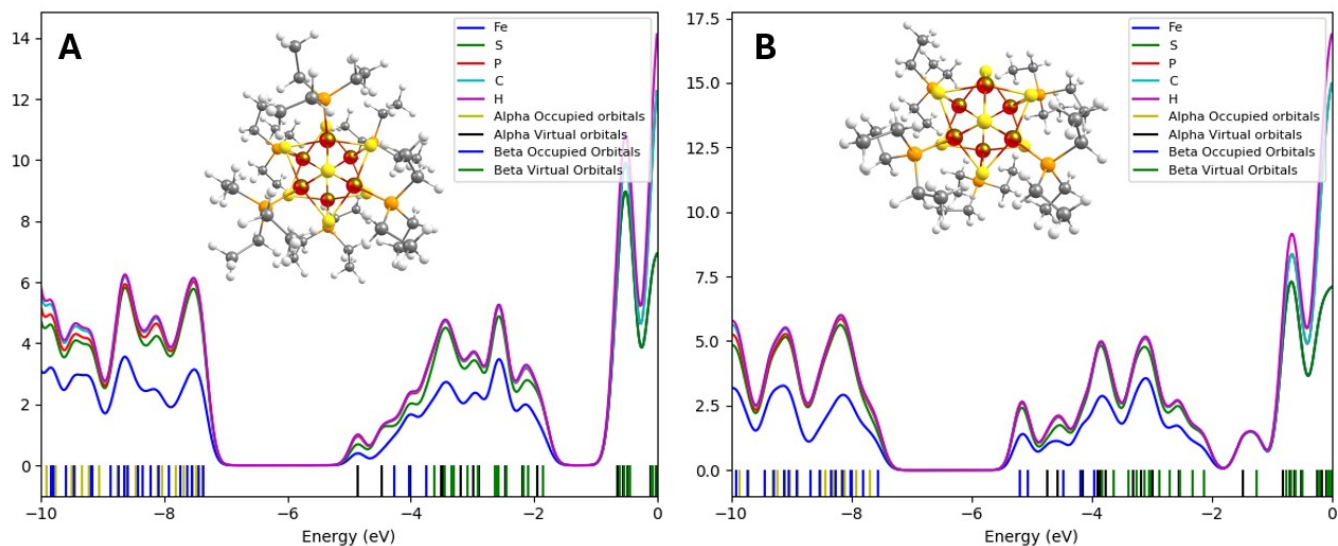


Figure S7. Partial density of States (PDOS) for (A) $[\text{Fe}_6\text{S}_8\text{L}_6]^+$ and (B) $[\text{Fe}_6\text{S}_8\text{L}_5]^+$ at the PBE0-D3/CEP-31G level of theory on the optimized geometry. FWHM = 0.30 eV

XYZ Coordinates of Considered Systems

Name: [number of][Metal]_[Total charge]_[Multiplicity]_[Site where ligand is removed]_[Which metal the ligand is removed from]

3Fe_1_1_M1_Fe

C	1.218746000	-0.371376000	-4.997955000
C	0.622052000	-1.766312000	-4.943565000
C	3.536066000	-0.930105000	-3.371430000
C	4.425216000	-0.976544000	-4.602880000
H	5.280220000	-1.631757000	-4.423504000
C	2.872422000	-3.915690000	0.446176000
C	3.970183000	-3.317045000	-0.414504000
H	4.302129000	-4.037620000	-1.164084000
C	4.344134000	-3.124120000	3.280856000
H	1.375447000	-2.523908000	-4.718621000
H	-0.153158000	-1.830276000	-4.179392000
H	4.093290000	-0.600662000	-2.490388000
H	3.154646000	-1.924838000	-3.129152000
H	3.894660000	-1.367290000	-5.472820000
H	4.819130000	0.007310000	-4.865023000
H	2.063317000	-4.310609000	-0.172894000
H	3.253368000	-4.746379000	1.048278000
H	3.617135000	-2.424985000	-0.932245000
H	4.840027000	-3.034609000	0.181433000
H	3.772004000	-3.728054000	3.987732000
H	4.814978000	-3.801005000	2.565662000

H	1.835462000	-4.624529000	3.018532000
H	0.379253000	-4.273144000	2.094851000
H	0.438733000	0.372077000	-5.182125000
H	0.170189000	-2.022279000	-5.903728000
H	1.940982000	-0.286192000	-5.815482000
P	2.071594000	0.159649000	-3.471835000
P	2.100331000	-2.723765000	1.591761000
C	3.479733000	-2.079474000	2.595286000
H	3.031617000	-1.397503000	3.321772000
H	4.069231000	-1.453264000	1.920468000
H	5.143702000	-2.637108000	3.842692000
C	1.162130000	-3.819777000	2.708004000
C	0.559138000	-3.120774000	3.911008000
Fe	-1.090918000	-0.961469000	-1.110210000
Fe	0.872427000	0.207169000	-1.626314000
H	1.906501000	2.467663000	-4.009416000
C	2.754636000	1.779595000	-3.976473000
H	3.130629000	1.681602000	-4.999544000
Co	0.908458000	-1.180171000	0.637097000
H	-0.097367000	-2.310852000	3.593237000
H	-0.026150000	-3.823224000	4.507430000
H	1.326832000	-2.692632000	4.558625000
S	-1.038580000	0.513103000	-2.705435000
S	-2.764951000	0.192151000	-0.186002000
S	0.813673000	-1.978328000	-1.428634000
S	-1.118129000	-2.102178000	0.807364000
S	0.765683000	2.438538000	-1.250574000
S	2.509034000	0.192629000	-0.095627000
C	3.833085000	2.307347000	-3.048214000
H	4.117320000	3.322981000	-3.330520000
H	4.732866000	1.690249000	-3.083786000
H	3.480135000	2.328245000	-2.016943000
S	0.797146000	0.121589000	2.414930000
Co	-1.284687000	1.689811000	-0.857252000
Fe	-1.094528000	-0.005146000	1.355853000
Co	0.966863000	1.540689000	0.736822000
P	-2.508695000	3.247763000	-1.655020000
S	-1.089129000	2.249607000	1.253781000
P	-2.352171000	-0.141001000	3.166521000
P	2.120532000	3.117311000	1.616033000
H	-3.403313000	1.975909000	-3.444079000
C	-1.635523000	4.448928000	-2.718437000
H	-2.339052000	5.257029000	-2.941567000
C	-3.306954000	4.332329000	-0.422749000
H	-2.502650000	4.716627000	0.209576000
H	-3.732237000	5.187451000	-0.956878000

H	-4.426283000	1.907720000	-2.036931000
C	-3.872422000	2.598481000	-2.678215000
H	-0.841460000	4.875080000	-2.099640000
H	-3.303857000	2.026267000	3.012006000
H	-4.283421000	0.831269000	2.203925000
C	-3.748608000	1.036163000	3.134594000
C	-3.152978000	-1.759248000	3.454944000
H	-3.577423000	-1.741468000	4.463448000
H	-2.356693000	-2.506985000	3.456781000
C	-1.529115000	0.194634000	4.764613000
H	-0.686038000	-0.496730000	4.833115000
H	-2.231775000	-0.075131000	5.558615000
H	3.028442000	3.950085000	-0.401216000
C	1.191422000	4.633561000	2.032046000
H	0.411641000	4.323659000	2.732649000
H	1.873963000	5.292467000	2.577720000
C	3.490496000	3.674834000	0.549593000
H	4.088574000	2.782974000	0.344029000
H	2.098867000	2.352403000	3.863277000
C	2.904019000	2.702651000	3.212103000
H	3.290225000	3.628656000	3.648524000
C	-4.785076000	3.644142000	-3.297290000
H	-1.835801000	3.456683000	-4.642821000
C	-1.057998000	3.865885000	-3.995347000
H	-0.528774000	4.637325000	-4.557991000
H	-0.355155000	3.063199000	-3.770346000
C	-4.360238000	3.633499000	0.417305000
H	-4.721453000	4.295864000	1.206358000
H	-3.951467000	2.737095000	0.883618000
H	-5.221186000	3.334206000	-0.183264000
H	-5.566889000	3.158800000	-3.884726000
H	-5.279312000	4.257176000	-2.541075000
H	-4.242082000	4.312400000	-3.968506000
C	-4.684125000	0.995985000	4.330669000
H	-5.483474000	1.729116000	4.203504000
H	-4.169161000	1.235553000	5.262969000
H	-5.155838000	0.019071000	4.450387000
H	-5.059388000	-1.427745000	2.462805000
H	-3.811952000	-2.097043000	1.413647000
C	-4.214251000	-2.117348000	2.427669000
H	-4.597993000	-3.121371000	2.617041000
C	-1.054843000	1.628535000	4.931443000
H	-1.890290000	2.330615000	4.950187000
H	-0.507067000	1.739689000	5.869199000
H	-0.395165000	1.923346000	4.113728000
C	4.345373000	4.803862000	1.099590000

C	0.581081000	5.350186000	0.841305000
H	0.004342000	6.215409000	1.174010000
H	1.345002000	5.705933000	0.147073000
H	-0.083978000	4.683003000	0.291647000
H	4.812150000	4.539783000	2.050468000
H	3.764099000	5.715022000	1.252646000
H	5.146646000	5.043216000	0.397650000
C	3.993901000	1.652163000	3.097434000
H	4.344210000	1.352664000	4.086969000
H	4.855218000	2.024014000	2.539409000
H	3.621449000	0.766121000	2.583231000

3Fe_1_1_M5_Fe

C	-1.499828000	-4.342992000	-2.340350000
C	-0.942975000	-5.121543000	-1.162524000
H	-0.457851000	-6.035863000	-1.509871000
C	1.163945000	-0.291037000	-5.014922000
C	0.637024000	-1.713730000	-5.032722000
C	3.487110000	-0.927412000	-3.424700000
C	4.357595000	-0.935200000	-4.670128000
H	5.210492000	-1.601633000	-4.525782000
C	3.047202000	-3.947710000	0.287527000
C	4.112345000	-3.279572000	-0.562445000
H	4.479106000	-3.966235000	-1.327711000
C	4.491290000	-3.091475000	3.124514000
H	-2.224265000	-4.947049000	-2.895210000
H	-0.701183000	-4.081401000	-3.039387000
H	-0.207682000	-4.528535000	-0.617528000
H	-1.726930000	-5.406960000	-0.458593000
H	-4.129738000	-5.290573000	-1.605952000
H	-2.268100000	-1.966770000	-4.149807000
H	-3.469734000	-3.237098000	-3.969606000
H	1.443715000	-2.447248000	-4.974068000
H	-0.029932000	-1.886319000	-4.187046000
H	4.055853000	-0.622296000	-2.542374000
H	3.108167000	-1.928161000	-3.206037000
H	3.811639000	-1.291796000	-5.545446000
H	4.754352000	0.054844000	-4.902578000
H	2.261057000	-4.374246000	-0.340470000
H	3.469855000	-4.767942000	0.875463000
H	3.715388000	-2.394403000	-1.058941000
H	4.967869000	-2.966496000	0.038789000
H	3.957683000	-3.735923000	3.825334000
H	5.003834000	-3.730569000	2.403029000
H	2.118272000	-4.737485000	2.853769000
H	0.612655000	-4.486974000	1.980623000

P	-2.337008000	-2.774256000	-1.910851000
H	0.342501000	0.421864000	-5.124489000
H	0.081289000	-1.904395000	-5.952958000
H	1.853394000	-0.117456000	-5.846171000
P	2.028022000	0.169283000	-3.472360000
P	2.215107000	-2.813938000	1.451368000
C	3.561569000	-2.096637000	2.450699000
H	3.068959000	-1.458626000	3.187810000
H	4.107764000	-1.423935000	1.784796000
H	5.258302000	-2.559735000	3.691255000
H	-5.487728000	-4.545302000	-0.773911000
C	-3.753358000	-3.275560000	-0.871332000
C	-4.658364000	-4.347496000	-1.455773000
C	-3.086499000	-2.317645000	-3.516794000
C	-4.175718000	-1.263474000	-3.431700000
C	1.376020000	-3.981663000	2.578103000
C	0.760084000	-3.354799000	3.815923000
H	-3.330793000	-3.593269000	0.084674000
H	-4.306636000	-2.357650000	-0.657847000
Fe	-1.079026000	-1.227840000	-0.946925000
Fe	0.835908000	0.140124000	-1.623279000
H	1.875643000	2.502697000	-3.905209000
C	2.717998000	1.807348000	-3.901852000
H	3.096324000	1.750882000	-4.927240000
Co	0.906414000	-1.336286000	0.554831000
H	-5.088133000	-4.047042000	-2.413092000
H	-4.532941000	-1.008668000	-4.431499000
H	-5.032854000	-1.611350000	-2.852540000
H	-3.804003000	-0.352499000	-2.963448000
H	0.003831000	-2.614508000	3.553835000
H	0.283734000	-4.123853000	4.426825000
H	1.510376000	-2.858426000	4.434435000
S	-1.069048000	0.306793000	-2.628908000
S	-2.832044000	0.088913000	-0.293340000
S	0.834897000	-2.071499000	-1.533013000
S	-1.048580000	-2.283280000	0.968700000
S	0.687872000	2.372900000	-1.200733000
S	2.471419000	0.146830000	-0.114246000
C	3.797027000	2.287313000	-2.948411000
H	4.084335000	3.313846000	-3.184003000
H	4.695351000	1.670211000	-3.011073000
H	3.442581000	2.261144000	-1.918063000
S	0.591970000	-0.074433000	2.368913000
Co	-1.353514000	1.623285000	-0.892964000
Fe	-1.241327000	-0.101262000	1.133075000
Co	0.890840000	1.427084000	0.781633000

P	-2.515529000	3.197180000	-1.731026000
S	-1.151337000	2.136906000	1.244825000
P	2.019996000	2.998751000	1.698653000
H	-3.424533000	1.944565000	-3.525163000
C	-1.599033000	4.351948000	-2.805796000
H	-2.271033000	5.175009000	-3.067360000
C	-3.294662000	4.298717000	-0.504178000
H	-2.479362000	4.701436000	0.101967000
H	-3.736367000	5.139023000	-1.049147000
H	-4.462609000	1.902560000	-2.123979000
C	-3.886860000	2.577008000	-2.762902000
H	-0.800486000	4.768336000	-2.186852000
H	3.028787000	3.811002000	-0.278509000
C	1.086548000	4.524301000	2.069023000
H	0.279209000	4.222705000	2.741031000
H	1.755221000	5.176584000	2.639421000
C	3.442869000	3.542024000	0.696254000
H	4.047630000	2.646784000	0.528814000
H	1.869687000	2.221357000	3.931190000
C	2.712312000	2.581073000	3.335040000
H	3.066741000	3.506210000	3.799536000
C	-4.775464000	3.637997000	-3.390086000
H	-1.804617000	3.320563000	-4.709251000
C	-1.022031000	3.701704000	-4.050270000
H	-0.431831000	4.422589000	-4.619149000
H	-0.372543000	2.867219000	-3.781356000
C	-4.326136000	3.614581000	0.376469000
H	-4.722187000	4.319358000	1.109583000
H	-3.885201000	2.777889000	0.920511000
H	-5.168736000	3.236376000	-0.205842000
H	-5.558964000	3.167144000	-3.987170000
H	-5.267836000	4.254650000	-2.635928000
H	-4.215429000	4.300445000	-4.053026000
C	4.272451000	4.674630000	1.277381000
C	0.529577000	5.247414000	0.856991000
H	-0.045399000	6.121533000	1.169262000
H	1.322716000	5.591171000	0.189744000
H	-0.124737000	4.587675000	0.286047000
H	4.684005000	4.420931000	2.256276000
H	3.688283000	5.590129000	1.386965000
H	5.113038000	4.901650000	0.618539000
C	3.811822000	1.537113000	3.277488000
H	4.098332000	1.224103000	4.283186000
H	4.706187000	1.918617000	2.781259000
H	3.474422000	0.658559000	2.728598000

3Fe_1_1_M6_Co

C	-1.365745000	-4.219628000	-2.473108000
C	-0.907157000	-5.015427000	-1.262507000
H	-0.293859000	-5.862657000	-1.575512000
C	1.130080000	-0.321768000	-4.993383000
C	0.608721000	-1.746218000	-4.993964000
C	3.438106000	-0.942863000	-3.375670000
C	4.324065000	-0.956909000	-4.609906000
H	5.171517000	-1.627807000	-4.454592000
C	2.975342000	-4.048466000	0.340623000
C	4.046749000	-3.392374000	-0.511970000
H	4.391203000	-4.077594000	-1.288674000
C	4.449991000	-3.279731000	3.195792000
H	-2.017494000	-4.824313000	-3.110748000
H	-0.508425000	-3.920182000	-3.080255000
H	-0.315972000	-4.394994000	-0.586571000
H	-1.752428000	-5.409106000	-0.695019000
H	-3.958344000	-5.271218000	-1.821745000
H	-2.257471000	-1.827873000	-4.278017000
H	-3.407190000	-3.149281000	-4.124350000
H	1.418832000	-2.476273000	-4.938775000
H	-0.043493000	-1.910945000	-4.136188000
H	3.997275000	-0.631559000	-2.489357000
H	3.055708000	-1.941815000	-3.153888000
H	3.787423000	-1.310546000	-5.492279000
H	4.729401000	0.030861000	-4.836786000
H	2.169270000	-4.440821000	-0.284341000
H	3.382785000	-4.890210000	0.908703000
H	3.661845000	-2.494262000	-0.996198000
H	4.914781000	-3.105092000	0.084028000
H	3.892941000	-3.910919000	3.890991000
H	4.935217000	-3.931210000	2.466394000
H	1.953655000	-4.851428000	2.899794000
H	0.477878000	-4.471359000	2.016514000
P	-2.271644000	-2.686319000	-2.056484000
H	0.306950000	0.387037000	-5.114213000
H	0.040680000	-1.948624000	-5.904134000
H	1.824872000	-0.154922000	-5.821472000
P	1.977724000	0.151911000	-3.447217000
P	2.189781000	-2.906400000	1.526036000
C	3.559245000	-2.242357000	2.532478000
H	3.098346000	-1.581294000	3.270352000
H	4.128354000	-1.586898000	1.868138000
H	5.238713000	-2.785453000	3.766232000
H	-5.339025000	-4.621955000	-0.946073000
C	-3.667707000	-3.265046000	-1.026718000

C	-4.529732000	-4.360890000	-1.631173000
C	-3.051256000	-2.231979000	-3.646398000
C	-4.174080000	-1.220309000	-3.494993000
C	1.274423000	-4.037798000	2.626891000
C	0.696424000	-3.376891000	3.864700000
H	-3.223574000	-3.582913000	-0.080433000
H	-4.254885000	-2.373306000	-0.793976000
Fe	-1.156091000	-1.116407000	-0.997259000
Fe	0.801812000	0.184671000	-1.589957000
H	1.821215000	2.477720000	-3.927011000
C	2.668788000	1.789631000	-3.883400000
H	3.069825000	1.711585000	-4.899113000
Co	1.025234000	-1.340891000	0.670984000
H	-4.986670000	-4.050670000	-2.572672000
H	-4.506685000	-0.867914000	-4.473276000
H	-5.038869000	-1.647947000	-2.984851000
H	-3.840536000	-0.357696000	-2.918028000
H	0.020026000	-2.567001000	3.589040000
H	0.136067000	-4.103538000	4.456086000
H	1.476673000	-2.959020000	4.503678000
S	-1.136666000	0.380993000	-2.625096000
S	-2.830839000	0.083182000	-0.078321000
S	0.822624000	-2.011416000	-1.408042000
S	-1.057281000	-2.069330000	1.015880000
S	0.662377000	2.371111000	-1.146188000
S	2.438993000	0.186815000	-0.062704000
C	3.726340000	2.305713000	-2.923719000
H	4.055339000	3.301359000	-3.226724000
H	4.605454000	1.658802000	-2.906126000
H	3.339161000	2.374663000	-1.906355000
S	0.752416000	-0.076656000	2.457378000
Co	-1.384332000	1.631108000	-0.837667000
Fe	-1.190416000	0.141482000	1.458890000
Co	0.738791000	1.309779000	0.766335000
P	-2.617440000	3.125399000	-1.731745000
S	-1.142425000	2.319822000	1.251270000
P	-2.380343000	0.171202000	3.293038000
H	-3.516274000	1.839288000	-3.502197000
C	-1.713289000	4.274470000	-2.824465000
H	-2.406810000	5.074532000	-3.101866000
C	-3.403723000	4.258171000	-0.538189000
H	-2.593335000	4.656127000	0.077477000
H	-3.823081000	5.096496000	-1.102774000
H	-4.545527000	1.796362000	-2.093197000
C	-3.984653000	2.471803000	-2.744602000
H	-0.935034000	4.724298000	-2.202661000

H	-3.445429000	2.266960000	2.979166000
H	-4.393415000	0.955578000	2.323653000
C	-3.833511000	1.271894000	3.207552000
C	-3.072818000	-1.459082000	3.746079000
H	-3.470349000	-1.374870000	4.762519000
H	-2.226203000	-2.148304000	3.787711000
C	-1.510818000	0.663792000	4.820133000
H	-0.711705000	-0.068310000	4.962874000
H	-2.216698000	0.532742000	5.646153000
C	-4.890485000	3.512175000	-3.382002000
H	-1.870095000	3.201826000	-4.709388000
C	-1.106758000	3.632777000	-4.058510000
H	-0.555223000	4.374921000	-4.638753000
H	-0.417728000	2.834246000	-3.781367000
C	-4.461520000	3.592627000	0.323042000
H	-4.806654000	4.274961000	1.101969000
H	-4.064504000	2.697724000	0.802829000
H	-5.331566000	3.295537000	-0.265622000
H	-5.671492000	3.021752000	-3.966468000
H	-5.385690000	4.137192000	-2.636633000
H	-4.341561000	4.168866000	-4.059594000
C	-4.718832000	1.302726000	4.442344000
H	-5.564357000	1.973873000	4.278065000
H	-4.180987000	1.667251000	5.319210000
H	-5.126776000	0.319039000	4.682301000
H	-5.022176000	-1.341138000	2.793293000
H	-3.750597000	-2.008324000	1.767406000
C	-4.132388000	-1.973519000	2.788595000
H	-4.441251000	-2.981662000	3.071350000
C	-0.947406000	2.073669000	4.804158000
H	-1.727045000	2.820710000	4.642438000
H	-0.467358000	2.297039000	5.758677000
H	-0.204484000	2.191551000	4.015213000

3Fe_1_3_M1_Fe

C	1.391458000	-0.114556000	-5.185661000
C	0.839583000	-1.528869000	-5.239735000
C	3.666274000	-0.905752000	-3.553243000
C	4.598743000	-0.934021000	-4.752267000
H	5.392646000	-1.667796000	-4.598349000
C	2.831286000	-3.960983000	0.347655000
C	3.880651000	-3.342303000	-0.558576000
H	4.197713000	-4.058225000	-1.319063000
C	4.395324000	-3.193719000	3.155152000
H	1.636515000	-2.274582000	-5.209627000
H	0.166289000	-1.722291000	-4.403122000

H	4.205775000	-0.665424000	-2.632575000
H	3.208567000	-1.883878000	-3.381669000
H	4.072958000	-1.209457000	-5.668503000
H	5.076730000	0.033488000	-4.918772000
H	1.995397000	-4.352909000	-0.237234000
H	3.245829000	-4.796311000	0.920197000
H	3.484491000	-2.460583000	-1.063397000
H	4.767752000	-3.038861000	0.000782000
H	3.841301000	-3.803166000	3.871513000
H	4.847264000	-3.865103000	2.422582000
H	1.890817000	-4.682800000	2.966918000
H	0.397860000	-4.329365000	2.104163000
H	0.579315000	0.614836000	-5.255447000
H	0.281346000	-1.680335000	-6.165119000
H	2.070129000	0.077393000	-6.022735000
P	2.279957000	0.275455000	-3.639157000
P	2.102837000	-2.781697000	1.534085000
C	3.513079000	-2.144488000	2.499693000
H	3.082264000	-1.468723000	3.242369000
H	4.085821000	-1.513363000	1.815516000
H	5.209372000	-2.711511000	3.700221000
C	1.205834000	-3.877343000	2.684451000
C	0.654503000	-3.179318000	3.914200000
Fe	-1.359439000	-1.126868000	-0.967423000
Fe	0.934735000	0.248159000	-1.722914000
H	2.205920000	2.611847000	-4.025636000
C	3.035782000	1.900638000	-3.987390000
H	3.483941000	1.870985000	-4.985299000
Co	0.919794000	-1.227512000	0.618634000
H	-0.019676000	-2.370385000	3.629453000
H	0.099369000	-3.886370000	4.533673000
H	1.448918000	-2.751192000	4.528864000
S	-1.133781000	0.317243000	-2.696762000
S	-2.939077000	0.243211000	-0.121382000
S	0.666061000	-2.013455000	-1.482080000
S	-1.119391000	-2.100298000	1.050353000
S	0.693816000	2.462449000	-1.257882000
S	2.497621000	0.182064000	-0.072704000
C	4.049192000	2.326634000	-2.939314000
H	4.398424000	3.342327000	-3.134711000
H	4.922846000	1.671943000	-2.933095000
H	3.607547000	2.303643000	-1.942360000
S	0.702136000	0.065781000	2.389674000
Co	-1.318195000	1.624012000	-0.865412000
Fe	-1.348893000	0.112394000	1.493669000
Co	0.916676000	1.523236000	0.737792000

P	-2.578125000	3.129584000	-1.735888000
S	-1.109585000	2.311700000	1.216655000
P	-2.493414000	-0.007358000	3.350965000
P	2.077399000	3.073824000	1.677886000
H	-3.521204000	1.767635000	-3.432903000
C	-1.719100000	4.263076000	-2.881481000
H	-2.437623000	5.037583000	-3.167711000
C	-3.334434000	4.288937000	-0.547148000
H	-2.506382000	4.713759000	0.026079000
H	-3.780898000	5.104973000	-1.123689000
H	-4.514327000	1.788166000	-2.004232000
C	-3.968055000	2.436872000	-2.693386000
H	-0.938356000	4.752240000	-2.292720000
H	-3.441391000	2.158127000	3.176304000
H	-4.462933000	0.947217000	2.447781000
C	-3.886222000	1.174630000	3.348324000
C	-3.260449000	-1.625843000	3.706660000
H	-3.683416000	-1.581906000	4.715198000
H	-2.444351000	-2.352503000	3.732499000
C	-1.575692000	0.363956000	4.886788000
H	-0.757289000	-0.358683000	4.937093000
H	-2.236806000	0.163213000	5.735142000
H	3.028625000	3.923959000	-0.313302000
C	1.168189000	4.602522000	2.096208000
H	0.358490000	4.298646000	2.764371000
H	1.847738000	5.233148000	2.677914000
C	3.471690000	3.625456000	0.639898000
H	4.059084000	2.728150000	0.428680000
H	2.006202000	2.269891000	3.909458000
C	2.827000000	2.624025000	3.280800000
H	3.215726000	3.537949000	3.739988000
C	-4.884756000	3.455767000	-3.349476000
H	-1.887660000	3.120605000	-4.723782000
C	-1.122629000	3.598957000	-4.109154000
H	-0.614701000	4.340227000	-4.729325000
H	-0.397142000	2.835998000	-3.823916000
C	-4.353692000	3.651774000	0.379414000
H	-4.698898000	4.375979000	1.119668000
H	-3.919337000	2.803528000	0.909189000
H	-5.228000000	3.294143000	-0.167488000
H	-5.682729000	2.945085000	-3.891827000
H	-5.357806000	4.113155000	-2.617337000
H	-4.351545000	4.081117000	-4.068067000
C	-4.767826000	1.172257000	4.585593000
H	-5.567083000	1.908762000	4.480383000
H	-4.206557000	1.426872000	5.486752000

H	-5.239470000	0.201217000	4.747691000
H	-5.165609000	-1.362797000	2.693125000
H	-3.896941000	-2.056833000	1.680407000
C	-4.310576000	-2.041628000	2.690170000
H	-4.682576000	-3.042188000	2.917261000
C	-1.035056000	1.782238000	4.940343000
H	-1.839557000	2.519815000	4.964422000
H	-0.425226000	1.926622000	5.834228000
H	-0.418067000	1.992044000	4.064602000
C	4.335767000	4.731679000	1.222030000
C	0.616847000	5.359953000	0.901757000
H	0.039776000	6.224543000	1.235546000
H	1.414142000	5.724058000	0.250716000
H	-0.036823000	4.720835000	0.306057000
H	4.782957000	4.442272000	2.174915000
H	3.767013000	5.649136000	1.383811000
H	5.151965000	4.970776000	0.537385000
C	3.905400000	1.562098000	3.168020000
H	4.235556000	1.244029000	4.158718000
H	4.780415000	1.929502000	2.628662000
H	3.527313000	0.688284000	2.637340000

3Fe_1_3_M3_Co

C	-1.568821000	-4.290738000	-2.403163000
C	-0.995937000	-5.070589000	-1.233182000
H	-0.442147000	-5.936799000	-1.599424000
C	1.323566000	-0.264623000	-5.069809000
C	0.726373000	-1.660375000	-5.064383000
C	3.593441000	-0.935837000	-3.384421000
C	4.529421000	-0.990520000	-4.579837000
H	5.339984000	-1.697024000	-4.390281000
H	-2.240088000	-4.916405000	-3.000602000
H	-0.770609000	-3.949223000	-3.067562000
H	-0.312770000	-4.457161000	-0.644889000
H	-1.780187000	-5.436658000	-0.567750000
H	-4.159344000	-5.385391000	-1.639666000
H	-2.474799000	-1.950676000	-4.159133000
H	-3.687381000	-3.217996000	-3.992216000
H	1.493850000	-2.429682000	-4.957483000
H	0.021827000	-1.773535000	-4.239161000
H	4.122520000	-0.642063000	-2.473702000
H	3.166474000	-1.918576000	-3.168612000
H	4.015916000	-1.320555000	-5.485093000
H	4.985650000	-0.020749000	-4.788310000
P	-2.513106000	-2.797586000	-1.947512000
H	0.540531000	0.484472000	-5.216844000

H	0.195055000	-1.849870000	-5.999354000
H	2.037357000	-0.148082000	-5.891029000
P	2.175912000	0.206595000	-3.523009000
H	-5.525849000	-4.737684000	-0.740432000
C	-3.868613000	-3.369105000	-0.874632000
C	-4.735265000	-4.478496000	-1.447327000
C	-3.289102000	-2.311590000	-3.525557000
C	-4.362053000	-1.248171000	-3.378896000
H	-3.393907000	-3.673886000	0.061334000
H	-4.458190000	-2.479893000	-0.636812000
Fe	-1.253474000	-1.155292000	-0.964025000
Fe	0.935499000	0.270524000	-1.727829000
H	2.068849000	2.512063000	-4.071882000
C	2.908906000	1.818733000	-3.976477000
H	3.359901000	1.719463000	-4.968812000
Co	0.987851000	-1.209765000	0.592507000
H	-5.215988000	-4.180019000	-2.380912000
H	-4.721930000	-0.934650000	-4.360556000
H	-5.220169000	-1.614540000	-2.812343000
H	-3.968836000	-0.372179000	-2.863214000
S	-1.089774000	0.309155000	-2.680896000
S	-2.926145000	0.123306000	-0.178770000
S	0.817164000	-1.965100000	-1.522369000
S	-1.012190000	-2.182423000	1.026650000
S	0.652939000	2.438051000	-1.232704000
S	2.504343000	0.278242000	-0.096655000
C	3.916815000	2.339274000	-2.968131000
H	4.259652000	3.336844000	-3.249239000
H	4.794059000	1.692547000	-2.904515000
H	3.472760000	2.398229000	-1.974042000
S	0.680605000	0.028681000	2.412137000
Co	-1.350540000	1.555499000	-0.858681000
Fe	-1.334096000	0.044939000	1.408440000
Co	0.858741000	1.543708000	0.760435000
P	-2.545998000	3.129460000	-1.725235000
S	-1.175700000	2.263964000	1.228158000
P	-2.481848000	0.057507000	3.287120000
P	2.041971000	3.064615000	1.709044000
H	-3.478143000	1.839595000	-3.478275000
C	-1.648232000	4.267400000	-2.836215000
H	-2.339091000	5.069638000	-3.113090000
C	-3.317098000	4.276838000	-0.533056000
H	-2.503572000	4.655452000	0.090690000
H	-3.717684000	5.126879000	-1.093497000
H	-4.507458000	1.843795000	-2.069836000
C	-3.930987000	2.496078000	-2.731011000

H	-0.856193000	4.716588000	-2.231648000
H	-3.527963000	2.164019000	2.999252000
H	-4.508976000	0.868889000	2.364098000
C	-3.925823000	1.174469000	3.237178000
C	-3.171197000	-1.573897000	3.738719000
H	-3.574065000	-1.506736000	4.753906000
H	-2.318578000	-2.257147000	3.773723000
C	-1.582032000	0.530262000	4.804142000
H	-0.758412000	-0.181618000	4.899545000
H	-2.253860000	0.361801000	5.651186000
H	2.960037000	3.974040000	-0.271382000
C	1.128960000	4.578199000	2.169937000
H	0.317930000	4.253205000	2.826417000
H	1.801535000	5.198383000	2.770538000
C	3.419169000	3.645862000	0.664497000
H	4.001835000	2.755259000	0.415784000
H	1.994609000	2.235709000	3.932515000
C	2.811952000	2.568325000	3.287491000
H	3.236000000	3.467700000	3.744963000
C	-4.814881000	3.545400000	-3.383584000
H	-1.837638000	3.174677000	-4.706536000
C	-1.062307000	3.607175000	-4.071010000
H	-0.513824000	4.338667000	-4.667680000
H	-0.372755000	2.808539000	-3.793107000
C	-4.389954000	3.629800000	0.324431000
H	-4.728382000	4.319567000	1.099932000
H	-4.007668000	2.731895000	0.811081000
H	-5.261664000	3.345066000	-0.267800000
H	-5.613831000	3.064349000	-3.951613000
H	-5.287187000	4.198536000	-2.647283000
H	-4.255502000	4.174139000	-4.078907000
C	-4.784227000	1.213367000	4.490264000
H	-5.624762000	1.896108000	4.349541000
H	-4.221458000	1.564900000	5.356994000
H	-5.198632000	0.233380000	4.734804000
H	-5.124394000	-1.461744000	2.793830000
H	-3.842989000	-2.067280000	1.744208000
C	-4.223028000	-2.077382000	2.766333000
H	-4.513852000	-3.100340000	3.012610000
C	-1.056336000	1.954372000	4.801890000
H	-1.864513000	2.686938000	4.751336000
H	-0.487500000	2.149958000	5.713045000
H	-0.401717000	2.121598000	3.945355000
C	4.295290000	4.731801000	1.266264000
C	0.578942000	5.359662000	0.989839000
H	-0.016396000	6.205649000	1.338818000

H	1.378294000	5.754080000	0.359312000
H	-0.054645000	4.726629000	0.366614000
H	4.769022000	4.405143000	2.193797000
H	3.729419000	5.640550000	1.479860000
H	5.092118000	5.000008000	0.569702000
C	3.860162000	1.477324000	3.151599000
H	4.234173000	1.188865000	4.135511000
H	4.713534000	1.810081000	2.557585000
H	3.444098000	0.588656000	2.674931000

3Fe_1_3_M5_Fe

C	-1.535743000	-4.372993000	-2.290084000
C	-0.960440000	-5.084104000	-1.078459000
H	-0.380085000	-5.955512000	-1.388106000
C	1.379240000	-0.111273000	-5.194759000
C	0.804455000	-1.517491000	-5.195267000
C	3.673758000	-0.868148000	-3.572922000
C	4.584587000	-0.920889000	-4.787380000
H	5.385625000	-1.646048000	-4.629225000
C	2.889504000	-3.970955000	0.333740000
C	3.959766000	-3.324960000	-0.528121000
H	4.313306000	-4.026440000	-1.286158000
C	4.357075000	-3.226806000	3.193966000
H	-2.212948000	-5.030800000	-2.843562000
H	-0.737817000	-4.080574000	-2.978074000
H	-0.306511000	-4.417455000	-0.514467000
H	-1.745257000	-5.429842000	-0.402835000
H	-4.142116000	-5.409789000	-1.527599000
H	-2.370412000	-2.096543000	-4.157282000
H	-3.583072000	-3.357825000	-3.964558000
H	1.589041000	-2.275973000	-5.159109000
H	0.153834000	-1.667434000	-4.331925000
H	4.227354000	-0.604762000	-2.667077000
H	3.221133000	-1.842505000	-3.369428000
H	4.043848000	-1.222503000	-5.686545000
H	5.053483000	0.044759000	-4.986901000
H	2.083215000	-4.369023000	-0.287053000
H	3.297124000	-4.808350000	0.908217000
H	3.568980000	-2.442312000	-1.035695000
H	4.822688000	-3.016564000	0.065121000
H	3.793398000	-3.857886000	3.883489000
H	4.842549000	-3.876747000	2.463471000
H	1.883649000	-4.761458000	2.893497000
H	0.400840000	-4.402091000	2.017778000
P	-2.451950000	-2.838907000	-1.905473000
H	0.574452000	0.624977000	-5.276212000

H	0.219146000	-1.688832000	-6.100661000
H	2.048002000	0.045128000	-6.046741000
P	2.281427000	0.308476000	-3.663586000
P	2.102956000	-2.824373000	1.516722000
C	3.476043000	-2.181127000	2.531522000
H	3.014207000	-1.526210000	3.274199000
H	4.056486000	-1.529126000	1.873996000
H	5.145798000	-2.739688000	3.770968000
H	-5.533419000	-4.699683000	-0.718449000
C	-3.850436000	-3.360950000	-0.855614000
C	-4.711166000	-4.486296000	-1.404176000
C	-3.197099000	-2.432820000	-3.525429000
C	-4.277798000	-1.368381000	-3.455495000
C	1.194034000	-3.955636000	2.622791000
C	0.615380000	-3.297598000	3.862605000
H	-3.416831000	-3.622728000	0.112771000
H	-4.437652000	-2.456055000	-0.676992000
Fe	-1.275361000	-1.205025000	-1.043523000
Fe	0.976683000	0.243173000	-1.727904000
H	2.190401000	2.635807000	-4.091662000
C	3.025147000	1.930483000	-4.044708000
H	3.473365000	1.893160000	-5.042316000
Co	0.932751000	-1.250811000	0.602257000
H	-5.149727000	-4.231717000	-2.371096000
H	-4.611700000	-1.096345000	-4.458622000
H	-5.150312000	-1.715245000	-2.898727000
H	-3.904008000	-0.468939000	-2.965146000
H	-0.078284000	-2.498199000	3.599278000
H	0.071688000	-4.032895000	4.458436000
H	1.395763000	-2.870638000	4.495544000
S	-1.096907000	0.323872000	-2.688983000
S	-2.905372000	0.156326000	-0.205460000
S	0.773406000	-2.001231000	-1.493941000
S	-1.112731000	-2.137109000	1.012574000
S	0.699819000	2.447941000	-1.260139000
S	2.521266000	0.143649000	-0.052510000
C	4.033203000	2.372976000	-2.998266000
H	4.360218000	3.397147000	-3.187248000
H	4.920511000	1.736796000	-2.999585000
H	3.593974000	2.333043000	-2.000430000
S	0.683080000	0.038940000	2.402915000
Co	-1.304237000	1.579554000	-0.878930000
Fe	-1.356201000	0.058001000	1.423849000
Co	0.944743000	1.501679000	0.729212000
P	-2.587437000	3.110548000	-1.669759000
S	-1.087628000	2.286122000	1.231347000

P	2.093284000	3.057628000	1.668121000
H	-3.459542000	1.848146000	-3.474205000
C	-1.734608000	4.326488000	-2.731811000
H	-2.451304000	5.121019000	-2.961389000
C	-3.399690000	4.170349000	-0.427343000
H	-2.595276000	4.617162000	0.162831000
H	-3.891319000	4.984797000	-0.968869000
H	-4.483640000	1.744408000	-2.065262000
C	-3.940846000	2.449937000	-2.699239000
H	-0.950565000	4.768697000	-2.111816000
H	3.066194000	3.887558000	-0.321219000
C	1.186354000	4.591155000	2.069221000
H	0.377028000	4.295438000	2.741447000
H	1.868856000	5.222997000	2.646222000
C	3.499504000	3.593182000	0.637788000
H	4.083559000	2.691008000	0.438338000
H	1.979463000	2.265935000	3.898310000
C	2.815221000	2.607289000	3.282099000
H	3.205193000	3.520694000	3.741453000
C	-4.875488000	3.484052000	-3.303877000
H	-1.915718000	3.336092000	-4.658387000
C	-1.143198000	3.741658000	-4.002244000
H	-0.605136000	4.511219000	-4.558952000
H	-0.445575000	2.935739000	-3.769175000
C	-4.383366000	3.445479000	0.474111000
H	-4.805317000	4.139105000	1.203542000
H	-3.897104000	2.636081000	1.020572000
H	-5.212262000	3.018006000	-0.093405000
H	-5.641209000	2.989879000	-3.905172000
H	-5.389601000	4.066976000	-2.537594000
H	-4.346271000	4.179257000	-3.958393000
C	4.364818000	4.699084000	1.218735000
C	0.638404000	5.343318000	0.870026000
H	0.076780000	6.219913000	1.198562000
H	1.435986000	5.688026000	0.208771000
H	-0.028862000	4.707544000	0.286239000
H	4.799978000	4.415600000	2.178932000
H	3.800606000	5.621782000	1.365646000
H	5.189704000	4.926024000	0.540374000
C	3.886918000	1.536455000	3.192935000
H	4.202616000	1.227555000	4.191102000
H	4.770905000	1.892052000	2.660130000
H	3.509877000	0.658737000	2.667711000

3Fe_1_3_M6_Co

C	-1.673153000	-4.420856000	-2.359960000
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C	-1.065497000	-5.150688000	-1.175234000
H	-0.505192000	-6.022379000	-1.518610000
C	1.424919000	0.059353000	-5.115728000
C	0.877593000	-1.343801000	-5.311327000
C	3.621950000	-0.893804000	-3.463380000
C	4.604092000	-0.832193000	-4.620932000
H	5.368931000	-1.602353000	-4.503189000
C	2.955569000	-4.026433000	0.330461000
C	3.979254000	-3.406907000	-0.602678000
H	4.319817000	-4.138141000	-1.338151000
C	4.479544000	-3.082344000	3.121486000
H	-2.361025000	-5.070070000	-2.911171000
H	-0.892293000	-4.108653000	-3.058669000
H	-0.385088000	-4.498047000	-0.626564000
H	-1.830143000	-5.499870000	-0.478641000
H	-4.281524000	-5.457703000	-1.549694000
H	-2.534753000	-2.097759000	-4.160343000
H	-3.761244000	-3.351141000	-3.981296000
H	1.674130000	-2.090158000	-5.321334000
H	0.181252000	-1.604894000	-4.512625000
H	4.122199000	-0.735131000	-2.504784000
H	3.141035000	-1.872683000	-3.394598000
H	4.114998000	-1.002035000	-5.582123000
H	5.116313000	0.130402000	-4.668937000
H	2.134982000	-4.471655000	-0.238454000
H	3.400815000	-4.823696000	0.933419000
H	3.548276000	-2.559427000	-1.136156000
H	4.855846000	-3.050928000	-0.058219000
H	3.944377000	-3.672558000	3.867863000
H	4.955215000	-3.774929000	2.424135000
H	2.060880000	-4.701840000	2.952623000
H	0.557655000	-4.452987000	2.074104000
P	-2.590642000	-2.901048000	-1.935173000
H	0.617839000	0.795555000	-5.152140000
H	0.348259000	-1.411091000	-6.263492000
H	2.137003000	0.317403000	-5.906270000
P	2.267314000	0.320346000	-3.518545000
P	2.182521000	-2.831357000	1.473995000
C	3.563664000	-2.097848000	2.414226000
H	3.105439000	-1.399220000	3.118771000
H	4.113959000	-1.476758000	1.702749000
H	5.275350000	-2.545415000	3.641311000
H	-5.639789000	-4.755472000	-0.679308000
C	-3.954578000	-3.424402000	-0.847696000
C	-4.840368000	-4.533904000	-1.389088000
C	-3.356982000	-2.441328000	-3.526571000

C	-4.420586000	-1.364585000	-3.405543000
C	1.333798000	-3.941624000	2.650063000
C	0.732377000	-3.257881000	3.863911000
H	-3.484464000	-3.709171000	0.096953000
H	-4.527931000	-2.518202000	-0.634789000
Fe	-1.315277000	-1.218898000	-1.017041000
Fe	0.867518000	0.161286000	-1.751722000
H	2.239831000	2.670726000	-3.793198000
C	3.058014000	1.949867000	-3.719621000
H	3.570894000	1.938246000	-4.687053000
Co	0.927226000	-1.373832000	0.523326000
H	-5.310117000	-4.256408000	-2.334679000
H	-4.769364000	-1.063192000	-4.394970000
H	-5.286854000	-1.714296000	-2.840817000
H	-4.023819000	-0.483883000	-2.899949000
H	0.007694000	-2.499994000	3.564379000
H	0.225392000	-3.989361000	4.496498000
H	1.494055000	-2.764398000	4.470547000
S	-1.163849000	0.219648000	-2.771490000
S	-2.953187000	0.096499000	-0.207660000
S	0.725156000	-2.088107000	-1.605950000
S	-1.083435000	-2.219288000	0.968924000
S	0.643798000	2.348581000	-1.305252000
S	2.465177000	0.080774000	-0.163110000
C	4.009147000	2.331990000	-2.599693000
H	4.422670000	3.324820000	-2.784918000
H	4.844890000	1.634018000	-2.521371000
H	3.497407000	2.353863000	-1.636608000
S	0.682385000	-0.106524000	2.320477000
Co	-1.382940000	1.498921000	-0.938909000
Fe	-1.361152000	-0.014131000	1.390171000
Co	0.838650000	1.346052000	0.655237000
P	-2.584791000	3.071593000	-1.776368000
S	-1.149470000	2.211891000	1.147532000
P	-2.445627000	0.111597000	3.306645000
H	-3.526692000	1.790497000	-3.533128000
C	-1.691267000	4.216079000	-2.883426000
H	-2.383013000	5.021893000	-3.147694000
C	-3.344038000	4.207412000	-0.568026000
H	-2.522184000	4.582435000	0.046829000
H	-3.752656000	5.059120000	-1.120367000
H	-4.542680000	1.779237000	-2.114900000
C	-3.974729000	2.438897000	-2.776010000
H	-0.896713000	4.660091000	-2.278321000
H	-3.428332000	2.244838000	3.010942000
H	-4.464479000	0.972590000	2.418664000

C	-3.852944000	1.273181000	3.273991000
C	-3.182636000	-1.491420000	3.792632000
H	-3.574862000	-1.394331000	4.809656000
H	-2.353302000	-2.202337000	3.834273000
C	-1.489468000	0.572485000	4.790987000
H	-0.691125000	-0.168742000	4.879147000
H	-2.147308000	0.444377000	5.656331000
C	-4.867581000	3.492163000	-3.410264000
H	-1.894543000	3.141369000	-4.762637000
C	-1.114496000	3.568016000	-4.128831000
H	-0.571047000	4.305902000	-4.722243000
H	-0.423663000	2.767115000	-3.861474000
C	-4.406154000	3.554179000	0.297737000
H	-4.744344000	4.244816000	1.072508000
H	-4.012023000	2.662531000	0.785694000
H	-5.279747000	3.260145000	-0.287382000
H	-5.668547000	3.014052000	-3.977939000
H	-5.337291000	4.134527000	-2.663002000
H	-4.315802000	4.131210000	-4.102232000
C	-4.682161000	1.357667000	4.544229000
H	-5.504777000	2.063352000	4.410639000
H	-4.090308000	1.705659000	5.392770000
H	-5.120582000	0.394468000	4.812939000
H	-5.126382000	-1.323254000	2.835542000
H	-3.873396000	-2.033585000	1.817194000
C	-4.256268000	-1.982850000	2.837512000
H	-4.597840000	-2.979345000	3.124440000
C	-0.910262000	1.975768000	4.748225000
H	-1.692728000	2.734117000	4.677775000
H	-0.337917000	2.174389000	5.656225000
H	-0.243895000	2.101459000	3.893803000

3Fe_1_5_M1_Fe

C	1.209837000	-0.005002000	-5.124065000
C	0.700589000	-1.432321000	-5.228148000
C	3.510987000	-0.816714000	-3.563689000
C	4.400271000	-0.794342000	-4.795898000
H	5.215530000	-1.511805000	-4.682569000
C	3.013174000	-3.978642000	0.316902000
C	4.026519000	-3.300922000	-0.587577000
H	4.384400000	-3.998346000	-1.347198000
C	4.527462000	-3.207107000	3.153516000
H	1.520394000	-2.153201000	-5.234453000
H	0.043923000	-1.678756000	-4.392583000
H	4.077395000	-0.589367000	-2.656647000
H	3.076377000	-1.806521000	-3.403777000

H	3.851014000	-1.065443000	-5.699298000
H	4.850313000	0.187012000	-4.958464000
H	2.194271000	-4.403395000	-0.269167000
H	3.471657000	-4.800058000	0.876199000
H	3.582983000	-2.442519000	-1.093687000
H	4.894454000	-2.947646000	-0.027273000
H	3.992332000	-3.866055000	3.839772000
H	5.023362000	-3.830356000	2.407017000
H	2.077851000	-4.801228000	2.909337000
H	0.584080000	-4.483313000	2.034898000
H	0.380181000	0.704961000	-5.171338000
H	0.136508000	-1.565346000	-6.152791000
H	1.884657000	0.232803000	-5.952358000
P	2.104896000	0.349328000	-3.574000000
P	2.231686000	-2.857080000	1.524515000
C	3.604206000	-2.181915000	2.517112000
H	3.136773000	-1.546947000	3.273659000
H	4.151872000	-1.507025000	1.854525000
H	5.307861000	-2.703807000	3.727894000
C	1.365647000	-4.015311000	2.638876000
C	0.770641000	-3.373388000	3.879277000
Fe	-1.308258000	-1.224620000	-0.938794000
Fe	0.975796000	0.154028000	-1.716416000
H	2.039136000	2.707364000	-3.856781000
C	2.856779000	1.983302000	-3.884649000
H	3.255113000	1.983960000	-4.903753000
Co	0.946989000	-1.369955000	0.652708000
H	0.063448000	-2.587574000	3.609217000
H	0.242010000	-4.120602000	4.474164000
H	1.539176000	-2.926838000	4.513384000
S	-1.093368000	0.232137000	-2.647163000
S	-2.926396000	0.094720000	-0.093270000
S	0.722118000	-2.076381000	-1.467363000
S	-1.093316000	-2.202997000	1.068590000
S	0.712498000	2.331724000	-1.195355000
S	2.477355000	0.081601000	-0.054043000
C	3.929407000	2.350814000	-2.874380000
H	4.240278000	3.389093000	-3.004828000
H	4.816638000	1.724206000	-2.982438000
H	3.557492000	2.229933000	-1.856636000
S	0.688526000	-0.088245000	2.441426000
Co	-1.325987000	1.519758000	-0.818497000
Fe	-1.349760000	-0.012842000	1.531205000
Co	0.904737000	1.429226000	0.812196000
P	-2.490745000	3.085195000	-1.739346000
S	-1.117562000	2.208501000	1.277463000

P	-2.557376000	0.115770000	3.335151000
P	2.045900000	3.007899000	1.714921000
H	-3.424521000	1.727535000	-3.445042000
C	-1.581736000	4.191513000	-2.872057000
H	-2.267690000	4.990528000	-3.170181000
C	-3.257644000	4.266380000	-0.578040000
H	-2.443481000	4.659762000	0.035704000
H	-3.654118000	5.101336000	-1.163837000
H	-4.449581000	1.786001000	-2.041067000
C	-3.873497000	2.415326000	-2.724324000
H	-0.790692000	4.650996000	-2.273732000
H	-3.510797000	2.254735000	2.990261000
H	-4.522991000	0.985477000	2.347661000
C	-3.952121000	1.284558000	3.230778000
C	-3.304758000	-1.489433000	3.788061000
H	-3.750321000	-1.382160000	4.782319000
H	-2.468839000	-2.187846000	3.883865000
C	-1.659410000	0.570681000	4.858449000
H	-0.876713000	-0.182843000	4.978413000
H	-2.351997000	0.454044000	5.697661000
H	3.007924000	3.839199000	-0.277167000
C	1.127027000	4.535654000	2.110920000
H	0.316083000	4.235758000	2.779141000
H	1.800245000	5.177470000	2.687639000
C	3.445009000	3.553297000	0.682305000
H	4.037990000	2.656218000	0.486849000
H	1.959059000	2.202385000	3.945387000
C	2.782369000	2.566510000	3.326214000
H	3.154420000	3.485691000	3.789057000
C	-4.752457000	3.446285000	-3.412634000
H	-1.771153000	3.065811000	-4.721526000
C	-0.995052000	3.501620000	-4.089502000
H	-0.433372000	4.214621000	-4.696428000
H	-0.319563000	2.699168000	-3.790069000
C	-4.334757000	3.646817000	0.293740000
H	-4.667945000	4.356122000	1.053658000
H	-3.958100000	2.756807000	0.798356000
H	-5.208110000	3.354813000	-0.292161000
H	-5.553926000	2.947845000	-3.961374000
H	-5.220836000	4.128509000	-2.700460000
H	-4.191033000	4.046215000	-4.131633000
C	-4.840759000	1.370306000	4.460240000
H	-5.648639000	2.085006000	4.290741000
H	-4.287878000	1.706016000	5.339613000
H	-5.301408000	0.409852000	4.698790000
H	-5.184289000	-1.341580000	2.707741000

H	-3.882516000	-2.107111000	1.792560000
C	-4.322199000	-2.007080000	2.786145000
H	-4.689769000	-2.987761000	3.093052000
C	-1.055916000	1.963296000	4.839557000
H	-1.823008000	2.736893000	4.764742000
H	-0.490114000	2.144576000	5.755572000
H	-0.382376000	2.077596000	3.989076000
C	4.297001000	4.670893000	1.260520000
C	0.577043000	5.272057000	0.902628000
H	-0.015634000	6.132097000	1.220399000
H	1.375953000	5.639349000	0.255404000
H	-0.058602000	4.615155000	0.307541000
H	4.733747000	4.396532000	2.222665000
H	3.722306000	5.587912000	1.402634000
H	5.120407000	4.904188000	0.582570000
C	3.874636000	1.517295000	3.225143000
H	4.195751000	1.202339000	4.219744000
H	4.751960000	1.895709000	2.697417000
H	3.513650000	0.640409000	2.688124000

3Fe_1_5_M3_Co

C	-1.609112000	-4.320277000	-2.311335000
C	-1.026526000	-5.064655000	-1.123701000
H	-0.484638000	-5.947759000	-1.466695000
C	1.395573000	-0.224390000	-5.096991000
C	0.808190000	-1.624116000	-5.098755000
C	3.629216000	-0.914812000	-3.345201000
C	4.587986000	-0.999413000	-4.520958000
H	5.383717000	-1.713443000	-4.299977000
H	-2.292579000	-4.960289000	-2.879117000
H	-0.817540000	-4.005520000	-2.996497000
H	-0.331488000	-4.435632000	-0.566262000
H	-1.804559000	-5.399614000	-0.434995000
H	-4.220398000	-5.370922000	-1.550897000
H	-2.462785000	-2.005537000	-4.121339000
H	-3.682640000	-3.264423000	-3.944103000
H	1.581049000	-2.389072000	-5.001580000
H	0.108073000	-1.747241000	-4.271720000
H	4.137391000	-0.610579000	-2.426637000
H	3.174902000	-1.883695000	-3.123774000
H	4.089096000	-1.338460000	-5.430849000
H	5.061496000	-0.039005000	-4.733957000
P	-2.537612000	-2.806577000	-1.893114000
H	0.609029000	0.521095000	-5.242469000
H	0.275473000	-1.806600000	-6.034014000
H	2.116089000	-0.097085000	-5.911353000

P	2.239957000	0.246594000	-3.550782000
H	-5.592983000	-4.681893000	-0.693008000
C	-3.913906000	-3.341318000	-0.828900000
C	-4.786177000	-4.451335000	-1.391462000
C	-3.288721000	-2.348280000	-3.492761000
C	-4.361423000	-1.279400000	-3.391032000
H	-3.455780000	-3.632865000	0.118953000
H	-4.494769000	-2.439370000	-0.619118000
Fe	-1.301079000	-1.133554000	-0.963363000
Fe	0.900314000	0.265491000	-1.720277000
H	2.138244000	2.556421000	-4.057873000
C	2.976897000	1.861723000	-3.961643000
H	3.442397000	1.773715000	-4.948655000
Co	0.897567000	-1.167403000	0.546918000
H	-5.245870000	-4.169078000	-2.340527000
H	-4.705019000	-0.992298000	-4.386546000
H	-5.229094000	-1.630043000	-2.829072000
H	-3.976232000	-0.390124000	-2.892030000
S	-1.124640000	0.299171000	-2.731232000
S	-2.954256000	0.191010000	-0.221022000
S	0.762996000	-1.976542000	-1.508008000
S	-1.068293000	-2.121760000	1.022657000
S	0.659158000	2.472131000	-1.306418000
S	2.483063000	0.247263000	-0.102101000
C	3.967279000	2.358386000	-2.924914000
H	4.306487000	3.365174000	-3.174986000
H	4.847289000	1.715181000	-2.867187000
H	3.506660000	2.386827000	-1.937400000
S	0.666591000	0.098532000	2.343918000
Co	-1.348913000	1.576367000	-0.914568000
Fe	-1.366274000	0.095240000	1.374216000
Co	0.889876000	1.584432000	0.715628000
P	-2.583993000	3.152849000	-1.759635000
S	-1.152247000	2.300649000	1.179554000
P	-2.488061000	-0.019312000	3.288988000
P	2.073085000	3.081732000	1.677205000
H	-3.530413000	1.867148000	-3.509430000
C	-1.706168000	4.301605000	-2.877624000
H	-2.397896000	5.107212000	-3.141893000
C	-3.346220000	4.294912000	-0.555832000
H	-2.523224000	4.683626000	0.049620000
H	-3.769518000	5.139903000	-1.107107000
H	-4.544512000	1.861050000	-2.090785000
C	-3.978037000	2.519308000	-2.754794000
H	-0.904858000	4.747076000	-2.282014000
H	-3.508289000	2.103960000	3.029265000

H	-4.511623000	0.829491000	2.389074000
C	-3.918126000	1.117685000	3.260797000
C	-3.192013000	-1.650208000	3.707891000
H	-3.578508000	-1.603213000	4.730522000
H	-2.351747000	-2.349056000	3.710826000
C	-1.565410000	0.427341000	4.798845000
H	-0.727204000	-0.271128000	4.859049000
H	-2.218418000	0.227045000	5.653872000
H	2.998503000	4.000535000	-0.294134000
C	1.166011000	4.598351000	2.139501000
H	0.352225000	4.274100000	2.793032000
H	1.840008000	5.213824000	2.743449000
C	3.455946000	3.657769000	0.637379000
H	4.027558000	2.762680000	0.379280000
H	2.011613000	2.254956000	3.899452000
C	2.834676000	2.576089000	3.255992000
H	3.271800000	3.469960000	3.712139000
C	-4.874266000	3.565738000	-3.394545000
H	-1.920708000	3.219065000	-4.751234000
C	-1.136274000	3.645336000	-4.122575000
H	-0.591396000	4.376966000	-4.722569000
H	-0.448500000	2.841649000	-3.854721000
C	-4.390888000	3.638046000	0.328645000
H	-4.729985000	4.331612000	1.100612000
H	-3.981907000	2.754520000	0.820434000
H	-5.266610000	3.327355000	-0.244513000
H	-5.674194000	3.083788000	-3.960591000
H	-5.345570000	4.210054000	-2.649815000
H	-4.323935000	4.203822000	-4.088663000
C	-4.763083000	1.151654000	4.523411000
H	-5.597083000	1.845289000	4.397768000
H	-4.188111000	1.487026000	5.388469000
H	-5.186074000	0.173507000	4.760629000
H	-5.167858000	-1.493785000	2.819280000
H	-3.907642000	-2.027403000	1.706628000
C	-4.265289000	-2.102059000	2.733893000
H	-4.546170000	-3.139338000	2.925564000
C	-1.065676000	1.860764000	4.818412000
H	-1.888163000	2.578818000	4.811167000
H	-0.473232000	2.042991000	5.717097000
H	-0.440056000	2.059374000	3.947026000
C	4.345396000	4.728159000	1.247546000
C	0.622151000	5.385706000	0.960498000
H	0.034495000	6.236482000	1.310829000
H	1.424647000	5.774436000	0.330297000
H	-0.019095000	4.759634000	0.337742000

H	4.819101000	4.386293000	2.169568000
H	3.789364000	5.639980000	1.473592000
H	5.142491000	4.996473000	0.551248000
C	3.866124000	1.469590000	3.121599000
H	4.244445000	1.184961000	4.105013000
H	4.719198000	1.784181000	2.517120000
H	3.431412000	0.582484000	2.658530000

3Fe_1_5_M5_Fe

C	-1.617157000	-4.422884000	-2.370370000
C	-1.061193000	-5.143345000	-1.153940000
H	-0.461393000	-6.001466000	-1.463196000
C	1.378959000	0.017433000	-5.057647000
C	0.829208000	-1.392400000	-5.188359000
C	3.625132000	-0.848928000	-3.454842000
C	4.540634000	-0.847439000	-4.667082000
H	5.334573000	-1.586663000	-4.542030000
C	2.912508000	-3.995102000	0.339924000
C	3.945210000	-3.374588000	-0.582968000
H	4.260052000	-4.092331000	-1.342767000
C	4.496931000	-3.173306000	3.117998000
H	-2.276395000	-5.077594000	-2.948920000
H	-0.805610000	-4.113046000	-3.034710000
H	-0.430762000	-4.476745000	-0.563731000
H	-1.857703000	-5.511753000	-0.504550000
H	-4.256895000	-5.446096000	-1.610861000
H	-2.468811000	-2.111086000	-4.208892000
H	-3.703284000	-3.355478000	-4.037740000
H	1.625608000	-2.139170000	-5.179270000
H	0.145509000	-1.623105000	-4.369522000
H	4.178615000	-0.643448000	-2.534545000
H	3.160000000	-1.827501000	-3.310009000
H	4.003003000	-1.099034000	-5.583275000
H	5.019436000	0.122263000	-4.816975000
H	2.076921000	-4.403482000	-0.234147000
H	3.342054000	-4.819485000	0.917141000
H	3.535985000	-2.499573000	-1.088994000
H	4.835700000	-3.059253000	-0.035955000
H	3.960905000	-3.782930000	3.847556000
H	4.949636000	-3.845185000	2.386239000
H	2.029671000	-4.705256000	2.967308000
H	0.514172000	-4.394319000	2.130247000
P	-2.544473000	-2.900505000	-1.975799000
H	0.568567000	0.749344000	-5.113826000
H	0.284806000	-1.500893000	-6.128422000
H	2.072623000	0.241455000	-5.873888000

P	2.248137000	0.348300000	-3.482042000
P	2.179035000	-2.813500000	1.522572000
C	3.589832000	-2.144425000	2.464280000
H	3.155125000	-1.473217000	3.208802000
H	4.142194000	-1.506606000	1.769760000
H	5.310156000	-2.672815000	3.647447000
H	-5.616706000	-4.740516000	-0.744804000
C	-3.923681000	-3.416774000	-0.899543000
C	-4.812043000	-4.520134000	-1.449026000
C	-3.294962000	-2.450468000	-3.577528000
C	-4.350361000	-1.364301000	-3.458843000
C	1.319761000	-3.917774000	2.694875000
C	0.771470000	-3.232212000	3.933404000
H	-3.465896000	-3.701170000	0.051638000
H	-4.492653000	-2.507009000	-0.689384000
Fe	-1.316283000	-1.219324000	-0.965631000
Fe	0.922184000	0.186477000	-1.725021000
H	2.228887000	2.700743000	-3.781499000
C	3.035402000	1.963572000	-3.800248000
H	3.446680000	1.954582000	-4.813979000
Co	0.946199000	-1.302043000	0.613292000
H	-5.274523000	-4.236672000	-2.396525000
H	-4.685757000	-1.047528000	-4.448145000
H	-5.225964000	-1.711305000	-2.907114000
H	-3.950272000	-0.493346000	-2.938516000
H	0.051822000	-2.456554000	3.669316000
H	0.265676000	-3.959455000	4.571185000
H	1.563875000	-2.768749000	4.524589000
S	-1.109840000	0.252993000	-2.676030000
S	-2.958647000	0.158908000	-0.137933000
S	0.739088000	-2.026912000	-1.491446000
S	-1.089423000	-2.183240000	1.095926000
S	0.667301000	2.379069000	-1.288795000
S	2.486555000	0.111285000	-0.099934000
C	4.100179000	2.311631000	-2.775519000
H	4.425936000	3.347062000	-2.891615000
H	4.980722000	1.674585000	-2.877924000
H	3.715999000	2.184495000	-1.763741000
S	0.709807000	0.015771000	2.393283000
Co	-1.336655000	1.549637000	-0.883401000
Fe	-1.317158000	0.042387000	1.421402000
Co	0.916969000	1.462725000	0.703569000
P	-2.566029000	3.102862000	-1.707327000
S	-1.101458000	2.261979000	1.211784000
P	2.065737000	3.030008000	1.623953000
H	-3.511828000	1.808186000	-3.450763000

C	-1.696227000	4.250368000	-2.829885000
H	-2.399689000	5.044970000	-3.097026000
C	-3.318669000	4.232368000	-0.488830000
H	-2.488935000	4.653324000	0.084813000
H	-3.773307000	5.056510000	-1.047553000
H	-4.510164000	1.783771000	-2.020652000
C	-3.959407000	2.450842000	-2.688491000
H	-0.901042000	4.709503000	-2.237021000
H	3.058616000	3.845301000	-0.360737000
C	1.151604000	4.563879000	2.009481000
H	0.341008000	4.272372000	2.681726000
H	1.831397000	5.201707000	2.583004000
C	3.479120000	3.571082000	0.609397000
H	4.079906000	2.674770000	0.436450000
H	1.947364000	2.240499000	3.856136000
C	2.780827000	2.598038000	3.246461000
H	3.147331000	3.520703000	3.706496000
C	-4.873681000	3.492755000	-3.310776000
H	-1.901073000	3.154885000	-4.696917000
C	-1.121020000	3.593851000	-4.071797000
H	-0.586167000	4.328989000	-4.676214000
H	-0.421860000	2.800805000	-3.801190000
C	-4.329343000	3.577084000	0.435937000
H	-4.698481000	4.302255000	1.163255000
H	-3.882770000	2.746183000	0.984144000
H	-5.190429000	3.193382000	-0.114556000
H	-5.668511000	3.003680000	-3.877473000
H	-5.351304000	4.119870000	-2.555735000
H	-4.336916000	4.146264000	-4.001067000
C	4.319352000	4.697523000	1.187795000
C	0.606943000	5.304642000	0.802038000
H	0.032914000	6.176855000	1.120804000
H	1.407177000	5.654253000	0.146540000
H	-0.046058000	4.658061000	0.214483000
H	4.739256000	4.436834000	2.161150000
H	3.741731000	5.615825000	1.306929000
H	5.154577000	4.921987000	0.521283000
C	3.876104000	1.550431000	3.167166000
H	4.173995000	1.231406000	4.167624000
H	4.765168000	1.932438000	2.661968000
H	3.530437000	0.674883000	2.617616000

3Fe_1_5_M6_Co

C	-1.560858000	-4.411943000	-2.299163000
C	-0.963461000	-5.123557000	-1.098343000
H	-0.377326000	-5.986011000	-1.421656000

C	1.334670000	0.034806000	-5.100102000
C	0.764202000	-1.363257000	-5.260414000
C	3.558496000	-0.918649000	-3.487494000
C	4.513348000	-0.880766000	-4.668449000
H	5.272913000	-1.657453000	-4.559691000
C	2.942666000	-4.035638000	0.318946000
C	3.961517000	-3.421990000	-0.623535000
H	4.288493000	-4.154654000	-1.363788000
C	4.508032000	-3.118786000	3.090081000
H	-2.240708000	-5.070477000	-2.848649000
H	-0.774223000	-4.106081000	-2.993729000
H	-0.310185000	-4.452353000	-0.538907000
H	-1.736007000	-5.483345000	-0.415841000
H	-4.145349000	-5.482438000	-1.519671000
H	-2.430295000	-2.103119000	-4.125568000
H	-3.631669000	-3.378616000	-3.946546000
H	1.549753000	-2.121067000	-5.275857000
H	0.083871000	-1.601127000	-4.440785000
H	4.082261000	-0.753300000	-2.542754000
H	3.069699000	-1.891487000	-3.394746000
H	4.000207000	-1.056764000	-5.615924000
H	5.034090000	0.075804000	-4.740180000
H	2.112407000	-4.471494000	-0.242780000
H	3.387035000	-4.838931000	0.914506000
H	3.531952000	-2.570088000	-1.150911000
H	4.846695000	-3.074020000	-0.087855000
H	3.976995000	-3.709565000	3.838967000
H	4.968316000	-3.810678000	2.381837000
H	2.065442000	-4.705589000	2.957930000
H	0.557383000	-4.441768000	2.091361000
P	-2.485388000	-2.891118000	-1.890464000
H	0.536816000	0.781083000	-5.130570000
H	0.211133000	-1.439125000	-6.198328000
H	2.032821000	0.270239000	-5.909774000
P	2.214007000	0.307675000	-3.524865000
P	2.192286000	-2.836237000	1.472884000
C	3.592192000	-2.121511000	2.400963000
H	3.151094000	-1.423427000	3.117130000
H	4.138694000	-1.500526000	1.686520000
H	5.315476000	-2.593010000	3.603341000
H	-5.535636000	-4.793886000	-0.690091000
C	-3.866444000	-3.437623000	-0.832492000
C	-4.722332000	-4.566092000	-1.382062000
C	-3.249038000	-2.458535000	-3.494081000
C	-4.337015000	-1.403609000	-3.393087000
C	1.344894000	-3.938029000	2.658433000

C	0.761405000	-3.242219000	3.874511000
H	-3.414814000	-3.707437000	0.125358000
H	-4.461736000	-2.540824000	-0.640089000
Fe	-1.314151000	-1.176830000	-1.002920000
Fe	0.859442000	0.181034000	-1.728759000
H	2.207542000	2.655541000	-3.825565000
C	3.018119000	1.925221000	-3.763651000
H	3.508550000	1.897245000	-4.742287000
Co	0.939785000	-1.356423000	0.554697000
H	-5.172907000	-4.306454000	-2.342032000
H	-4.684208000	-1.119397000	-4.388225000
H	-5.200620000	-1.766804000	-2.832720000
H	-3.965510000	-0.508076000	-2.893300000
H	0.040742000	-2.480019000	3.575534000
H	0.252971000	-3.965184000	4.515752000
H	1.533443000	-2.753594000	4.472095000
S	-1.177357000	0.269816000	-2.701717000
S	-2.944439000	0.135282000	-0.179619000
S	0.705061000	-2.050314000	-1.561236000
S	-1.085474000	-2.184514000	1.014254000
S	0.670517000	2.373479000	-1.300288000
S	2.490392000	0.070683000	-0.171521000
C	3.998642000	2.305954000	-2.668650000
H	4.415322000	3.294589000	-2.868481000
H	4.830503000	1.601798000	-2.606040000
H	3.508626000	2.336200000	-1.694486000
S	0.741220000	-0.049829000	2.339989000
Co	-1.371470000	1.549001000	-0.896586000
Fe	-1.303744000	0.025128000	1.379236000
Co	0.910727000	1.383328000	0.668902000
P	-2.568261000	3.122026000	-1.756719000
S	-1.066735000	2.253144000	1.210349000
P	-2.514654000	0.091701000	3.288651000
H	-3.558031000	1.827947000	-3.477860000
C	-1.679474000	4.242178000	-2.892527000
H	-2.366015000	5.050169000	-3.163526000
C	-3.292636000	4.286014000	-0.551451000
H	-2.455449000	4.648819000	0.050349000
H	-3.692127000	5.143307000	-1.101624000
H	-4.552122000	1.857495000	-2.045978000
C	-3.984083000	2.497551000	-2.726260000
H	-0.873682000	4.688613000	-2.304118000
H	-3.444330000	2.242883000	2.984403000
H	-4.484384000	0.994863000	2.343978000
C	-3.894861000	1.276196000	3.220437000
C	-3.268051000	-1.517873000	3.705430000

H	-3.676640000	-1.437957000	4.717878000
H	-2.443255000	-2.233687000	3.742272000
C	-1.572860000	0.507965000	4.793470000
H	-0.774656000	-0.235190000	4.864271000
H	-2.245832000	0.344800000	5.641712000
C	-4.869315000	3.553503000	-3.366351000
H	-1.910160000	3.131118000	-4.747776000
C	-1.120858000	3.567574000	-4.132242000
H	-0.582192000	4.291322000	-4.747144000
H	-0.429977000	2.769386000	-3.857520000
C	-4.354698000	3.656576000	0.331952000
H	-4.660491000	4.350226000	1.117551000
H	-3.975119000	2.750185000	0.803781000
H	-5.246409000	3.389120000	-0.238344000
H	-5.690247000	3.079847000	-3.908719000
H	-5.311968000	4.221097000	-2.624535000
H	-4.318682000	4.167159000	-4.081843000
C	-4.754704000	1.353065000	4.471209000
H	-5.560321000	2.075629000	4.326300000
H	-4.179701000	1.676620000	5.340699000
H	-5.217390000	0.393590000	4.710633000
H	-5.192438000	-1.305917000	2.718973000
H	-3.925653000	-1.999978000	1.705620000
C	-4.327824000	-1.972373000	2.718677000
H	-4.680703000	-2.973025000	2.975041000
C	-0.998653000	1.912964000	4.814793000
H	-1.781688000	2.671748000	4.758877000
H	-0.446242000	2.074928000	5.742004000
H	-0.315184000	2.072348000	3.980153000

3Fe_1_7_M1_Fe

C	1.186414000	-0.087015000	-5.082309000
C	0.671657000	-1.515320000	-5.117967000
C	3.502606000	-0.809864000	-3.503585000
C	4.375171000	-0.837021000	-4.747383000
H	5.202796000	-1.535844000	-4.609128000
C	2.969320000	-3.957546000	0.346834000
C	4.008326000	-3.308746000	-0.550297000
H	4.342184000	-4.011074000	-1.316333000
C	4.521544000	-3.189127000	3.155042000
H	1.488171000	-2.239577000	-5.091667000
H	0.016053000	-1.718801000	-4.269972000
H	4.078214000	-0.534705000	-2.615835000
H	3.080302000	-1.795262000	-3.291850000
H	3.817859000	-1.162522000	-5.627560000
H	4.808142000	0.141045000	-4.966690000

H	2.143082000	-4.358453000	-0.245603000
H	3.399519000	-4.791518000	0.909722000
H	3.596995000	-2.430172000	-1.048820000
H	4.887458000	-2.992481000	0.014536000
H	3.983789000	-3.829821000	3.856381000
H	4.993686000	-3.830821000	2.408781000
H	2.048179000	-4.729882000	2.964941000
H	0.552789000	-4.411885000	2.094472000
H	0.358435000	0.622295000	-5.159919000
H	0.104713000	-1.689213000	-6.034124000
H	1.860160000	0.110854000	-5.921826000
P	2.082434000	0.338858000	-3.551249000
P	2.213376000	-2.808384000	1.545043000
C	3.609594000	-2.152867000	2.520340000
H	3.163450000	-1.503529000	3.277682000
H	4.162830000	-1.492797000	1.847464000
H	5.320508000	-2.695655000	3.712275000
C	1.343758000	-3.941019000	2.683659000
C	0.763849000	-3.268642000	3.915192000
Fe	-1.237922000	-1.132356000	-0.927539000
Fe	0.950337000	0.205961000	-1.645201000
H	1.989001000	2.683856000	-3.925017000
C	2.814048000	1.967773000	-3.932383000
H	3.204015000	1.933558000	-4.954257000
Co	0.966955000	-1.277138000	0.690487000
H	0.066077000	-2.478929000	3.632633000
H	0.228505000	-3.996862000	4.527574000
H	1.541669000	-2.820444000	4.536856000
S	-1.094926000	0.288596000	-2.634077000
S	-2.911533000	0.179854000	-0.129998000
S	0.755539000	-2.031282000	-1.410951000
S	-1.072904000	-2.170207000	1.074938000
S	0.724153000	2.398567000	-1.209021000
S	2.501935000	0.138888000	-0.046064000
C	3.890355000	2.385582000	-2.946298000
H	4.190176000	3.420605000	-3.121122000
H	4.782693000	1.763290000	-3.036221000
H	3.526870000	2.303108000	-1.921693000
S	0.740586000	0.035563000	2.456065000
Co	-1.297473000	1.588383000	-0.813417000
Fe	-1.278688000	0.049522000	1.460770000
Co	0.929157000	1.491120000	0.788788000
P	-2.493902000	3.111236000	-1.744897000
S	-1.078668000	2.288444000	1.274515000
P	-2.585069000	0.021351000	3.338037000
P	2.113691000	3.044592000	1.686376000

H	-3.451715000	1.731840000	-3.419633000
C	-1.605314000	4.212158000	-2.898886000
H	-2.300010000	5.005158000	-3.192862000
C	-3.246894000	4.304755000	-0.586005000
H	-2.420971000	4.724767000	-0.006172000
H	-3.672588000	5.120471000	-1.178264000
H	-4.463494000	1.819699000	-2.007460000
C	-3.889833000	2.434004000	-2.706006000
H	-0.808326000	4.680385000	-2.315407000
H	-3.470844000	2.203292000	3.128351000
H	-4.480008000	1.019722000	2.337659000
C	-3.946365000	1.229276000	3.268518000
C	-3.368086000	-1.596021000	3.649068000
H	-3.832519000	-1.551601000	4.639544000
H	-2.549244000	-2.318005000	3.706563000
C	-1.693805000	0.367958000	4.892320000
H	-0.891743000	-0.372620000	4.949050000
H	-2.380470000	0.169116000	5.721187000
H	3.048417000	3.886002000	-0.313885000
C	1.211899000	4.578583000	2.104275000
H	0.407931000	4.280624000	2.782263000
H	1.897245000	5.211056000	2.676985000
C	3.500198000	3.588995000	0.635499000
H	4.082585000	2.689001000	0.421820000
H	2.054821000	2.258947000	3.923883000
C	2.873257000	2.605890000	3.287831000
H	3.267327000	3.522038000	3.737897000
C	-4.770154000	3.458182000	-3.402169000
H	-1.813316000	3.070570000	-4.737152000
C	-1.031625000	3.516783000	-4.119382000
H	-0.483641000	4.229079000	-4.739479000
H	-0.347027000	2.720948000	-3.823517000
C	-4.288595000	3.691947000	0.332057000
H	-4.619322000	4.419748000	1.075418000
H	-3.878920000	2.828692000	0.857114000
H	-5.168727000	3.360937000	-0.222252000
H	-5.577710000	2.954852000	-3.937303000
H	-5.230655000	4.151605000	-2.695615000
H	-4.212722000	4.046179000	-4.133928000
C	-4.887941000	1.234115000	4.460744000
H	-5.662316000	1.991738000	4.324772000
H	-4.366355000	1.464049000	5.391944000
H	-5.390841000	0.273394000	4.585910000
H	-5.216984000	-1.322536000	2.537795000
H	-3.909591000	-2.051987000	1.601637000
C	-4.372687000	-2.012689000	2.588805000

H	-4.768444000	-3.003960000	2.815928000
C	-1.125718000	1.773611000	4.977338000
H	-1.913324000	2.529473000	4.972383000
H	-0.554415000	1.895515000	5.899418000
H	-0.462981000	1.973621000	4.133716000
C	4.372099000	4.695022000	1.205730000
C	0.651541000	5.331233000	0.910837000
H	0.069936000	6.192747000	1.244769000
H	1.444949000	5.698815000	0.257074000
H	0.003298000	4.686927000	0.314998000
H	4.825901000	4.409166000	2.156553000
H	3.807758000	5.615339000	1.366974000
H	5.183663000	4.927857000	0.513468000
C	3.948027000	1.540152000	3.175700000
H	4.278869000	1.222347000	4.166237000
H	4.823055000	1.904593000	2.634388000
H	3.568408000	0.667077000	2.644885000

3Fe_1_7_M3_Co

C	-1.545968000	-4.327888000	-2.413088000
C	-0.959964000	-5.084473000	-1.233963000
H	-0.391464000	-5.946051000	-1.588325000
C	1.286458000	-0.230504000	-5.065372000
C	0.701232000	-1.631312000	-5.071507000
C	3.572415000	-0.914694000	-3.405623000
C	4.498140000	-0.956439000	-4.609555000
H	5.311083000	-1.663529000	-4.432886000
H	-2.211261000	-4.968807000	-3.000737000
H	-0.752633000	-3.985638000	-3.083102000
H	-0.287534000	-4.451535000	-0.653670000
H	-1.738150000	-5.454517000	-0.563538000
H	-4.135387000	-5.434309000	-1.648744000
H	-2.462854000	-1.989722000	-4.177280000
H	-3.668702000	-3.263399000	-4.015461000
H	1.476219000	-2.395084000	-4.980982000
H	0.005347000	-1.761507000	-4.241576000
H	4.107854000	-0.628247000	-2.496241000
H	3.148626000	-1.899842000	-3.195568000
H	3.977349000	-1.279595000	-5.513134000
H	4.951497000	0.015611000	-4.813462000
P	-2.497393000	-2.837382000	-1.964635000
H	0.496348000	0.514021000	-5.195612000
H	0.163624000	-1.813180000	-6.004362000
H	1.992155000	-0.097886000	-5.891239000
P	2.152987000	0.227319000	-3.523464000
H	-5.508831000	-4.787470000	-0.759350000

C	-3.855466000	-3.412841000	-0.895204000
C	-4.715983000	-4.528761000	-1.463970000
C	-3.275229000	-2.357053000	-3.544772000
C	-4.353726000	-1.298866000	-3.395738000
H	-3.383478000	-3.709974000	0.044748000
H	-4.450053000	-2.525109000	-0.663517000
Fe	-1.260851000	-1.158929000	-0.968089000
Fe	0.932237000	0.281828000	-1.708073000
H	2.044602000	2.542449000	-4.034957000
C	2.882914000	1.844453000	-3.963051000
H	3.317150000	1.756612000	-4.963935000
Co	0.952365000	-1.200860000	0.551530000
H	-5.193539000	-4.237938000	-2.401685000
H	-4.711691000	-0.980215000	-4.376495000
H	-5.212401000	-1.672785000	-2.835004000
H	-3.967034000	-0.424178000	-2.872340000
S	-1.094040000	0.318791000	-2.671550000
S	-2.928020000	0.130857000	-0.159448000
S	0.833985000	-1.961553000	-1.545969000
S	-1.017251000	-2.171332000	1.035992000
S	0.659460000	2.445942000	-1.215148000
S	2.494586000	0.268042000	-0.076263000
C	3.910148000	2.345862000	-2.964522000
H	4.253301000	3.345333000	-3.238297000
H	4.784988000	1.694112000	-2.924179000
H	3.483124000	2.393956000	-1.962424000
S	0.694977000	0.003648000	2.401943000
Co	-1.347973000	1.558235000	-0.844888000
Fe	-1.327097000	0.054236000	1.418205000
Co	0.871357000	1.544860000	0.777922000
P	-2.547844000	3.118976000	-1.718215000
S	-1.161370000	2.271302000	1.243985000
P	-2.497312000	0.091033000	3.276361000
P	2.051895000	3.058143000	1.729771000
H	-3.488682000	1.807415000	-3.450678000
C	-1.654868000	4.248317000	-2.841419000
H	-2.352428000	5.041728000	-3.127047000
C	-3.311195000	4.276341000	-0.531356000
H	-2.494334000	4.656400000	0.087007000
H	-3.710529000	5.123137000	-1.097649000
H	-4.513279000	1.834049000	-2.039428000
C	-3.937049000	2.475531000	-2.711190000
H	-0.867401000	4.710732000	-2.240956000
H	-3.517399000	2.209392000	2.987490000
H	-4.510195000	0.925070000	2.346962000
C	-3.927284000	1.224162000	3.222385000

C	-3.205529000	-1.532715000	3.726762000
H	-3.620910000	-1.455834000	4.736291000
H	-2.358299000	-2.221705000	3.777781000
C	-1.594050000	0.547851000	4.796289000
H	-0.783244000	-0.178502000	4.892694000
H	-2.271557000	0.388904000	5.640735000
H	2.976116000	3.972985000	-0.245616000
C	1.144089000	4.573431000	2.193760000
H	0.326493000	4.249107000	2.842313000
H	1.816540000	5.184965000	2.803347000
C	3.432631000	3.636029000	0.688372000
H	4.009527000	2.743013000	0.435018000
H	1.998704000	2.210787000	3.946245000
C	2.817264000	2.551376000	3.307119000
H	3.235812000	3.449249000	3.772713000
C	-4.818442000	3.519955000	-3.375092000
H	-1.833968000	3.132424000	-4.698963000
C	-1.063026000	3.580749000	-4.069103000
H	-0.523314000	4.311729000	-4.674372000
H	-0.364767000	2.792787000	-3.782768000
C	-4.383548000	3.638623000	0.333331000
H	-4.714517000	4.333243000	1.107681000
H	-4.003518000	2.740697000	0.821101000
H	-5.259435000	3.356367000	-0.253817000
H	-5.622795000	3.034354000	-3.931412000
H	-5.283410000	4.187124000	-2.646752000
H	-4.259224000	4.134579000	-4.083026000
C	-4.790226000	1.270638000	4.472053000
H	-5.621045000	1.964838000	4.329639000
H	-4.226762000	1.612236000	5.342312000
H	-5.218711000	0.295524000	4.711516000
H	-5.136709000	-1.402660000	2.739017000
H	-3.846540000	-2.057568000	1.730478000
C	-4.247712000	-2.036672000	2.744389000
H	-4.564026000	-3.047785000	3.007533000
C	-1.044104000	1.962482000	4.799336000
H	-1.839568000	2.708598000	4.744342000
H	-0.478055000	2.147221000	5.714507000
H	-0.381372000	2.118742000	3.947092000
C	4.315341000	4.712688000	1.297323000
C	0.607574000	5.366669000	1.015323000
H	0.016189000	6.214507000	1.366478000
H	1.413873000	5.759760000	0.392871000
H	-0.026859000	4.742759000	0.383709000
H	4.785979000	4.377520000	2.223380000
H	3.755419000	5.624002000	1.515491000

H	5.114632000	4.979330000	0.603021000
C	3.870406000	1.465715000	3.167645000
H	4.242627000	1.173474000	4.151110000
H	4.724233000	1.805437000	2.578257000
H	3.459263000	0.577965000	2.685169000

3Fe_1_7_M5_Fe

C	-1.580314000	-4.400318000	-2.325559000
C	-1.024364000	-5.125737000	-1.112997000
H	-0.464964000	-6.009088000	-1.426821000
C	1.244630000	-0.074954000	-5.111618000
C	0.735981000	-1.505117000	-5.158490000
C	3.554370000	-0.800932000	-3.527356000
C	4.440521000	-0.803347000	-4.761467000
H	5.268803000	-1.502373000	-4.628278000
C	2.984601000	-3.969913000	0.349882000
C	4.016420000	-3.307868000	-0.545344000
H	4.371119000	-4.009002000	-1.303188000
C	4.477258000	-3.174607000	3.182781000
H	-2.257938000	-5.046391000	-2.892883000
H	-0.771478000	-4.108461000	-3.000923000
H	-0.354229000	-4.476864000	-0.547716000
H	-1.817833000	-5.456036000	-0.439935000
H	-4.229252000	-5.387962000	-1.567298000
H	-2.388653000	-2.094534000	-4.185750000
H	-3.626166000	-3.334472000	-4.006143000
H	1.555875000	-2.225959000	-5.155726000
H	0.103454000	-1.717912000	-4.295006000
H	4.119207000	-0.537910000	-2.628868000
H	3.137420000	-1.792839000	-3.335086000
H	3.893775000	-1.112725000	-5.654254000
H	4.872642000	0.179925000	-4.957512000
H	2.174361000	-4.397373000	-0.246465000
H	3.428667000	-4.788560000	0.924284000
H	3.592026000	-2.441030000	-1.053894000
H	4.884086000	-2.968840000	0.023794000
H	3.935457000	-3.821279000	3.875375000
H	4.973602000	-3.810448000	2.447132000
H	2.037221000	-4.765063000	2.927405000
H	0.538515000	-4.449492000	2.062267000
P	-2.488825000	-2.863756000	-1.945074000
H	0.412194000	0.629830000	-5.184829000
H	0.150352000	-1.672106000	-6.064546000
H	1.916865000	0.131334000	-5.949869000
P	2.126600000	0.339625000	-3.566469000
P	2.191771000	-2.829403000	1.535002000

C	3.562914000	-2.152479000	2.529184000
H	3.093490000	-1.508750000	3.276964000
H	4.118133000	-1.486208000	1.864209000
H	5.257491000	-2.667751000	3.754259000
H	-5.594894000	-4.652355000	-0.736953000
C	-3.885692000	-3.351582000	-0.879336000
C	-4.775756000	-4.452954000	-1.430576000
C	-3.221342000	-2.421923000	-3.557545000
C	-4.277905000	-1.335124000	-3.468203000
C	1.324867000	-3.978721000	2.658329000
C	0.738809000	-3.330397000	3.899868000
H	-3.445677000	-3.629722000	0.081478000
H	-4.448072000	-2.433385000	-0.690519000
Fe	-1.250938000	-1.201846000	-0.972634000
Fe	0.957799000	0.173324000	-1.685168000
H	2.016971000	2.685690000	-3.916281000
C	2.848349000	1.976667000	-3.928136000
H	3.246631000	1.960102000	-4.947133000
Co	0.943480000	-1.323981000	0.637090000
H	-5.218926000	-4.179032000	-2.389931000
H	-4.604599000	-1.039530000	-4.466907000
H	-5.157941000	-1.671503000	-2.917097000
H	-3.882584000	-0.453412000	-2.963308000
H	0.023004000	-2.550227000	3.638199000
H	0.220197000	-4.076653000	4.504494000
H	1.512597000	-2.878949000	4.523945000
S	-1.067999000	0.241166000	-2.681063000
S	-2.930537000	0.144840000	-0.182470000
S	0.788055000	-2.044006000	-1.459271000
S	-1.097708000	-2.204650000	1.063212000
S	0.715626000	2.365029000	-1.232491000
S	2.486248000	0.109380000	-0.048932000
C	3.912624000	2.388908000	-2.926345000
H	4.200812000	3.430759000	-3.078131000
H	4.813219000	1.779445000	-3.021768000
H	3.542879000	2.280979000	-1.906308000
S	0.672668000	-0.014857000	2.429254000
Co	-1.304943000	1.530884000	-0.882870000
Fe	-1.318933000	0.016483000	1.401968000
Co	0.910901000	1.458339000	0.758123000
P	-2.506207000	3.100059000	-1.724622000
S	-1.116877000	2.240707000	1.223625000
P	2.055309000	3.019395000	1.683385000
H	-3.435256000	1.823574000	-3.490895000
C	-1.608950000	4.242768000	-2.830572000
H	-2.295381000	5.050732000	-3.101736000

C	-3.273810000	4.232377000	-0.517979000
H	-2.453010000	4.646942000	0.072828000
H	-3.713547000	5.060573000	-1.082504000
H	-4.456258000	1.798946000	-2.076548000
C	-3.889694000	2.465274000	-2.731845000
H	-0.811919000	4.683546000	-2.226693000
H	3.051376000	3.836447000	-0.299080000
C	1.141701000	4.555496000	2.060515000
H	0.320993000	4.263638000	2.720409000
H	1.813965000	5.191252000	2.645074000
C	3.472886000	3.551281000	0.667679000
H	4.062630000	2.649395000	0.484578000
H	1.922436000	2.235921000	3.915474000
C	2.761275000	2.587925000	3.309688000
H	3.131039000	3.509155000	3.770068000
C	-4.787144000	3.516331000	-3.362913000
H	-1.813908000	3.169862000	-4.710311000
C	-1.032140000	3.581349000	-4.068817000
H	-0.465909000	4.305050000	-4.658372000
H	-0.361925000	2.765514000	-3.792918000
C	-4.304803000	3.578450000	0.385238000
H	-4.680453000	4.300572000	1.112236000
H	-3.873053000	2.740388000	0.934649000
H	-5.159676000	3.205384000	-0.182064000
H	-5.575972000	3.035658000	-3.945101000
H	-5.272987000	4.142195000	-2.612123000
H	-4.235879000	4.170772000	-4.040922000
C	4.325450000	4.665932000	1.250737000
C	0.614950000	5.299415000	0.846966000
H	0.034567000	6.169818000	1.159172000
H	1.425254000	5.652431000	0.205781000
H	-0.026948000	4.653616000	0.246539000
H	4.748858000	4.393409000	2.219315000
H	3.755482000	5.587532000	1.381690000
H	5.158573000	4.890407000	0.581612000
C	3.849913000	1.533011000	3.238003000
H	4.147336000	1.220982000	4.240823000
H	4.740482000	1.904845000	2.727842000
H	3.497241000	0.655095000	2.697089000

3Fe_1_7_M6_Co

C	-1.554743000	-4.412943000	-2.288385000
C	-0.955318000	-5.116554000	-1.083994000
H	-0.366087000	-5.978756000	-1.402302000
C	1.347695000	0.057411000	-5.104122000
C	0.776313000	-1.340046000	-5.267988000

C	3.566775000	-0.904401000	-3.490646000
C	4.526214000	-0.863911000	-4.667741000
H	5.282599000	-1.643948000	-4.560480000
C	2.934032000	-4.032061000	0.299249000
C	3.955456000	-3.412439000	-0.636516000
H	4.281556000	-4.139441000	-1.382720000
C	4.495883000	-3.153519000	3.084829000
H	-2.232454000	-5.076418000	-2.834544000
H	-0.769171000	-4.108111000	-2.984630000
H	-0.304583000	-4.440197000	-0.527665000
H	-1.726895000	-5.475298000	-0.399829000
H	-4.143352000	-5.484291000	-1.512090000
H	-2.426487000	-2.115211000	-4.125312000
H	-3.625344000	-3.392492000	-3.942403000
H	1.561487000	-2.098240000	-5.285045000
H	0.095292000	-1.579838000	-4.449412000
H	4.087325000	-0.744884000	-2.543103000
H	3.075353000	-1.876528000	-3.404145000
H	4.015890000	-1.032914000	-5.618027000
H	5.050667000	0.091133000	-4.732461000
H	2.102720000	-4.459580000	-0.267238000
H	3.375291000	-4.842772000	0.886994000
H	3.528602000	-2.554897000	-1.156999000
H	4.840794000	-3.071266000	-0.096797000
H	3.959250000	-3.749893000	3.825261000
H	4.955068000	-3.839885000	2.370505000
H	2.044692000	-4.726226000	2.930454000
H	0.540702000	-4.443922000	2.062754000
P	-2.483097000	-2.892503000	-1.886470000
H	0.550158000	0.804063000	-5.134120000
H	0.223540000	-1.413576000	-6.206280000
H	2.046369000	0.293926000	-5.913026000
P	2.224835000	0.325278000	-3.526648000
P	2.187204000	-2.842044000	1.465040000
C	3.587720000	-2.143780000	2.403674000
H	3.148294000	-1.450398000	3.125393000
H	4.139532000	-1.518382000	1.697240000
H	5.304273000	-2.637822000	3.606729000
H	-5.534422000	-4.794266000	-0.685066000
C	-3.864865000	-3.438289000	-0.828480000
C	-4.720430000	-4.567670000	-1.376622000
C	-3.245428000	-2.469626000	-3.493415000
C	-4.335896000	-1.416828000	-3.398553000
C	1.330049000	-3.951011000	2.636716000
C	0.748124000	-3.262926000	3.857924000
H	-3.413985000	-3.706510000	0.130216000

H	-4.460207000	-2.541177000	-0.637453000
Fe	-1.318754000	-1.171588000	-1.003670000
Fe	0.868038000	0.189399000	-1.728079000
H	2.224402000	2.673250000	-3.824836000
C	3.033486000	1.941452000	-3.759544000
H	3.530187000	1.915431000	-4.735049000
Co	0.942390000	-1.346717000	0.559620000
H	-5.170070000	-4.309873000	-2.337559000
H	-4.681399000	-1.136172000	-4.395293000
H	-5.200069000	-1.780095000	-2.839082000
H	-3.967239000	-0.519266000	-2.900438000
H	0.035663000	-2.490884000	3.564454000
H	0.230613000	-3.987977000	4.489447000
H	1.522397000	-2.787921000	4.463499000
S	-1.173275000	0.274990000	-2.702524000
S	-2.944136000	0.145884000	-0.181336000
S	0.704891000	-2.037799000	-1.562670000
S	-1.091027000	-2.169380000	1.018874000
S	0.664129000	2.388844000	-1.302462000
S	2.500368000	0.069143000	-0.160599000
C	4.007205000	2.317406000	-2.656839000
H	4.425840000	3.306616000	-2.849602000
H	4.838211000	1.612423000	-2.591938000
H	3.511373000	2.343902000	-1.685428000
S	0.750995000	-0.048737000	2.347301000
Co	-1.369803000	1.555048000	-0.900050000
Fe	-1.307424000	0.034301000	1.387561000
Co	0.867566000	1.335078000	0.634842000
P	-2.577484000	3.110220000	-1.763896000
S	-1.071893000	2.270924000	1.198616000
P	-2.511077000	0.108543000	3.306924000
H	-3.555486000	1.799688000	-3.478669000
C	-1.696382000	4.231700000	-2.903671000
H	-2.390670000	5.032159000	-3.177372000
C	-3.309994000	4.272983000	-0.563344000
H	-2.474999000	4.649812000	0.032823000
H	-3.719874000	5.121046000	-1.120153000
H	-4.551015000	1.828024000	-2.047406000
C	-3.987395000	2.469056000	-2.730314000
H	-0.895189000	4.687803000	-2.316418000
H	-3.443655000	2.259794000	3.010478000
H	-4.481928000	1.012845000	2.365535000
C	-3.893009000	1.291707000	3.243274000
C	-3.262228000	-1.501659000	3.726614000
H	-3.671284000	-1.422130000	4.738944000
H	-2.436379000	-2.216215000	3.764317000

C	-1.562494000	0.528294000	4.806201000
H	-0.766695000	-0.217524000	4.877409000
H	-2.230827000	0.373800000	5.659655000
C	-4.879854000	3.515586000	-3.375828000
H	-1.916775000	3.112629000	-4.755485000
C	-1.131694000	3.558403000	-4.141255000
H	-0.600018000	4.285567000	-4.758161000
H	-0.433145000	2.767804000	-3.864164000
C	-4.363261000	3.640176000	0.327892000
H	-4.677765000	4.339677000	1.104780000
H	-3.971347000	2.745111000	0.810919000
H	-5.251516000	3.353651000	-0.238548000
H	-5.694893000	3.032699000	-3.918846000
H	-5.330540000	4.181304000	-2.637214000
H	-4.332587000	4.131642000	-4.091790000
C	-4.753616000	1.363510000	4.493761000
H	-5.559840000	2.085941000	4.351490000
H	-4.179071000	1.684092000	5.364656000
H	-5.215473000	0.402679000	4.729378000
H	-5.186760000	-1.294165000	2.739240000
H	-3.918568000	-1.986413000	1.726164000
C	-4.320795000	-1.958855000	2.739449000
H	-4.671952000	-2.960044000	2.996113000
C	-0.982063000	1.931114000	4.813248000
H	-1.762463000	2.692654000	4.757328000
H	-0.421878000	2.098025000	5.734892000
H	-0.303974000	2.081392000	3.972411000

3Fe_1_9_M1_Fe

6	1.370699000	-0.103466000	-5.252428000
6	0.831603000	-1.524534000	-5.265255000
6	3.710274000	-0.866493000	-3.695056000
6	4.603817000	-0.886527000	-4.923457000
1	5.411404000	-1.610544000	-4.796238000
6	2.939464000	-3.935807000	0.332207000
6	3.945497000	-3.278934000	-0.595986000
1	4.280708000	-3.988253000	-1.354952000
6	4.523154000	-3.178856000	3.130073000
1	1.637620000	-2.261105000	-5.263638000
1	0.202114000	-1.714280000	-4.394158000
1	4.277570000	-0.617987000	-2.793084000
1	3.272596000	-1.850622000	-3.504844000
1	4.050375000	-1.168624000	-5.821218000
1	5.063742000	0.086849000	-5.106218000
1	2.102526000	-4.350393000	-0.235077000
1	3.395773000	-4.760995000	0.887601000

1	3.504094000	-2.419962000	-1.103299000
1	4.827862000	-2.932404000	-0.054274000
1	3.990098000	-3.820927000	3.833605000
1	4.988279000	-3.818150000	2.377409000
1	2.045843000	-4.720583000	2.954139000
1	0.534552000	-4.383354000	2.117921000
1	0.547142000	0.615460000	-5.295873000
1	0.231519000	-1.695026000	-6.160694000
1	2.009666000	0.087324000	-6.120245000
15	2.304932000	0.299280000	-3.735500000
15	2.200985000	-2.793677000	1.547501000
6	3.607853000	-2.138468000	2.506551000
1	3.170798000	-1.489105000	3.268934000
1	4.155587000	-1.479873000	1.828100000
1	5.327178000	-2.688255000	3.682396000
6	1.341771000	-3.924097000	2.693903000
6	0.794965000	-3.253797000	3.941735000
26	-1.325165000	-1.136813000	-0.839996000
26	0.947144000	0.207464000	-1.721440000
1	2.191103000	2.633389000	-4.125066000
6	3.032647000	1.934894000	-4.098330000
1	3.472664000	1.922063000	-5.100083000
27	0.955981000	-1.263041000	0.695620000
1	0.101237000	-2.453472000	3.679694000
1	0.261903000	-3.980624000	4.557540000
1	1.590757000	-2.822200000	4.552277000
16	-1.153370000	0.265013000	-2.610687000
16	-2.938771000	0.238597000	-0.072092000
16	0.678191000	-2.039583000	-1.395654000
16	-1.069979000	-2.131174000	1.154853000
16	0.710403000	2.414495000	-1.225795000
16	2.493575000	0.157262000	-0.047705000
6	4.045734000	2.371363000	-3.052933000
1	4.366229000	3.399447000	-3.232518000
1	4.937062000	1.740902000	-3.068038000
1	3.615262000	2.318074000	-2.051661000
16	0.746569000	0.054623000	2.461334000
27	-1.314592000	1.607101000	-0.813845000
26	-1.316178000	0.123421000	1.559097000
27	0.928285000	1.512689000	0.783339000
15	-2.533516000	3.122873000	-1.725069000
16	-1.080232000	2.339747000	1.261097000
15	-2.726011000	-0.002831000	3.496226000
15	2.116038000	3.068465000	1.670797000
1	-3.510993000	1.746952000	-3.390378000
6	-1.654845000	4.212430000	-2.897163000

1	-2.357434000	4.994564000	-3.201796000
6	-3.266156000	4.320364000	-0.558692000
1	-2.429040000	4.749617000	-0.002198000
1	-3.708253000	5.127834000	-1.150463000
1	-4.497346000	1.816229000	-1.959135000
6	-3.941455000	2.440055000	-2.663473000
1	-0.862367000	4.698035000	-2.321616000
1	-3.586725000	2.196679000	3.321222000
1	-4.598772000	1.043594000	2.494982000
6	-4.075684000	1.225392000	3.438445000
6	-3.532223000	-1.613199000	3.789874000
1	-4.032960000	-1.588673000	4.762665000
1	-2.718881000	-2.341370000	3.865428000
6	-1.830982000	0.318077000	5.057270000
1	-1.044387000	-0.440658000	5.109678000
1	-2.505315000	0.139871000	5.900522000
1	3.065346000	3.874792000	-0.338725000
6	1.226290000	4.613051000	2.070604000
1	0.421851000	4.329150000	2.754025000
1	1.918836000	5.245887000	2.634397000
6	3.510514000	3.584104000	0.615832000
1	4.082307000	2.674687000	0.414234000
1	2.035409000	2.295766000	3.910538000
6	2.861553000	2.632887000	3.279016000
1	3.258017000	3.549800000	3.725530000
6	-4.841910000	3.463390000	-3.334851000
1	-1.852678000	3.035591000	-4.714693000
6	-1.075344000	3.505075000	-4.108690000
1	-0.545215000	4.217694000	-4.743762000
1	-0.372323000	2.727626000	-3.805625000
6	-4.284891000	3.714295000	0.389538000
1	-4.615064000	4.456936000	1.118207000
1	-3.855915000	2.871204000	0.932375000
1	-5.168148000	3.356893000	-0.143039000
1	-5.652387000	2.957513000	-3.863034000
1	-5.298484000	4.144203000	-2.613731000
1	-4.301211000	4.064319000	-4.068587000
6	-5.038507000	1.224922000	4.612818000
1	-5.795331000	2.001971000	4.486019000
1	-4.526900000	1.417328000	5.558129000
1	-5.562410000	0.271563000	4.704695000
1	-5.336346000	-1.323357000	2.610127000
1	-3.989983000	-2.029204000	1.712576000
6	-4.492734000	-2.012998000	2.681431000
1	-4.896268000	-3.009675000	2.868321000
6	-1.223169000	1.709650000	5.121982000

1	-1.991784000	2.485054000	5.125554000
1	-0.631059000	1.827011000	6.031599000
1	-0.572067000	1.887267000	4.263542000
6	4.393396000	4.685954000	1.177319000
6	0.670150000	5.356279000	0.869525000
1	0.099024000	6.227947000	1.194899000
1	1.465016000	5.707098000	0.208397000
1	0.011775000	4.711172000	0.285598000
1	4.837893000	4.405976000	2.134288000
1	3.840455000	5.615564000	1.323872000
1	5.211913000	4.899227000	0.487011000
6	3.931193000	1.560694000	3.181841000
1	4.250831000	1.246639000	4.177199000
1	4.813187000	1.917617000	2.646880000
1	3.550942000	0.686440000	2.653159000

3Fe_1_9_M2

C	-1.629939000	-4.386452000	-2.295874000
C	-1.084905000	-5.136674000	-1.094019000
H	-0.546759000	-6.027817000	-1.422477000
C	3.089006000	-3.863487000	0.279842000
C	4.091650000	-3.135551000	-0.597758000
H	4.552363000	-3.833072000	-1.299526000
C	4.439806000	-3.176517000	3.209438000
H	-2.313764000	-5.016834000	-2.873575000
H	-0.817727000	-4.090616000	-2.964540000
H	-0.394996000	-4.508436000	-0.529395000
H	-1.881243000	-5.458707000	-0.420051000
H	-4.248828000	-5.392400000	-1.517899000
H	-2.462043000	-2.054796000	-4.128156000
H	-3.678818000	-3.318638000	-3.951981000
H	2.311153000	-4.331041000	-0.329369000
H	3.574341000	-4.659935000	0.852806000
H	3.609884000	-2.344050000	-1.173446000
H	4.890802000	-2.682026000	-0.008248000
H	3.887497000	-3.874415000	3.841886000
H	4.988140000	-3.757011000	2.465412000
H	2.031236000	-4.818511000	2.756971000
H	0.560612000	-4.450372000	1.862810000
P	-2.535099000	-2.851092000	-1.899751000
P	2.222184000	-2.800627000	1.481130000
C	3.530027000	-2.143087000	2.567431000
H	3.016015000	-1.543108000	3.322166000
H	4.097367000	-1.437052000	1.956638000
H	5.178157000	-2.679642000	3.842075000

H	-5.610748000	-4.675697000	-0.665012000
C	-3.914469000	-3.357367000	-0.822830000
C	-4.802394000	-4.463798000	-1.367710000
C	-3.286849000	-2.401756000	-3.500568000
C	-4.362628000	-1.335745000	-3.395699000
C	1.328066000	-4.017394000	2.509137000
C	0.704641000	-3.434908000	3.764833000
H	-3.457169000	-3.642482000	0.127786000
H	-4.485343000	-2.447095000	-0.621787000
Fe	-1.241387000	-1.176049000	-0.986243000
Fe	0.980363000	0.209753000	-1.686178000
Co	0.957508000	-1.288981000	0.624488000
H	-5.260096000	-4.188046000	-2.319555000
H	-4.704523000	-1.045261000	-4.390733000
H	-5.230891000	-1.690041000	-2.836775000
H	-3.976694000	-0.447760000	-2.895248000
H	0.038793000	-2.605536000	3.519827000
H	0.124505000	-4.196152000	4.289889000
H	1.462660000	-3.060440000	4.455413000
S	-1.116631000	0.273205000	-2.748659000
S	-2.904316000	0.136636000	-0.199711000
S	0.794105000	-2.104807000	-1.476089000
S	-1.055018000	-2.174204000	1.017421000
S	0.705577000	2.474343000	-1.201971000
S	2.566060000	0.152360000	0.038976000
S	0.665202000	-0.034033000	2.405764000
Co	-1.303190000	1.536511000	-0.884239000
Fe	-1.356588000	0.017094000	1.441179000
Co	0.890381000	1.452902000	0.781199000
P	-2.502598000	3.088560000	-1.769820000
S	-1.141166000	2.225941000	1.207615000
P	-2.505197000	0.069417000	3.300308000
P	2.048689000	3.008059000	1.696308000
H	-3.464981000	1.781370000	-3.493434000
C	-1.616593000	4.215951000	-2.897055000
H	-2.324291000	5.003151000	-3.176097000
C	-3.253761000	4.243195000	-0.571725000
H	-2.431330000	4.623913000	0.038380000
H	-3.655971000	5.089860000	-1.136309000
H	-4.470957000	1.801482000	-2.068341000
C	-3.903810000	2.445361000	-2.745223000
H	-0.830988000	4.684257000	-2.298817000
H	-3.504998000	2.194958000	2.998210000
H	-4.514735000	0.916780000	2.374398000
C	-3.924321000	1.216486000	3.244649000
C	-3.230017000	-1.544206000	3.761999000

H	-3.636841000	-1.462346000	4.774545000
H	-2.393010000	-2.245994000	3.806410000
C	-1.593432000	0.532416000	4.813640000
H	-0.784936000	-0.196050000	4.913540000
H	-2.267039000	0.388251000	5.663752000
H	3.022186000	3.828914000	-0.300272000
C	1.138333000	4.538037000	2.111410000
H	0.323569000	4.231460000	2.772303000
H	1.818778000	5.155137000	2.706754000
C	3.451938000	3.540991000	0.661932000
H	4.036958000	2.638731000	0.467942000
H	1.949732000	2.231418000	3.937751000
C	2.778504000	2.576020000	3.314574000
H	3.154968000	3.501073000	3.761901000
C	-4.793584000	3.494311000	-3.391003000
H	-1.795295000	3.081342000	-4.743385000
C	-1.026700000	3.555278000	-4.129537000
H	-0.521455000	4.299883000	-4.747446000
H	-0.297660000	2.792138000	-3.855509000
C	-4.321712000	3.610349000	0.301464000
H	-4.647800000	4.309359000	1.074003000
H	-3.940276000	2.714311000	0.792161000
H	-5.200956000	3.326053000	-0.279587000
H	-5.606284000	3.010379000	-3.936525000
H	-5.247518000	4.159644000	-2.653986000
H	-4.244336000	4.109514000	-4.105908000
C	-4.779777000	1.283843000	4.498520000
H	-5.606964000	1.981665000	4.353085000
H	-4.208671000	1.632000000	5.361188000
H	-5.213102000	0.314436000	4.752358000
H	-5.170595000	-1.395169000	2.797121000
H	-3.893328000	-2.042815000	1.767265000
C	-4.284519000	-2.032964000	2.785142000
H	-4.603254000	-3.045751000	3.038933000
C	-1.035191000	1.943803000	4.794283000
H	-1.827341000	2.693460000	4.741566000
H	-0.455810000	2.136463000	5.699398000
H	-0.383330000	2.087098000	3.931210000
C	4.310639000	4.650863000	1.245658000
C	0.600867000	5.320805000	0.928007000
H	0.033328000	6.186352000	1.276000000
H	1.405286000	5.685656000	0.286489000
H	-0.052600000	4.699604000	0.314805000
H	4.746880000	4.369973000	2.206222000
H	3.743381000	5.572122000	1.390994000
H	5.134913000	4.879748000	0.567473000

C	3.864203000	1.519317000	3.243479000
H	4.184359000	1.233096000	4.247236000
H	4.742528000	1.877153000	2.703321000
H	3.498755000	0.630444000	2.730954000

3Fe_1_9_M3

C	-1.608168000	-4.388064000	-2.514275000
C	-1.007892000	-5.126315000	-1.328811000
H	-0.403416000	-5.967851000	-1.671863000
C	1.476895000	-0.302867000	-5.092835000
C	0.802447000	-1.662812000	-5.062539000
C	3.691620000	-0.944005000	-3.307636000
C	4.670407000	-1.044399000	-4.465364000
H	5.464645000	-1.752580000	-4.221568000
H	-2.262284000	-5.042956000	-3.098363000
H	-0.816971000	-4.044426000	-3.187668000
H	-0.368777000	-4.469024000	-0.737152000
H	-1.781628000	-5.524045000	-0.668835000
H	-4.194191000	-5.494638000	-1.721357000
H	-2.550804000	-2.048557000	-4.265018000
H	-3.771571000	-3.303902000	-4.093784000
H	1.505758000	-2.461797000	-4.820056000
H	0.006700000	-1.680504000	-4.317059000
H	4.190019000	-0.625369000	-2.388371000
H	3.245376000	-1.914895000	-3.077149000
H	4.188786000	-1.398325000	-5.378807000
H	5.144691000	-0.085812000	-4.684766000
P	-2.546666000	-2.891560000	-2.048321000
H	0.744553000	0.480626000	-5.308414000
H	0.364922000	-1.887929000	-6.037280000
H	2.232677000	-0.258815000	-5.883330000
P	2.293652000	0.204467000	-3.539023000
H	-5.550207000	-4.854222000	-0.799859000
C	-3.894908000	-3.479081000	-0.963971000
C	-4.770421000	-4.590213000	-1.517430000
C	-3.353798000	-2.412024000	-3.616907000
C	-4.410036000	-1.334864000	-3.433615000
H	-3.410003000	-3.780128000	-0.030874000
H	-4.484645000	-2.592040000	-0.714863000
Fe	-1.290317000	-1.117196000	-1.014264000
Fe	0.971346000	0.353886000	-1.805528000
H	2.199315000	2.486202000	-4.168521000
C	3.038631000	1.801303000	-4.018559000
H	3.525467000	1.667837000	-4.989796000
Co	0.969127000	-1.105094000	0.483537000
H	-5.265201000	-4.292862000	-2.444270000

H	-4.779243000	-0.989152000	-4.401188000
H	-5.266714000	-1.703676000	-2.866043000
H	-3.999109000	-0.477947000	-2.897909000
S	-1.085155000	0.388850000	-2.702019000
S	-2.917330000	0.237703000	-0.138630000
S	0.802142000	-1.891289000	-1.605134000
S	-0.951200000	-2.116887000	1.054892000
S	0.659836000	2.516980000	-1.312342000
S	2.528949000	0.345698000	-0.176295000
C	4.006013000	2.360163000	-2.991892000
H	4.358118000	3.347939000	-3.294865000
H	4.880953000	1.718350000	-2.871219000
H	3.521726000	2.452587000	-2.019695000
S	0.815662000	0.118761000	2.342295000
Co	-1.324609000	1.645017000	-0.870760000
Fe	-1.292783000	0.150470000	1.481435000
Co	0.922620000	1.621334000	0.695535000
P	-2.576025000	3.173036000	-1.719865000
S	-1.098728000	2.383866000	1.206089000
P	-2.622919000	0.025261000	3.481529000
P	2.122180000	3.149032000	1.621814000
H	-3.514207000	1.836541000	-3.435794000
C	-1.729950000	4.325219000	-2.855492000
H	-2.452169000	5.102890000	-3.122698000
C	-3.339662000	4.309503000	-0.513340000
H	-2.514245000	4.732301000	0.065229000
H	-3.793653000	5.131308000	-1.075524000
H	-4.508659000	1.831346000	-2.004399000
C	-3.965440000	2.490999000	-2.685790000
H	-0.942397000	4.804835000	-2.268301000
H	-3.568690000	2.190597000	3.305020000
H	-4.586737000	0.985791000	2.565769000
C	-4.016231000	1.206803000	3.472831000
C	-3.363689000	-1.607185000	3.825244000
H	-3.822152000	-1.596622000	4.818726000
H	-2.524825000	-2.308480000	3.865342000
C	-1.677035000	0.393552000	5.001307000
H	-0.868587000	-0.342747000	5.033558000
H	-2.312348000	0.210764000	5.873249000
H	3.023942000	4.043481000	-0.371950000
C	1.221919000	4.669247000	2.085574000
H	0.424847000	4.353311000	2.763541000
H	1.910670000	5.290649000	2.666363000
C	3.491118000	3.717158000	0.560592000
H	4.067552000	2.822655000	0.311160000
H	2.087492000	2.324563000	3.845772000

C	2.901971000	2.660464000	3.198189000
H	3.319686000	3.564513000	3.652200000
C	-4.888564000	3.513116000	-3.327213000
H	-1.918986000	3.212466000	-4.714150000
C	-1.146731000	3.677442000	-4.098209000
H	-0.639342000	4.425392000	-4.710591000
H	-0.422015000	2.906618000	-3.830759000
C	-4.352278000	3.649899000	0.405464000
H	-4.702170000	4.360462000	1.156712000
H	-3.911369000	2.796690000	0.922100000
H	-5.225017000	3.294457000	-0.145655000
H	-5.684079000	3.006565000	-3.877295000
H	-5.364847000	4.156962000	-2.585288000
H	-4.358673000	4.151998000	-4.036122000
C	-4.909589000	1.205709000	4.701253000
H	-5.703355000	1.948570000	4.597097000
H	-4.351962000	1.447941000	5.608184000
H	-5.387818000	0.236002000	4.852800000
H	-5.234858000	-1.385892000	2.738713000
H	-3.900677000	-2.012863000	1.768856000
C	-4.358612000	-2.037289000	2.759581000
H	-4.707630000	-3.054344000	2.947755000
C	-1.107465000	1.802702000	5.021389000
H	-1.896893000	2.556872000	5.038374000
H	-0.487281000	1.952397000	5.907202000
H	-0.493173000	1.983935000	4.137113000
C	4.378890000	4.801153000	1.148743000
C	0.649412000	5.445341000	0.912739000
H	0.070582000	6.299226000	1.270028000
H	1.435945000	5.827799000	0.259199000
H	-0.006010000	4.813557000	0.311068000
H	4.854367000	4.478827000	2.076881000
H	3.821323000	5.716178000	1.356651000
H	5.174389000	5.056400000	0.445915000
C	3.959854000	1.578663000	3.063390000
H	4.332617000	1.291172000	4.047973000
H	4.812690000	1.920829000	2.474008000
H	3.554438000	0.686799000	2.583262000

3Fe_1_9_M4

C	-1.633167000	-4.320495000	-2.291657000
C	-1.012447000	-5.065877000	-1.123841000
H	-0.462712000	-5.939044000	-1.480705000
C	1.436754000	-0.120671000	-5.262765000
C	0.884539000	-1.536752000	-5.262785000
C	3.768588000	-0.870170000	-3.689731000

C	4.662292000	-0.907955000	-4.917442000
H	5.470408000	-1.629676000	-4.780222000
C	2.985685000	-3.918176000	0.280142000
C	4.018683000	-3.240413000	-0.602151000
H	4.379550000	-3.932283000	-1.365481000
C	4.484830000	-3.183902000	3.129096000
H	-2.340578000	-4.958387000	-2.830800000
H	-0.862776000	-4.019780000	-3.006664000
H	-0.318038000	-4.422535000	-0.580773000
H	-1.768376000	-5.415253000	-0.417713000
H	-4.250485000	-5.326618000	-1.523404000
H	-2.497956000	-2.053957000	-4.094386000
H	-3.765788000	-3.244574000	-3.829195000
H	1.682636000	-2.281956000	-5.252723000
H	0.257142000	-1.708401000	-4.386050000
H	4.337156000	-0.608935000	-2.792085000
H	3.330675000	-1.851309000	-3.484745000
H	4.109031000	-1.202594000	-5.811356000
H	5.121669000	0.062845000	-5.114236000
H	2.172812000	-4.327763000	-0.324667000
H	3.426565000	-4.750762000	0.836827000
H	3.590955000	-2.371878000	-1.104235000
H	4.882761000	-2.903869000	-0.025967000
H	3.940464000	-3.837793000	3.812901000
H	4.975392000	-3.811266000	2.382536000
H	2.034578000	-4.751997000	2.858568000
H	0.539267000	-4.416612000	1.992921000
P	-2.519300000	-2.786764000	-1.839219000
H	0.619696000	0.604426000	-5.318969000
H	0.281321000	-1.710261000	-6.155941000
H	2.081179000	0.053534000	-6.129820000
P	2.363311000	0.295419000	-3.743830000
P	2.201830000	-2.799641000	1.489592000
C	3.576519000	-2.144984000	2.493388000
H	3.112940000	-1.508611000	3.250964000
H	4.136047000	-1.473308000	1.837706000
H	5.269712000	-2.691230000	3.706526000
H	-5.573255000	-4.644658000	-0.585323000
C	-3.878347000	-3.326233000	-0.749751000
C	-4.792199000	-4.403468000	-1.309046000
C	-3.312673000	-2.335464000	-3.421195000
C	-4.333695000	-1.216291000	-3.321080000
C	1.327554000	-3.958973000	2.595959000
C	0.741912000	-3.319146000	3.842211000
H	-3.400335000	-3.650347000	0.177854000
H	-4.436509000	-2.420708000	-0.498241000

Fe	-1.272483000	-1.226252000	-0.980160000
Fe	0.998323000	0.242582000	-1.762326000
H	2.244970000	2.621118000	-4.165445000
C	3.089851000	1.927313000	-4.122128000
H	3.540396000	1.905790000	-5.119041000
Co	0.962452000	-1.270792000	0.622083000
H	-5.286576000	-4.082129000	-2.227505000
H	-4.745018000	-0.992531000	-4.306989000
H	-5.166577000	-1.486334000	-2.668757000
H	-3.881230000	-0.304458000	-2.928885000
H	0.041335000	-2.525426000	3.579243000
H	0.207796000	-4.065193000	4.433790000
H	1.516732000	-2.885087000	4.477193000
S	-1.080368000	0.260082000	-2.694840000
S	-2.927466000	0.109450000	-0.193225000
S	0.771929000	-2.003761000	-1.486267000
S	-1.040371000	-2.177093000	1.028931000
S	0.696477000	2.455549000	-1.243934000
S	2.510490000	0.177423000	-0.054844000
C	4.090563000	2.380647000	-3.071598000
H	4.413823000	3.405247000	-3.264809000
H	4.981467000	1.749248000	-3.064479000
H	3.648189000	2.345807000	-2.074387000
S	0.720880000	0.002020000	2.417664000
Co	-1.281129000	1.497589000	-0.842779000
Fe	-1.352570000	0.028353000	1.508018000
Co	0.902663000	1.488959000	0.767718000
S	-1.144851000	2.277064000	1.232296000
P	-2.701725000	-0.025544000	3.493754000
P	2.066570000	3.051895000	1.689901000
H	-3.654295000	2.106742000	3.098628000
H	-4.662296000	0.834510000	2.476300000
C	-4.099472000	1.142928000	3.362318000
C	-3.438943000	-1.637230000	3.936153000
H	-3.904740000	-1.566758000	4.923817000
H	-2.598288000	-2.332072000	4.026345000
C	-1.802070000	0.443054000	5.014637000
H	-0.995471000	-0.289022000	5.118485000
H	-2.465661000	0.313156000	5.875021000
H	3.004010000	3.908885000	-0.305625000
C	1.156288000	4.574332000	2.123737000
H	0.346214000	4.264783000	2.789542000
H	1.839235000	5.190155000	2.717766000
C	3.453118000	3.606205000	0.643491000
H	4.039671000	2.710273000	0.424622000
H	2.002362000	2.239461000	3.917166000

C	2.822600000	2.593953000	3.287551000
H	3.211809000	3.507334000	3.747438000
C	-4.997599000	1.259055000	4.581633000
H	-5.801375000	1.974535000	4.396151000
H	-4.446797000	1.606218000	5.458155000
H	-5.462621000	0.304316000	4.836058000
H	-5.309629000	-1.499158000	2.839407000
H	-3.962086000	-2.147942000	1.903612000
C	-4.423765000	-2.135070000	2.892104000
H	-4.756973000	-3.147933000	3.126246000
C	-1.228172000	1.849560000	4.970112000
H	-2.013834000	2.605673000	4.913037000
H	-0.640059000	2.050811000	5.867726000
H	-0.580605000	1.974365000	4.100263000
C	4.318589000	4.711895000	1.224758000
C	0.611866000	5.357661000	0.942826000
H	0.064397000	6.233824000	1.294885000
H	1.412088000	5.708582000	0.288239000
H	-0.069390000	4.751538000	0.344409000
H	4.772594000	4.419681000	2.173601000
H	3.748980000	5.627541000	1.392976000
H	5.129628000	4.954715000	0.535388000
C	3.902052000	1.534107000	3.170136000
H	4.235293000	1.214485000	4.159345000
H	4.774849000	1.904316000	2.629129000
H	3.525087000	0.660871000	2.637783000

3Fe_1_9_M5_Fe

C	-1.595718000	-4.443705000	-2.509226000
C	-1.072827000	-5.180430000	-1.286222000
H	-0.424012000	-6.005960000	-1.585240000
C	1.317531000	-0.174631000	-5.163122000
C	0.742964000	-1.580567000	-5.120200000
C	3.656336000	-0.904509000	-3.593436000
C	4.521014000	-0.996651000	-4.838734000
H	5.330470000	-1.714324000	-4.689084000
C	2.965431000	-3.932502000	0.437658000
C	4.007417000	-3.285405000	-0.457204000
H	4.356464000	-3.994932000	-1.209766000
C	4.469891000	-3.139319000	3.264046000
H	-2.202429000	-5.101518000	-3.138827000
H	-0.761661000	-4.088153000	-3.121487000
H	-0.498978000	-4.507595000	-0.646074000
H	-1.886329000	-5.598246000	-0.689830000
H	-4.235861000	-5.548008000	-1.872266000
H	-2.466319000	-2.095905000	-4.298256000

H	-3.697880000	-3.350139000	-4.196820000
H	1.528784000	-2.338166000	-5.090661000
H	0.117626000	-1.713405000	-4.235358000
H	4.245155000	-0.614104000	-2.718165000
H	3.213378000	-1.871964000	-3.340275000
H	3.946626000	-1.328391000	-5.705932000
H	4.978056000	-0.036771000	-5.087961000
H	2.150100000	-4.351205000	-0.157717000
H	3.398159000	-4.753682000	1.017191000
H	3.592358000	-2.418355000	-0.972840000
H	4.877323000	-2.953754000	0.112960000
H	3.923397000	-3.774359000	3.963612000
H	4.954939000	-3.786126000	2.530539000
H	2.007964000	-4.699289000	3.026269000
H	0.514027000	-4.376103000	2.155477000
P	-2.568497000	-2.953150000	-2.089984000
H	0.510721000	0.560579000	-5.234639000
H	0.132729000	-1.770713000	-6.005311000
H	1.960823000	-0.034543000	-6.037196000
P	2.259369000	0.269112000	-3.661439000
P	2.186271000	-2.780222000	1.618883000
C	3.565386000	-2.110154000	2.607352000
H	3.105447000	-1.456796000	3.352562000
H	4.127372000	-1.455039000	1.937108000
H	5.258806000	-2.638014000	3.828409000
H	-5.623873000	-4.921823000	-0.988617000
C	-3.961823000	-3.545875000	-1.069768000
C	-4.818361000	-4.646364000	-1.672449000
C	-3.299632000	-2.464504000	-3.692576000
C	-4.361097000	-1.385337000	-3.547929000
C	1.303669000	-3.908378000	2.749163000
C	0.723401000	-3.242018000	3.983654000
H	-3.517433000	-3.857371000	-0.119996000
H	-4.556238000	-2.658878000	-0.831844000
Fe	-1.315845000	-1.201082000	-0.934100000
Fe	0.935616000	0.213785000	-1.672125000
H	2.152799000	2.586028000	-4.138895000
C	2.992338000	1.886111000	-4.089677000
H	3.428472000	1.835193000	-5.092007000
Co	0.964705000	-1.258406000	0.714939000
H	-5.278499000	-4.332419000	-2.611627000
H	-4.694052000	-1.039587000	-4.528483000
H	-5.238191000	-1.752740000	-3.011770000
H	-3.968365000	-0.527476000	-2.999395000
H	0.013647000	-2.459336000	3.713178000
H	0.197985000	-3.977652000	4.595257000

H	1.500934000	-2.791371000	4.603687000
S	-1.124455000	0.352326000	-2.623128000
S	-2.922355000	0.197748000	-0.102231000
S	0.798280000	-2.033114000	-1.364722000
S	-1.075048000	-2.143428000	1.123289000
S	0.710689000	2.433437000	-1.188862000
S	2.498566000	0.173180000	-0.002804000
C	4.010559000	2.357259000	-3.064899000
H	4.337271000	3.375235000	-3.285706000
H	4.897480000	1.720489000	-3.056450000
H	3.581038000	2.346798000	-2.061771000
S	0.689947000	0.063412000	2.485527000
Co	-1.308852000	1.613478000	-0.794883000
Fe	-1.316586000	0.071948000	1.481331000
Co	0.933895000	1.523292000	0.805674000
P	-2.559540000	3.156565000	-1.611489000
S	-1.092237000	2.295049000	1.308740000
P	2.106320000	3.085830000	1.690390000
H	-3.449903000	1.889227000	-3.403518000
C	-1.688514000	4.345794000	-2.689438000
H	-2.395753000	5.144475000	-2.933900000
C	-3.354827000	4.245722000	-0.383138000
H	-2.543915000	4.683401000	0.204990000
H	-3.828651000	5.064190000	-0.934336000
H	-4.469392000	1.802515000	-1.992182000
C	-3.923215000	2.500709000	-2.631396000
H	-0.902365000	4.789275000	-2.073089000
H	3.058120000	3.880741000	-0.323763000
C	1.204998000	4.624871000	2.081321000
H	0.410000000	4.339396000	2.774839000
H	1.897819000	5.267707000	2.633398000
C	3.500941000	3.602156000	0.635539000
H	4.081315000	2.695731000	0.444962000
H	2.015070000	2.319141000	3.929245000
C	2.844612000	2.654873000	3.301707000
H	3.237339000	3.574317000	3.746448000
C	-4.850032000	3.540395000	-3.238485000
H	-1.871387000	3.327664000	-4.601198000
C	-1.097891000	3.737839000	-3.949040000
H	-0.554013000	4.496098000	-4.515682000
H	-0.405233000	2.931565000	-3.702781000
C	-4.355051000	3.548565000	0.521917000
H	-4.761776000	4.255258000	1.247404000
H	-3.887305000	2.731094000	1.072672000
H	-5.192922000	3.136722000	-0.043898000
H	-5.622211000	3.050308000	-3.834814000

H	-5.356467000	4.132781000	-2.474273000
H	-4.316332000	4.226812000	-3.898671000
C	4.372525000	4.716798000	1.189581000
C	0.631525000	5.354130000	0.880210000
H	0.076003000	6.236552000	1.203428000
H	1.414525000	5.685579000	0.195257000
H	-0.046476000	4.705621000	0.323538000
H	4.812882000	4.451534000	2.152579000
H	3.811837000	5.643994000	1.321156000
H	5.193731000	4.927573000	0.501690000
C	3.916919000	1.584895000	3.212897000
H	4.236792000	1.279980000	4.210927000
H	4.798407000	1.939233000	2.675172000
H	3.538426000	0.705345000	2.692065000

3Fe_1_9_M6_Co

C	-1.595103000	-4.386262000	-2.397237000
C	-1.062370000	-5.142344000	-1.191338000
H	-0.441338000	-5.980693000	-1.512848000
C	1.334641000	-0.167723000	-5.239203000
C	0.739282000	-1.565676000	-5.194591000
C	3.671177000	-0.897900000	-3.661694000
C	4.560489000	-0.949922000	-4.891746000
H	5.372344000	-1.665879000	-4.746552000
C	3.031366000	-3.949253000	0.426276000
C	4.051390000	-3.306290000	-0.496567000
H	4.403388000	-4.028837000	-1.235202000
C	4.550398000	-3.065630000	3.236744000
H	-2.223666000	-5.030491000	-3.019801000
H	-0.768386000	-4.038069000	-3.022727000
H	-0.456529000	-4.489447000	-0.560440000
H	-1.871114000	-5.545936000	-0.578601000
H	-4.204453000	-5.495881000	-1.729875000
H	-2.470819000	-2.024669000	-4.170074000
H	-3.687372000	-3.293909000	-4.060762000
H	1.514433000	-2.334095000	-5.160531000
H	0.110240000	-1.687870000	-4.310121000
H	4.240172000	-0.621435000	-2.769077000
H	3.236824000	-1.877035000	-3.439096000
H	4.005813000	-1.260218000	-5.779597000
H	5.015061000	0.019956000	-5.103614000
H	2.211906000	-4.387845000	-0.149530000
H	3.482627000	-4.755723000	1.012517000
H	3.615924000	-2.459005000	-1.027949000
H	4.921693000	-2.946085000	0.055090000
H	4.018989000	-3.686166000	3.960936000

H	5.035537000	-3.728933000	2.517931000
H	2.119535000	-4.681325000	3.054098000
H	0.627787000	-4.423320000	2.158149000
P	-2.552447000	-2.889473000	-1.965346000
H	0.537280000	0.577621000	-5.317217000
H	0.127385000	-1.751524000	-6.079542000
H	1.981878000	-0.038126000	-6.111788000
P	2.262137000	0.262016000	-3.724130000
P	2.252663000	-2.788060000	1.598270000
C	3.626596000	-2.068087000	2.558534000
H	3.165041000	-1.393138000	3.283874000
H	4.170536000	-1.422600000	1.864195000
H	5.338957000	-2.538082000	3.776720000
H	-5.598493000	-4.868750000	-0.857169000
C	-3.941969000	-3.485956000	-0.942344000
C	-4.791289000	-4.595156000	-1.539953000
C	-3.297457000	-2.401747000	-3.561242000
C	-4.371792000	-1.336852000	-3.413717000
C	1.396596000	-3.918221000	2.749233000
C	0.780076000	-3.242981000	3.960642000
H	-3.494621000	-3.792945000	0.007378000
H	-4.544627000	-2.602357000	-0.713106000
Fe	-1.230735000	-1.163691000	-0.952958000
Fe	0.971938000	0.229762000	-1.669793000
H	2.129202000	2.584563000	-4.169623000
C	2.978191000	1.896860000	-4.110580000
H	3.435161000	1.864876000	-5.104661000
Co	0.979662000	-1.314113000	0.702269000
H	-5.249225000	-4.290783000	-2.483209000
H	-4.706641000	-0.991834000	-4.393823000
H	-5.245724000	-1.716567000	-2.880839000
H	-3.990377000	-0.476432000	-2.861712000
H	0.060340000	-2.481714000	3.654969000
H	0.261896000	-3.977263000	4.580709000
H	1.534809000	-2.757025000	4.581979000
S	-1.133027000	0.348075000	-2.625520000
S	-2.911438000	0.148997000	-0.083671000
S	0.810637000	-2.051984000	-1.395001000
S	-1.056735000	-2.162467000	1.105036000
S	0.684473000	2.425984000	-1.203214000
S	2.536058000	0.105366000	-0.038205000
C	3.967798000	2.372784000	-3.059255000
H	4.310601000	3.383504000	-3.287457000
H	4.847997000	1.728284000	-3.014063000
H	3.510002000	2.387290000	-2.068223000
S	0.743311000	0.005385000	2.466797000

Co	-1.344352000	1.593498000	-0.791752000
Fe	-1.287105000	0.045702000	1.479683000
Co	0.865577000	1.359354000	0.731057000
P	-2.524781000	3.155408000	-1.679268000
S	-1.060687000	2.283320000	1.307834000
P	-2.560111000	0.067982000	3.340950000
H	-3.520025000	1.833571000	-3.375218000
C	-1.639458000	4.260229000	-2.830614000
H	-2.331829000	5.064261000	-3.099343000
C	-3.242688000	4.331471000	-0.482522000
H	-2.402307000	4.706698000	0.106968000
H	-3.648641000	5.178550000	-1.043699000
H	-4.507463000	1.882631000	-1.939381000
C	-3.942940000	2.513195000	-2.631227000
H	-0.830433000	4.712711000	-2.251571000
H	-3.472026000	2.230477000	3.067703000
H	-4.487261000	1.007117000	2.343060000
C	-3.933571000	1.257697000	3.251354000
C	-3.324409000	-1.550909000	3.690798000
H	-3.768293000	-1.488533000	4.689718000
H	-2.500144000	-2.266188000	3.745095000
C	-1.659371000	0.450853000	4.877859000
H	-0.856221000	-0.287026000	4.947485000
H	-2.352226000	0.258245000	5.703786000
C	-4.830794000	3.560890000	-3.281660000
H	-1.885701000	3.140033000	-4.678431000
C	-1.091554000	3.581521000	-4.072772000
H	-0.563663000	4.306718000	-4.695167000
H	-0.393561000	2.787640000	-3.804652000
C	-4.297450000	3.711945000	0.415855000
H	-4.597907000	4.414625000	1.195325000
H	-3.912276000	2.812116000	0.896073000
H	-5.192888000	3.436532000	-0.144640000
H	-5.654123000	3.078748000	-3.812597000
H	-5.269834000	4.239596000	-2.547835000
H	-4.283456000	4.163132000	-4.009128000
C	-4.844226000	1.293366000	4.467790000
H	-5.636702000	2.029052000	4.317226000
H	-4.304490000	1.576809000	5.373113000
H	-5.324624000	0.329863000	4.648494000
H	-5.205600000	-1.313651000	2.628612000
H	-3.907770000	-2.021231000	1.664159000
C	-4.349073000	-1.989705000	2.660642000
H	-4.722572000	-2.986594000	2.901696000
C	-1.101204000	1.860503000	4.949327000
H	-1.891943000	2.612042000	4.908134000

H	-0.561520000	1.999185000	5.887565000
H	-0.409056000	2.052949000	4.128734000

3Fe_1_11_M1_Fe

C	1.429922000	-0.202044000	-5.281023000
C	0.888572000	-1.622074000	-5.263705000
C	3.729651000	-0.859844000	-3.619892000
C	4.661883000	-0.894512000	-4.818553000
H	5.484893000	-1.590243000	-4.641455000
C	2.934861000	-3.956115000	0.347570000
C	3.976823000	-3.325587000	-0.558903000
H	4.311519000	-4.045245000	-1.308217000
C	4.503189000	-3.137070000	3.128084000
H	1.690741000	-2.360316000	-5.201031000
H	0.223697000	-1.777314000	-4.412283000
H	4.260273000	-0.568125000	-2.708644000
H	3.309882000	-1.847948000	-3.411121000
H	4.145467000	-1.223178000	-5.722458000
H	5.100326000	0.084822000	-5.021740000
H	2.108282000	-4.366034000	-0.237424000
H	3.362854000	-4.778945000	0.928585000
H	3.563022000	-2.461273000	-1.079574000
H	4.854912000	-2.998900000	0.001576000
H	3.971600000	-3.756665000	3.852416000
H	4.962826000	-3.799451000	2.392306000
H	2.050729000	-4.684091000	2.974338000
H	0.527576000	-4.376754000	2.146263000
H	0.608553000	0.513604000	-5.383598000
H	0.324570000	-1.824630000	-6.175816000
H	2.104498000	-0.041931000	-6.127777000
P	2.293492000	0.261234000	-3.741314000
P	2.184220000	-2.790266000	1.532474000
C	3.588046000	-2.111414000	2.480098000
H	3.148401000	-1.448595000	3.228872000
H	4.137474000	-1.466959000	1.789715000
H	5.311160000	-2.632818000	3.662067000
C	1.335379000	-3.900181000	2.706363000
C	0.793446000	-3.214159000	3.947073000
Fe	-1.317546000	-1.135112000	-0.941441000
Fe	0.943044000	0.212853000	-1.739414000
H	2.126203000	2.585617000	-4.177512000
C	2.984302000	1.909238000	-4.123909000
H	3.438424000	1.887572000	-5.119301000
Co	0.937640000	-1.280119000	0.642546000
H	0.077433000	-2.437697000	3.674538000
H	0.284534000	-3.939228000	4.585132000

H	1.587922000	-2.753296000	4.537794000
S	-1.128260000	0.376074000	-2.726973000
S	-3.004556000	0.280753000	-0.102757000
S	0.780577000	-2.058958000	-1.471180000
S	-1.076918000	-2.181060000	1.140581000
S	0.690455000	2.412576000	-1.243182000
S	2.486077000	0.139339000	-0.071888000
C	3.971925000	2.390838000	-3.074790000
H	4.257582000	3.428093000	-3.260654000
H	4.884579000	1.791583000	-3.076773000
H	3.534068000	2.330262000	-2.077348000
S	0.711713000	0.027389000	2.407591000
Co	-1.332310000	1.601779000	-0.845709000
Fe	-1.365216000	0.065263000	1.488667000
Co	0.923848000	1.495503000	0.758726000
P	-2.545417000	3.143775000	-1.710981000
S	-1.087108000	2.297437000	1.239730000
P	-2.720800000	-0.018655000	3.472471000
P	2.100386000	3.048761000	1.645671000
H	-3.497943000	1.831827000	-3.438820000
C	-1.659010000	4.290630000	-2.822151000
H	-2.361676000	5.090379000	-3.076869000
C	-3.287591000	4.297177000	-0.505655000
H	-2.453120000	4.709061000	0.067700000
H	-3.722938000	5.123226000	-1.076600000
H	-4.501583000	1.843095000	-2.015105000
C	-3.939484000	2.493279000	-2.689665000
H	-0.867338000	4.741434000	-2.217824000
H	-3.568144000	2.187022000	3.308769000
H	-4.620001000	1.035949000	2.532068000
C	-4.060649000	1.221306000	3.453433000
C	-3.530331000	-1.621835000	3.791664000
H	-4.011209000	-1.590511000	4.774256000
H	-2.719455000	-2.353975000	3.851014000
C	-1.781329000	0.299670000	5.008350000
H	-0.991201000	-0.456311000	5.037011000
H	-2.432161000	0.116353000	5.868729000
H	3.046996000	3.855513000	-0.364615000
C	1.204224000	4.588592000	2.046328000
H	0.409135000	4.302861000	2.739654000
H	1.901285000	5.225087000	2.600551000
C	3.492462000	3.565838000	0.589894000
H	4.067569000	2.658509000	0.388579000
H	2.016273000	2.268536000	3.882431000
C	2.842316000	2.610963000	3.253939000
H	3.232051000	3.529932000	3.702279000

C	-4.833088000	3.543035000	-3.329129000
H	-1.859590000	3.229005000	-4.707398000
C	-1.081047000	3.660856000	-4.075841000
H	-0.553679000	4.413774000	-4.665060000
H	-0.380783000	2.863758000	-3.824566000
C	-4.315261000	3.671685000	0.418990000
H	-4.656362000	4.402764000	1.154555000
H	-3.892412000	2.819281000	0.950816000
H	-5.190582000	3.320089000	-0.130258000
H	-5.634899000	3.057692000	-3.888829000
H	-5.301843000	4.190950000	-2.585862000
H	-4.284903000	4.175623000	-4.029951000
C	-4.976181000	1.239996000	4.665054000
H	-5.732408000	2.020792000	4.559369000
H	-4.426654000	1.439499000	5.587338000
H	-5.502136000	0.291311000	4.788096000
H	-5.354395000	-1.321666000	2.645256000
H	-4.028945000	-2.038620000	1.725270000
C	-4.514639000	-2.017267000	2.702764000
H	-4.921405000	-3.010737000	2.899208000
C	-1.177855000	1.693500000	5.063170000
H	-1.949091000	2.465853000	5.089584000
H	-0.562467000	1.809793000	5.957445000
H	-0.550808000	1.877418000	4.188408000
C	4.370506000	4.671327000	1.152608000
C	0.632230000	5.326815000	0.850218000
H	0.069543000	6.202193000	1.180113000
H	1.417077000	5.670828000	0.173823000
H	-0.039021000	4.680389000	0.282665000
H	4.813843000	4.394661000	2.111004000
H	3.814546000	5.599680000	1.295248000
H	5.189650000	4.884948000	0.463297000
C	3.918126000	1.545710000	3.155735000
H	4.235790000	1.228536000	4.150635000
H	4.800060000	1.909462000	2.625440000
H	3.543596000	0.672655000	2.621591000

3Fe_1_11_M5_Fe

C	-1.632906000	-4.454791000	-2.545085000
C	-1.073513000	-5.170409000	-1.325924000
H	-0.434155000	-6.000334000	-1.632470000
C	1.374787000	-0.246069000	-5.181112000
C	0.787270000	-1.646188000	-5.122233000
C	3.701685000	-0.891528000	-3.550181000
C	4.600537000	-0.967900000	-4.772100000
H	5.425624000	-1.660900000	-4.594358000

C	2.966052000	-3.975792000	0.461012000
C	4.033920000	-3.362757000	-0.427621000
H	4.374462000	-4.088849000	-1.168186000
C	4.485516000	-3.105862000	3.257458000
H	-2.263270000	-5.120063000	-3.143144000
H	-0.819846000	-4.110095000	-3.190592000
H	-0.481944000	-4.485897000	-0.715278000
H	-1.868728000	-5.578487000	-0.699002000
H	-4.292928000	-5.521848000	-1.825600000
H	-2.514722000	-2.102216000	-4.329678000
H	-3.769299000	-3.332893000	-4.201704000
H	1.564044000	-2.409837000	-5.044883000
H	0.129018000	-1.750320000	-4.257583000
H	4.257432000	-0.577338000	-2.661767000
H	3.277942000	-1.868092000	-3.299420000
H	4.059034000	-1.323937000	-5.650619000
H	5.036820000	0.002314000	-5.018880000
H	2.152155000	-4.389357000	-0.139583000
H	3.374927000	-4.794566000	1.061118000
H	3.642426000	-2.494212000	-0.958729000
H	4.904719000	-3.046586000	0.149803000
H	3.941834000	-3.703008000	3.991564000
H	4.951587000	-3.790163000	2.546045000
H	2.043459000	-4.664504000	3.075608000
H	0.528972000	-4.369842000	2.227713000
P	-2.593832000	-2.960619000	-2.124207000
H	0.576054000	0.492925000	-5.293185000
H	0.207259000	-1.852836000	-6.023865000
H	2.045422000	-0.131431000	-6.038142000
P	2.272901000	0.237035000	-3.666850000
P	2.193130000	-2.790015000	1.613879000
C	3.583042000	-2.094693000	2.570367000
H	3.131478000	-1.415109000	3.296746000
H	4.145579000	-1.465939000	1.875901000
H	5.288630000	-2.590264000	3.787962000
H	-5.646317000	-4.856256000	-0.917811000
C	-3.963750000	-3.514465000	-1.055708000
C	-4.853225000	-4.606410000	-1.625362000
C	-3.344112000	-2.453268000	-3.708747000
C	-4.380580000	-1.353362000	-3.542540000
C	1.329721000	-3.884672000	2.791051000
C	0.772272000	-3.186394000	4.018184000
H	-3.495971000	-3.821944000	-0.116175000
H	-4.534763000	-2.613688000	-0.813072000
Fe	-1.285306000	-1.209436000	-1.028476000
Fe	0.954111000	0.224123000	-1.671457000

H	2.100190000	2.549951000	-4.146306000
C	2.959053000	1.874620000	-4.092566000
H	3.397901000	1.830627000	-5.094175000
Co	0.970256000	-1.284351000	0.670061000
H	-5.330686000	-4.295650000	-2.556834000
H	-4.726140000	-1.003866000	-4.517196000
H	-5.253222000	-1.702768000	-2.987460000
H	-3.958726000	-0.503059000	-3.004114000
H	0.043582000	-2.425155000	3.737897000
H	0.272180000	-3.909678000	4.664933000
H	1.558410000	-2.706930000	4.605152000
S	-1.081037000	0.427164000	-2.735202000
S	-2.987937000	0.224770000	-0.122064000
S	0.896082000	-2.056698000	-1.437572000
S	-1.060605000	-2.208183000	1.138176000
S	0.694239000	2.421655000	-1.213923000
S	2.511258000	0.146131000	-0.023833000
C	3.963350000	2.374575000	-3.068386000
H	4.252762000	3.404806000	-3.284194000
H	4.871999000	1.769332000	-3.067552000
H	3.537973000	2.342441000	-2.064164000
S	0.670953000	0.033300000	2.431323000
Co	-1.319128000	1.592387000	-0.835646000
Fe	-1.345602000	0.005719000	1.409840000
Co	0.936279000	1.489109000	0.772256000
P	-2.574247000	3.153755000	-1.608892000
S	-1.090498000	2.237666000	1.274391000
P	2.096060000	3.057491000	1.668048000
H	-3.458184000	1.934072000	-3.434783000
C	-1.703186000	4.385531000	-2.639504000
H	-2.411289000	5.195800000	-2.839580000
C	-3.366178000	4.213813000	-0.351403000
H	-2.550747000	4.637658000	0.240812000
H	-3.836169000	5.045514000	-0.886167000
H	-4.484864000	1.818124000	-2.027746000
C	-3.933769000	2.527486000	-2.650046000
H	-0.915493000	4.799996000	-2.004963000
H	3.049897000	3.863568000	-0.340704000
C	1.183440000	4.589946000	2.058297000
H	0.393181000	4.299917000	2.755283000
H	1.874266000	5.238042000	2.606763000
C	3.491094000	3.583839000	0.618892000
H	4.076931000	2.681129000	0.427314000
H	2.001638000	2.284912000	3.905212000
C	2.830276000	2.630764000	3.282056000
H	3.210380000	3.553912000	3.730105000

C	-4.853719000	3.586684000	-3.234060000
H	-1.896637000	3.475653000	-4.602964000
C	-1.118683000	3.843826000	-3.931363000
H	-0.571530000	4.629526000	-4.456038000
H	-0.434996000	3.017268000	-3.733578000
C	-4.368670000	3.512098000	0.546503000
H	-4.769226000	4.214706000	1.279621000
H	-3.907449000	2.683062000	1.084303000
H	-5.209867000	3.112220000	-0.022946000
H	-5.627945000	3.114855000	-3.842338000
H	-5.357972000	4.163177000	-2.456394000
H	-4.316055000	4.285810000	-3.877507000
C	4.355140000	4.701479000	1.178957000
C	0.600488000	5.313910000	0.858948000
H	0.046160000	6.196775000	1.182913000
H	1.377574000	5.643684000	0.166488000
H	-0.081750000	4.662434000	0.311017000
H	4.793499000	4.436409000	2.142922000
H	3.789366000	5.625567000	1.310243000
H	5.177640000	4.917620000	0.494304000
C	3.914765000	1.573339000	3.195202000
H	4.231655000	1.266674000	4.193599000
H	4.795722000	1.939634000	2.664769000
H	3.549016000	0.692920000	2.667242000

3Fe_1_11_M6_Co

C	-1.663018000	-4.394217000	-2.398440000
C	-1.117835000	-5.151516000	-1.198537000
H	-0.503608000	-5.992807000	-1.525636000
C	1.351219000	-0.202437000	-5.272971000
C	0.758075000	-1.601063000	-5.216038000
C	3.704813000	-0.928353000	-3.719544000
C	4.574561000	-0.994867000	-4.962971000
H	5.388000000	-1.709998000	-4.822896000
C	3.089372000	-3.903648000	0.415509000
C	4.091421000	-3.259856000	-0.525818000
H	4.441377000	-3.986236000	-1.261614000
C	4.637060000	-2.991218000	3.205972000
H	-2.294350000	-5.039151000	-3.017317000
H	-0.841158000	-4.045972000	-3.031051000
H	-0.502881000	-4.500645000	-0.574294000
H	-1.920764000	-5.551946000	-0.576004000
H	-4.281598000	-5.493843000	-1.734517000
H	-2.520591000	-2.043120000	-4.164503000
H	-3.756737000	-3.291337000	-4.050563000
H	1.534659000	-2.368177000	-5.184984000

H	0.135601000	-1.720526000	-4.326688000
H	4.289363000	-0.644230000	-2.839373000
H	3.272554000	-1.904683000	-3.481166000
H	4.005309000	-1.314479000	-5.838147000
H	5.026420000	-0.027834000	-5.192763000
H	2.264610000	-4.351886000	-0.145047000
H	3.554832000	-4.702975000	1.000456000
H	3.641323000	-2.422371000	-1.060694000
H	4.964994000	-2.885838000	0.011356000
H	4.117993000	-3.608180000	3.941895000
H	5.117269000	-3.657660000	2.486739000
H	2.220908000	-4.622274000	3.060385000
H	0.715468000	-4.387162000	2.181603000
P	-2.610733000	-2.892924000	-1.953765000
H	0.552053000	0.541697000	-5.344224000
H	0.139550000	-1.792073000	-6.095209000
H	1.987299000	-0.075298000	-6.154028000
P	2.297714000	0.234815000	-3.771767000
P	2.319630000	-2.742053000	1.592378000
C	3.699395000	-2.004541000	2.530672000
H	3.241435000	-1.327532000	3.256458000
H	4.231849000	-1.360958000	1.825888000
H	5.428916000	-2.454173000	3.731476000
H	-5.670165000	-4.865329000	-0.853851000
C	-4.004964000	-3.491110000	-0.935499000
C	-4.863105000	-4.591295000	-1.536687000
C	-3.352465000	-2.404725000	-3.552712000
C	-4.409036000	-1.321235000	-3.410630000
C	1.485071000	-3.869432000	2.760626000
C	0.876057000	-3.193421000	3.975652000
H	-3.560238000	-3.807222000	0.012742000
H	-4.602512000	-2.605850000	-0.698121000
Fe	-1.227148000	-1.146371000	-0.934316000
Fe	1.011697000	0.229953000	-1.699025000
H	2.167565000	2.555911000	-4.228774000
C	3.014438000	1.864875000	-4.178621000
H	3.455775000	1.825841000	-5.179426000
Co	1.030172000	-1.279825000	0.695229000
H	-5.321515000	-4.278072000	-2.476865000
H	-4.745836000	-0.981285000	-4.391954000
H	-5.285211000	-1.681919000	-2.868044000
H	-4.011539000	-0.460853000	-2.869755000
H	0.136536000	-2.449110000	3.676444000
H	0.382001000	-3.932213000	4.609756000
H	1.632002000	-2.689740000	4.581302000
S	-1.089169000	0.340197000	-2.641212000

S	-2.901860000	0.240407000	-0.129313000
S	0.813615000	-2.039037000	-1.394882000
S	-0.994762000	-2.164916000	1.125812000
S	0.754105000	2.430079000	-1.233762000
S	2.565627000	0.138020000	-0.059802000
C	4.022414000	2.343521000	-3.145956000
H	4.364270000	3.352048000	-3.384913000
H	4.901688000	1.697062000	-3.112161000
H	3.581654000	2.364700000	-2.147358000
S	0.771751000	0.038934000	2.467464000
Co	-1.280373000	1.635531000	-0.834399000
Fe	-1.277533000	0.065461000	1.450545000
Co	0.887488000	1.379494000	0.711791000
P	-2.469683000	3.192989000	-1.716509000
S	-1.032248000	2.331974000	1.267925000
P	-2.686806000	0.009621000	3.477808000
H	-3.445220000	1.871059000	-3.424647000
C	-1.574552000	4.300121000	-2.857070000
H	-2.260078000	5.108783000	-3.129449000
C	-3.199490000	4.357310000	-0.516697000
H	-2.361084000	4.755595000	0.060566000
H	-3.627499000	5.190951000	-1.081935000
H	-4.443245000	1.910474000	-1.996209000
C	-3.876556000	2.546125000	-2.681303000
H	-0.766755000	4.746589000	-2.271653000
H	-3.592795000	2.182602000	3.248082000
H	-4.588864000	0.990183000	2.459014000
C	-4.062091000	1.205569000	3.393237000
C	-3.454650000	-1.616259000	3.795125000
H	-3.942566000	-1.595033000	4.774447000
H	-2.624746000	-2.325907000	3.864190000
C	-1.799202000	0.373603000	5.031071000
H	-0.984941000	-0.355212000	5.085914000
H	-2.470016000	0.169590000	5.871616000
C	-4.764915000	3.592592000	-3.332824000
H	-1.817674000	3.190326000	-4.711250000
C	-1.023297000	3.617373000	-4.095764000
H	-0.477476000	4.335916000	-4.710189000
H	-0.339958000	2.811830000	-3.823333000
C	-4.233669000	3.728137000	0.399685000
H	-4.561030000	4.447078000	1.152926000
H	-3.818755000	2.860434000	0.914058000
H	-5.117059000	3.402039000	-0.152777000
H	-5.575196000	3.107633000	-3.880894000
H	-5.221896000	4.257177000	-2.597148000
H	-4.213902000	4.209013000	-4.045551000

C	-5.014062000	1.217791000	4.576960000
H	-5.792976000	1.969177000	4.431061000
H	-4.498910000	1.457682000	5.509168000
H	-5.510424000	0.254100000	4.707775000
H	-5.286777000	-1.377258000	2.649427000
H	-3.932167000	-2.031514000	1.726921000
C	-4.421285000	-2.040804000	2.702429000
H	-4.790528000	-3.051217000	2.888132000
C	-1.246591000	1.787742000	5.097768000
H	-2.044418000	2.533027000	5.088966000
H	-0.675755000	1.927556000	6.017304000
H	-0.584714000	1.993840000	4.254914000

3Fe_1_13_M6_Co

C	-1.749390000	-4.493330000	-2.347758000
C	-1.181024000	-5.200868000	-1.128248000
H	-0.521536000	-6.014908000	-1.434649000
C	1.510652000	-0.010380000	-5.284616000
C	0.916320000	-1.407910000	-5.350880000
C	3.768368000	-0.896589000	-3.658789000
C	4.725937000	-0.900777000	-4.837846000
H	5.491622000	-1.667526000	-4.702654000
C	3.015037000	-3.958466000	0.383828000
C	4.008153000	-3.365767000	-0.599245000
H	4.321714000	-4.120282000	-1.323154000
C	4.658021000	-2.968708000	3.096492000
H	-2.351928000	-5.171813000	-2.959365000
H	-0.939695000	-4.117845000	-2.980235000
H	-0.609033000	-4.506744000	-0.509478000
H	-1.969648000	-5.630434000	-0.507084000
H	-4.380826000	-5.644414000	-1.712422000
H	-2.615321000	-2.160988000	-4.126298000
H	-3.872772000	-3.392890000	-4.046456000
H	1.691634000	-2.176608000	-5.348400000
H	0.258537000	-1.591182000	-4.498897000
H	4.292366000	-0.699678000	-2.719078000
H	3.285509000	-1.868954000	-3.527331000
H	4.212406000	-1.112996000	-5.777772000
H	5.238706000	0.057033000	-4.945453000
H	2.167136000	-4.403226000	-0.143912000
H	3.475932000	-4.750225000	0.982538000
H	3.559507000	-2.535184000	-1.145368000
H	4.903958000	-2.998789000	-0.094706000
H	4.154047000	-3.533596000	3.882829000
H	5.093348000	-3.683743000	2.395457000
H	2.239168000	-4.579343000	3.062417000

H	0.688195000	-4.330408000	2.267299000
P	-2.758182000	-3.029646000	-1.932398000
H	0.716948000	0.741244000	-5.329670000
H	0.333216000	-1.529123000	-6.265688000
H	2.181776000	0.176892000	-6.128661000
P	2.411869000	0.319381000	-3.731202000
P	2.298302000	-2.744226000	1.542669000
C	3.719311000	-1.993123000	2.406133000
H	3.295821000	-1.275802000	3.113941000
H	4.244705000	-1.393291000	1.659088000
H	5.482493000	-2.426104000	3.562888000
H	-5.787544000	-5.035943000	-0.846373000
C	-4.148454000	-3.633727000	-0.917156000
C	-4.980049000	-4.751572000	-1.524016000
C	-3.464478000	-2.516143000	-3.534673000
C	-4.504519000	-1.416328000	-3.393661000
C	1.502618000	-3.818234000	2.785871000
C	0.982022000	-3.096773000	4.015497000
H	-3.706206000	-3.935422000	0.036777000
H	-4.762338000	-2.756598000	-0.693212000
Fe	-1.454965000	-1.246466000	-0.854556000
Fe	0.959656000	0.201238000	-1.752490000
H	2.366772000	2.658837000	-4.077939000
C	3.192144000	1.944187000	-4.007449000
H	3.693983000	1.933208000	-4.980118000
Co	1.012927000	-1.288321000	0.622421000
H	-5.435837000	-4.448515000	-2.468711000
H	-4.820694000	-1.061117000	-4.376146000
H	-5.394251000	-1.768132000	-2.867692000
H	-4.099312000	-0.569010000	-2.837103000
H	0.240805000	-2.346900000	3.736615000
H	0.510617000	-3.808047000	4.696625000
H	1.782984000	-2.595203000	4.562294000
S	-1.097742000	0.298087000	-2.717942000
S	-2.985586000	0.349190000	-0.100211000
S	0.781640000	-2.046878000	-1.487435000
S	-0.970873000	-2.177669000	1.222016000
S	0.717633000	2.438171000	-1.362245000
S	2.579086000	0.096292000	-0.148818000
C	4.146330000	2.347940000	-2.895141000
H	4.542117000	3.348068000	-3.079480000
H	4.995056000	1.664844000	-2.823355000
H	3.641216000	2.359013000	-1.927500000
S	0.794437000	0.078611000	2.352834000
Co	-1.301547000	1.616901000	-0.908663000
Fe	-1.297958000	0.103955000	1.467910000

Co	0.931576000	1.395148000	0.578243000
P	-2.519859000	3.157867000	-1.774531000
S	-0.989135000	2.334153000	1.165810000
P	-2.690204000	0.025306000	3.469186000
H	-3.555029000	1.818088000	-3.430812000
C	-1.654218000	4.249282000	-2.954475000
H	-2.352513000	5.048726000	-3.221705000
C	-3.191489000	4.355673000	-0.572718000
H	-2.323687000	4.754683000	-0.040913000
H	-3.626302000	5.181005000	-1.145271000
H	-4.513824000	1.895958000	-1.975245000
C	-3.959260000	2.510857000	-2.688105000
H	-0.839088000	4.712299000	-2.392358000
H	-3.505869000	2.242311000	3.321115000
H	-4.569497000	1.115842000	2.525590000
C	-4.014146000	1.282851000	3.453051000
C	-3.524767000	-1.569008000	3.778627000
H	-4.032765000	-1.530146000	4.746901000
H	-2.721280000	-2.306858000	3.863889000
C	-1.753403000	0.316012000	5.011221000
H	-0.962918000	-0.440262000	5.027061000
H	-2.406164000	0.114631000	5.866364000
C	-4.851460000	3.558647000	-3.332650000
H	-1.927077000	3.117831000	-4.790507000
C	-1.123249000	3.558415000	-4.197079000
H	-0.598292000	4.276265000	-4.830465000
H	-0.429844000	2.759699000	-3.930840000
C	-4.199116000	3.777512000	0.403792000
H	-4.497714000	4.536381000	1.129479000
H	-3.773855000	2.932894000	0.946002000
H	-5.101342000	3.430502000	-0.103852000
H	-5.687491000	3.076585000	-3.843264000
H	-5.272676000	4.245029000	-2.595601000
H	-4.314694000	4.151466000	-4.075557000
C	-4.937647000	1.306257000	4.658463000
H	-5.677845000	2.102899000	4.557401000
H	-4.389968000	1.484902000	5.586015000
H	-5.482828000	0.366625000	4.768341000
H	-5.317850000	-1.266308000	2.585402000
H	-3.965824000	-1.976333000	1.702390000
C	-4.480616000	-1.962953000	2.664981000
H	-4.893570000	-2.957421000	2.845871000
C	-1.151374000	1.709304000	5.094781000
H	-1.923961000	2.480063000	5.127945000
H	-0.547544000	1.809277000	5.998422000
H	-0.509633000	1.913767000	4.235796000

3Fe_1_1Restricted

C	-1.323634000	-4.269461000	-2.471003000
C	-0.854171000	-5.046268000	-1.252043000
H	-0.214341000	-5.878168000	-1.552867000
C	1.088948000	-0.329594000	-4.978215000
C	0.581869000	-1.758925000	-4.958227000
C	3.427784000	-0.911917000	-3.394397000
C	4.285575000	-0.940465000	-4.647837000
H	5.144527000	-1.598569000	-4.500486000
C	2.971388000	-3.960105000	0.426360000
C	4.050557000	-3.324701000	-0.432412000
H	4.398195000	-4.026348000	-1.193089000
C	4.414223000	-3.181789000	3.291657000
H	-1.959504000	-4.891365000	-3.108043000
H	-0.468761000	-3.956112000	-3.074592000
H	-0.287271000	-4.404674000	-0.574968000
H	-1.693753000	-5.458993000	-0.689542000
H	-3.888820000	-5.370164000	-1.826459000
H	-2.253602000	-1.914325000	-4.292825000
H	-3.391302000	-3.242188000	-4.122593000
H	1.400548000	-2.480135000	-4.913865000
H	-0.049133000	-1.925239000	-4.084901000
H	4.002602000	-0.585628000	-2.523519000
H	3.056987000	-1.909783000	-3.148270000
H	3.732461000	-1.317090000	-5.510386000
H	4.673420000	0.047139000	-4.905123000
H	2.169664000	-4.361945000	-0.198207000
H	3.371788000	-4.792429000	1.013030000
H	3.672181000	-2.434195000	-0.935621000
H	4.915596000	-3.028038000	0.163837000
H	3.840497000	-3.795852000	3.988584000
H	4.900176000	-3.850156000	2.578239000
H	1.936016000	-4.718605000	2.986804000
H	0.470477000	-4.362629000	2.078187000
P	-2.253075000	-2.747649000	-2.058653000
H	0.256575000	0.370100000	-5.092747000
H	-0.002991000	-1.975007000	-5.854643000
H	1.766158000	-0.163710000	-5.820888000
P	1.955339000	0.169563000	-3.446847000
P	2.176328000	-2.791271000	1.582047000
C	3.544939000	-2.145515000	2.600451000
H	3.080994000	-1.470533000	3.323717000
H	4.135004000	-1.510958000	1.934168000
H	5.202357000	-2.689458000	3.865246000
H	-5.285711000	-4.750654000	-0.954467000

C	-3.644885000	-3.355382000	-1.038957000
C	-4.481296000	-4.472770000	-1.638902000
C	-3.042349000	-2.317315000	-3.653982000
C	-4.175330000	-1.314272000	-3.518063000
C	1.256061000	-3.913508000	2.691447000
C	0.654824000	-3.238368000	3.910592000
H	-3.199581000	-3.656048000	-0.087462000
H	-4.256307000	-2.477359000	-0.816653000
Fe	-1.145889000	-1.148145000	-1.030059000
Fe	0.764712000	0.176832000	-1.599139000
H	1.776565000	2.485763000	-3.960218000
C	2.627318000	1.800659000	-3.936722000
H	3.001551000	1.716829000	-4.961652000
Co	0.996243000	-1.260193000	0.671021000
H	-4.943624000	-4.175873000	-2.582224000
H	-4.531835000	-1.003844000	-4.502294000
H	-5.024785000	-1.732677000	-2.975256000
H	-3.844378000	-0.424796000	-2.981310000
H	-0.021536000	-2.435701000	3.613472000
H	0.091316000	-3.960218000	4.505234000
H	1.422925000	-2.804665000	4.554037000
S	-1.172803000	0.371669000	-2.590246000
S	-2.881611000	-0.005332000	-0.135953000
S	0.836455000	-2.005578000	-1.388001000
S	-1.021905000	-2.060897000	1.014323000
S	0.645417000	2.369696000	-1.197776000
S	2.488039000	0.197386000	-0.109741000
C	3.704884000	2.325178000	-3.006089000
H	3.971558000	3.351219000	-3.267579000
H	4.613418000	1.722444000	-3.061660000
H	3.362222000	2.314146000	-1.971610000
S	0.701992000	0.015733000	2.425838000
Co	-1.343951000	1.502545000	-0.706019000
Fe	-1.281478000	0.170238000	1.329139000
Co	0.960981000	1.509274000	0.786149000
P	-2.572667000	3.093727000	-1.553098000
S	-1.025448000	2.312746000	1.334486000
P	-2.541905000	0.140566000	3.134860000
P	2.181778000	3.035068000	1.660770000
H	-3.532836000	1.827734000	-3.311004000
C	-1.697995000	4.255002000	-2.661536000
H	-2.395693000	5.066983000	-2.888155000
C	-3.331338000	4.237920000	-0.348276000
H	-2.526754000	4.548767000	0.322084000
H	-3.668433000	5.128135000	-0.887157000
H	-4.546282000	1.820729000	-1.891882000

C	-3.972321000	2.477769000	-2.550794000
H	-0.885638000	4.683357000	-2.068988000
H	-3.562422000	2.265970000	2.904221000
H	-4.547763000	0.997387000	2.218005000
C	-3.971541000	1.273306000	3.105062000
C	-3.268153000	-1.487191000	3.546900000
H	-3.685619000	-1.412851000	4.555830000
H	-2.429581000	-2.186056000	3.595471000
C	-1.684554000	0.537515000	4.702152000
H	-0.885189000	-0.201379000	4.799107000
H	-2.395817000	0.350246000	5.512389000
H	3.041546000	3.913058000	-0.356715000
C	1.309315000	4.574524000	2.123889000
H	0.525117000	4.280996000	2.826626000
H	2.018659000	5.196688000	2.678400000
C	3.530569000	3.591750000	0.566381000
H	4.094545000	2.692312000	0.306496000
H	2.192418000	2.228689000	3.888803000
C	2.992727000	2.575915000	3.230012000
H	3.412307000	3.482489000	3.676412000
C	-4.852680000	3.541767000	-3.184953000
H	-1.953130000	3.231320000	-4.562457000
C	-1.155928000	3.637824000	-3.937028000
H	-0.622350000	4.388375000	-4.523575000
H	-0.464653000	2.826171000	-3.710278000
C	-4.466754000	3.603505000	0.433557000
H	-4.754204000	4.229593000	1.280262000
H	-4.170838000	2.627917000	0.816874000
H	-5.352258000	3.461729000	-0.188491000
H	-5.670371000	3.073084000	-3.736432000
H	-5.299611000	4.203876000	-2.440919000
H	-4.297446000	4.160781000	-3.892104000
C	-4.850718000	1.287231000	4.344086000
H	-5.679887000	1.984866000	4.207910000
H	-4.299578000	1.606890000	5.230280000
H	-5.282231000	0.306383000	4.552135000
H	-5.175830000	-1.317091000	2.518145000
H	-3.892656000	-2.057227000	1.560456000
C	-4.311577000	-1.982985000	2.563737000
H	-4.670630000	-2.971680000	2.856561000
C	-1.116860000	1.941194000	4.800609000
H	-1.893735000	2.703336000	4.708764000
H	-0.626822000	2.082550000	5.766318000
H	-0.379308000	2.117059000	4.016586000
C	4.435919000	4.679040000	1.119543000
C	0.716610000	5.341941000	0.955369000

H	0.164893000	6.213476000	1.313312000
H	1.489842000	5.696618000	0.270997000
H	0.031534000	4.712589000	0.385353000
H	4.927940000	4.370099000	2.043795000
H	3.887698000	5.600615000	1.323955000
H	5.218861000	4.919564000	0.397454000
C	4.049755000	1.499928000	3.064795000
H	4.413490000	1.163966000	4.037718000
H	4.908277000	1.861690000	2.495640000
H	3.638304000	0.640162000	2.536715000

3Fe_1_1Unrestricted

C	-1.323669000	-4.269377000	-2.468744000
C	-0.859074000	-5.049123000	-1.249800000
H	-0.219049000	-5.881045000	-1.550160000
C	1.085651000	-0.322794000	-4.978900000
C	0.572156000	-1.749870000	-4.961176000
C	3.422961000	-0.916655000	-3.397145000
C	4.277111000	-0.949913000	-4.652956000
H	5.133899000	-1.611203000	-4.507288000
C	2.974410000	-3.957180000	0.426162000
C	4.049931000	-3.319043000	-0.435168000
H	4.398236000	-4.020144000	-1.196040000
C	4.421406000	-3.179930000	3.284667000
H	-1.957987000	-4.889386000	-3.109164000
H	-0.466462000	-3.955637000	-3.068820000
H	-0.293858000	-4.409470000	-0.569514000
H	-1.700966000	-5.462160000	-0.690980000
H	-3.885869000	-5.371593000	-1.820075000
H	-2.254340000	-1.914835000	-4.290875000
H	-3.391969000	-3.242668000	-4.119901000
H	1.387575000	-2.474829000	-4.918046000
H	-0.059532000	-1.914764000	-4.088077000
H	4.001421000	-0.591421000	-2.528288000
H	3.049205000	-1.912851000	-3.148699000
H	3.720112000	-1.325308000	-5.513549000
H	4.668091000	0.035880000	-4.912403000
H	2.172798000	-4.362046000	-0.196579000
H	3.378570000	-4.787756000	1.012740000
H	3.667817000	-2.430046000	-0.938265000
H	4.915227000	-3.019324000	0.159174000
H	3.852369000	-3.800771000	3.979416000
H	4.908641000	-3.841813000	2.566082000
H	1.938313000	-4.718587000	2.985390000
H	0.472833000	-4.362856000	2.076583000
P	-2.253070000	-2.747521000	-2.056460000

H	0.256424000	0.380805000	-5.092305000
H	-0.013726000	-1.961871000	-5.857900000
H	1.763575000	-0.158622000	-5.821337000
P	1.954323000	0.170131000	-3.446796000
P	2.177815000	-2.789908000	1.582385000
C	3.545501000	-2.143717000	2.601758000
H	3.079853000	-1.475503000	3.330186000
H	4.130932000	-1.502107000	1.938147000
H	5.208713000	-2.687279000	3.859117000
H	-5.283827000	-4.752044000	-0.949829000
C	-3.644506000	-3.355109000	-1.036151000
C	-4.479420000	-4.474515000	-1.634416000
C	-3.042870000	-2.317658000	-3.651662000
C	-4.175811000	-1.314576000	-3.515662000
C	1.257902000	-3.913716000	2.690492000
C	0.655806000	-3.240045000	3.910027000
H	-3.199171000	-3.653595000	-0.083974000
H	-4.257020000	-2.477405000	-0.815592000
Fe	-1.145752000	-1.147701000	-1.028562000
Fe	0.764452000	0.177567000	-1.598609000
H	1.783926000	2.488519000	-3.953168000
C	2.631924000	1.799895000	-3.933333000
H	3.003763000	1.717489000	-4.959246000
Co	0.997116000	-1.259112000	0.671713000
H	-4.941655000	-4.179854000	-2.578486000
H	-4.532582000	-1.004371000	-4.499866000
H	-5.025119000	-1.732854000	-2.972533000
H	-3.844707000	-0.424973000	-2.979199000
H	-0.021257000	-2.437802000	3.613386000
H	0.092882000	-3.962866000	4.504046000
H	1.423386000	-2.806064000	4.553909000
S	-1.173486000	0.371892000	-2.588996000
S	-2.881218000	-0.005003000	-0.133864000
S	0.836624000	-2.004806000	-1.387140000
S	-1.020808000	-2.060040000	1.015922000
S	0.644953000	2.370450000	-1.197535000
S	2.488330000	0.198596000	-0.109873000
C	3.713514000	2.317300000	-3.003385000
H	3.983857000	3.342999000	-3.262439000
H	4.619454000	1.711011000	-3.062554000
H	3.372902000	2.304673000	-1.968255000
S	0.703336000	0.017014000	2.426473000
Co	-1.344086000	1.503094000	-0.704917000
Fe	-1.280534000	0.171135000	1.330560000
Co	0.961346000	1.510326000	0.786392000
P	-2.573497000	3.093878000	-1.551672000

S	-1.024947000	2.313704000	1.335337000
P	-2.540240000	0.141602000	3.136765000
P	2.182320000	3.036421000	1.660269000
H	-3.523535000	1.827264000	-3.314570000
C	-1.697416000	4.261064000	-2.652787000
H	-2.394872000	5.074203000	-2.875968000
C	-3.340060000	4.232109000	-0.346213000
H	-2.539166000	4.542389000	0.328807000
H	-3.676776000	5.123460000	-0.883456000
H	-4.545193000	1.820749000	-1.901331000
C	-3.967421000	2.477553000	-2.557136000
H	-0.885831000	4.686297000	-2.056926000
H	-3.558370000	2.268793000	2.912156000
H	-4.543386000	1.003760000	2.219000000
C	-3.968780000	1.275746000	3.108328000
C	-3.267907000	-1.485777000	3.547848000
H	-3.692777000	-1.409307000	4.553532000
H	-2.428998000	-2.183625000	3.604324000
C	-1.681881000	0.536667000	4.703986000
H	-0.879576000	-0.199515000	4.797303000
H	-2.391162000	0.344005000	5.514684000
H	3.051400000	3.902683000	-0.358291000
C	1.311462000	4.579208000	2.115222000
H	0.527723000	4.290391000	2.820407000
H	2.021797000	5.204156000	2.665324000
C	3.536168000	3.586648000	0.568859000
H	4.101242000	2.685681000	0.316745000
H	2.182910000	2.240470000	3.892052000
C	2.986728000	2.580650000	3.233860000
H	3.409581000	3.487214000	3.677173000
C	-4.844002000	3.541322000	-3.196893000
H	-1.950246000	3.247667000	-4.559501000
C	-1.153801000	3.650831000	-3.930946000
H	-0.619600000	4.404590000	-4.512799000
H	-0.462731000	2.838033000	-3.707787000
C	-4.477519000	3.592371000	0.428273000
H	-4.769963000	4.214643000	1.276079000
H	-4.181234000	2.615949000	0.809162000
H	-5.360012000	3.451109000	-0.198153000
H	-5.658513000	3.072448000	-3.752895000
H	-5.295180000	4.203823000	-2.455787000
H	-4.284607000	4.159941000	-3.901106000
C	-4.850558000	1.285675000	4.345546000
H	-5.679109000	1.984190000	4.210122000
H	-4.301127000	1.601929000	5.234009000
H	-5.282948000	0.304286000	4.549221000

H	-5.168085000	-1.320605000	2.504453000
H	-3.876925000	-2.061641000	1.558231000
C	-4.303405000	-1.985322000	2.558198000
H	-4.663455000	-2.973698000	2.850862000
C	-1.119542000	1.942224000	4.806293000
H	-1.899566000	2.701602000	4.718218000
H	-0.628544000	2.082261000	5.771711000
H	-0.383933000	2.123610000	4.021719000
C	4.439030000	4.677105000	1.119864000
C	0.718050000	5.339967000	0.942712000
H	0.166843000	6.213721000	1.295993000
H	1.490840000	5.690460000	0.255699000
H	0.032368000	4.707485000	0.376863000
H	4.926926000	4.373459000	2.048040000
H	3.889883000	5.599806000	1.316597000
H	5.225173000	4.913562000	0.399912000
C	4.038798000	1.498607000	3.076578000
H	4.398263000	1.165469000	4.052057000
H	4.900628000	1.853341000	2.508008000
H	3.624465000	0.638395000	2.551468000

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C	-1.551448000	-4.365806000	-2.360294000
C	-0.982925000	-5.107846000	-1.163808000
H	-0.387709000	-5.960054000	-1.497407000
C	1.289541000	-0.083775000	-5.088503000
C	0.753202000	-1.503130000	-5.148670000
C	3.581458000	-0.831655000	-3.494839000
C	4.478015000	-0.832238000	-4.721014000
H	5.300890000	-1.537748000	-4.587461000
C	2.947732000	-3.954018000	0.302263000
C	4.000703000	-3.299028000	-0.573270000
H	4.344597000	-3.992829000	-1.342812000
C	4.448101000	-3.192692000	3.137231000
H	-2.209441000	-5.013273000	-2.948602000
H	-0.746705000	-4.031507000	-3.020350000
H	-0.344566000	-4.451601000	-0.571081000
H	-1.771494000	-5.487900000	-0.511197000
H	-4.164358000	-5.445768000	-1.624993000
H	-2.424900000	-2.033574000	-4.157334000
H	-3.629796000	-3.311984000	-4.010745000
H	1.558020000	-2.240716000	-5.125097000
H	0.095845000	-1.701457000	-4.300515000
H	4.141096000	-0.576597000	-2.590642000
H	3.158600000	-1.822846000	-3.312120000
H	3.936192000	-1.130875000	-5.620573000

H	4.918252000	0.149527000	-4.906725000
H	2.135012000	-4.355014000	-0.308573000
H	3.368807000	-4.788862000	0.870672000
H	3.597943000	-2.413670000	-1.066321000
H	4.871886000	-2.990555000	0.007807000
H	3.899695000	-3.834814000	3.829151000
H	4.933426000	-3.833274000	2.398351000
H	1.994150000	-4.749496000	2.881032000
H	0.500392000	-4.415959000	2.011628000
P	-2.499340000	-2.862963000	-1.940765000
H	0.470907000	0.636240000	-5.169696000
H	0.186758000	-1.659210000	-6.069011000
H	1.975227000	0.112323000	-5.918329000
P	2.158601000	0.314162000	-3.529558000
P	2.167029000	-2.808201000	1.489873000
C	3.546204000	-2.156024000	2.489482000
H	3.084189000	-1.509737000	3.239565000
H	4.109075000	-1.492899000	1.827804000
H	5.237211000	-2.699179000	3.708372000
H	-5.544743000	-4.778515000	-0.761405000
C	-3.876361000	-3.420036000	-0.885599000
C	-4.738978000	-4.533079000	-1.456121000
C	-3.248876000	-2.400466000	-3.539634000
C	-4.333463000	-1.344673000	-3.419500000
C	1.291001000	-3.955933000	2.609925000
C	0.707586000	-3.302752000	3.849704000
H	-3.418515000	-3.710987000	0.063286000
H	-4.464627000	-2.524122000	-0.669592000
Fe	-1.278664000	-1.191084000	-0.977785000
Fe	0.960396000	0.216743000	-1.723523000
H	2.066703000	2.656412000	-3.907741000
C	2.896169000	1.944869000	-3.899781000
H	3.309767000	1.916731000	-4.912431000
Co	0.934037000	-1.285870000	0.608652000
H	-5.199703000	-4.246778000	-2.403633000
H	-4.672493000	-1.033817000	-4.409454000
H	-5.201778000	-1.717423000	-2.872968000
H	-3.958624000	-0.466019000	-2.894242000
H	0.020449000	-2.500119000	3.578144000
H	0.160966000	-4.037492000	4.444272000
H	1.484849000	-2.873009000	4.484701000
S	-1.082219000	0.274560000	-2.685464000
S	-2.935064000	0.130963000	-0.165417000
S	0.788273000	-2.007936000	-1.500597000
S	-1.077376000	-2.176925000	1.029323000
S	0.687544000	2.384564000	-1.225581000

S	2.480342000	0.153308000	-0.070179000
C	3.946338000	2.367528000	-2.887916000
H	4.251145000	3.402158000	-3.057040000
H	4.840801000	1.744670000	-2.951471000
H	3.555814000	2.286881000	-1.873268000
S	0.673948000	-0.031777000	2.402982000
Co	-1.326751000	1.528965000	-0.852101000
Fe	-1.362827000	0.025631000	1.457064000
Co	0.878995000	1.457027000	0.770273000
P	-2.514500000	3.082976000	-1.736557000
S	-1.146384000	2.239366000	1.227219000
P	-2.498351000	0.104664000	3.334215000
P	2.031148000	3.003988000	1.703118000
H	-3.434510000	1.782524000	-3.487411000
C	-1.613708000	4.218735000	-2.847636000
H	-2.304831000	5.019845000	-3.127580000
C	-3.293678000	4.238961000	-0.557988000
H	-2.482420000	4.632768000	0.059173000
H	-3.700608000	5.076911000	-1.132140000
H	-4.467604000	1.787687000	-2.082199000
C	-3.893273000	2.440061000	-2.744904000
H	-0.824168000	4.669033000	-2.240763000
H	-3.479036000	2.241073000	3.046566000
H	-4.501399000	0.974535000	2.421484000
C	-3.906900000	1.265898000	3.291919000
C	-3.240859000	-1.503267000	3.792598000
H	-3.655705000	-1.418956000	4.801762000
H	-2.409047000	-2.210950000	3.843572000
C	-1.576108000	0.549973000	4.847245000
H	-0.773906000	-0.186774000	4.937979000
H	-2.243756000	0.411663000	5.703031000
H	2.980978000	3.872027000	-0.279425000
C	1.117892000	4.530632000	2.124266000
H	0.299969000	4.222053000	2.779850000
H	1.789990000	5.157541000	2.718485000
C	3.425048000	3.570015000	0.671982000
H	4.016771000	2.676906000	0.455864000
H	1.968809000	2.196479000	3.934654000
C	2.785403000	2.559207000	3.306004000
H	3.167481000	3.475343000	3.766413000
C	-4.778824000	3.483696000	-3.404006000
H	-1.796306000	3.127553000	-4.718969000
C	-1.023107000	3.557841000	-4.079367000
H	-0.469025000	4.287917000	-4.672781000
H	-0.339127000	2.756455000	-3.796542000
C	-4.361120000	3.597411000	0.309715000

H	-4.706107000	4.297808000	1.072811000
H	-3.969976000	2.711658000	0.810870000
H	-5.229611000	3.293944000	-0.278017000
H	-5.570966000	2.996937000	-3.976765000
H	-5.260301000	4.134344000	-2.671401000
H	-4.219026000	4.115476000	-4.096385000
C	-4.759979000	1.336787000	4.546773000
H	-5.579266000	2.045362000	4.407678000
H	-4.183465000	1.671972000	5.411160000
H	-5.204263000	0.370787000	4.794913000
H	-5.164052000	-1.334021000	2.795370000
H	-3.884196000	-2.022605000	1.795592000
C	-4.290157000	-1.988588000	2.807652000
H	-4.631548000	-2.990941000	3.073638000
C	-1.001294000	1.954896000	4.824082000
H	-1.785345000	2.713388000	4.774857000
H	-0.413817000	2.142347000	5.725222000
H	-0.353967000	2.088472000	3.956072000
C	4.282538000	4.677238000	1.261309000
C	0.580545000	5.295601000	0.928152000
H	-0.010597000	6.151703000	1.259656000
H	1.386141000	5.672770000	0.294947000
H	-0.053644000	4.655485000	0.313321000
H	4.733101000	4.383641000	2.211376000
H	3.708257000	5.589893000	1.431190000
H	5.096261000	4.926939000	0.577320000
C	3.870656000	1.505094000	3.187863000
H	4.199730000	1.179350000	4.176568000
H	4.744885000	1.881871000	2.653704000
H	3.498249000	0.635820000	2.646536000

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C	-1.537891000	-4.338664000	-2.329958000
C	-0.965318000	-5.085854000	-1.139110000
H	-0.382096000	-5.943918000	-1.478860000
C	1.254287000	-0.137259000	-5.082116000
C	0.703417000	-1.551623000	-5.121677000
C	3.558408000	-0.880721000	-3.501902000
C	4.440596000	-0.899714000	-4.738331000
H	5.262840000	-1.606044000	-4.605294000
C	2.977802000	-3.935749000	0.300075000
C	4.028009000	-3.271848000	-0.571928000
H	4.375301000	-3.959814000	-1.345210000
C	4.476542000	-3.173159000	3.133388000
H	-2.204484000	-4.981261000	-2.914034000
H	-0.736608000	-4.008384000	-2.995991000

H	-0.313908000	-4.435805000	-0.553993000
H	-1.750785000	-5.457943000	-0.478251000
H	-4.145048000	-5.414362000	-1.595951000
H	-2.401343000	-2.012521000	-4.127096000
H	-3.613362000	-3.282803000	-3.970109000
H	1.500573000	-2.297374000	-5.092741000
H	0.049364000	-1.731325000	-4.266944000
H	4.129365000	-0.614540000	-2.608017000
H	3.135799000	-1.868443000	-3.301268000
H	3.887266000	-1.208380000	-5.627442000
H	4.881645000	0.078135000	-4.941743000
H	2.167679000	-4.338456000	-0.313115000
H	3.402590000	-4.770688000	0.865505000
H	3.621829000	-2.385327000	-1.059820000
H	4.897701000	-2.962482000	0.010900000
H	3.933834000	-3.822721000	3.822850000
H	4.965591000	-3.806513000	2.390711000
H	2.030796000	-4.741423000	2.878826000
H	0.536373000	-4.419766000	2.006553000
P	-2.478857000	-2.832852000	-1.906526000
H	0.442012000	0.589752000	-5.164028000
H	0.130062000	-1.713596000	-6.036745000
H	1.934818000	0.043135000	-5.919674000
P	2.139402000	0.268936000	-3.534691000
P	2.190560000	-2.796931000	1.490165000
C	3.566007000	-2.140166000	2.491989000
H	3.099896000	-1.501549000	3.246115000
H	4.122765000	-1.468875000	1.833378000
H	5.262748000	-2.676600000	3.705896000
H	-5.528002000	-4.745168000	-0.738284000
C	-3.859119000	-3.388375000	-0.855564000
C	-4.719534000	-4.501075000	-1.430309000
C	-3.226804000	-2.369882000	-3.506190000
C	-4.305396000	-1.307663000	-3.393868000
C	1.321629000	-3.953464000	2.607118000
C	0.729654000	-3.307016000	3.846399000
H	-3.405308000	-3.680690000	0.094481000
H	-4.448326000	-2.492508000	-0.642816000
Fe	-1.266850000	-1.162575000	-0.942018000
Fe	0.955309000	0.224701000	-1.713685000
H	2.050574000	2.605991000	-3.941468000
C	2.879862000	1.894215000	-3.925783000
H	3.290945000	1.852740000	-4.939115000
Co	0.946358000	-1.281474000	0.614904000
H	-5.176698000	-4.214835000	-2.379472000
H	-4.646382000	-1.007419000	-4.386438000

H	-5.173611000	-1.669339000	-2.839758000
H	-3.923956000	-0.424537000	-2.881230000
H	0.036345000	-2.509809000	3.574389000
H	0.188067000	-4.047076000	4.438962000
H	1.501684000	-2.871159000	4.483589000
S	-1.081582000	0.291502000	-2.666408000
S	-2.935488000	0.134033000	-0.166332000
S	0.790837000	-1.990946000	-1.491641000
S	-1.059589000	-2.184005000	1.030741000
S	0.685963000	2.394966000	-1.206435000
S	2.482507000	0.174484000	-0.058667000
C	3.933177000	2.331224000	-2.923243000
H	4.250827000	3.356815000	-3.121401000
H	4.820151000	1.696024000	-2.967740000
H	3.540338000	2.284763000	-1.907175000
S	0.675371000	-0.033749000	2.413859000
Co	-1.332149000	1.543643000	-0.844041000
Fe	-1.339795000	0.026283000	1.441968000
Co	0.875855000	1.462378000	0.785289000
P	-2.507744000	3.108567000	-1.723626000
S	-1.154681000	2.237638000	1.247108000
P	-2.510491000	0.071341000	3.289216000
P	2.030543000	3.012026000	1.711896000
H	-3.437904000	1.815392000	-3.474875000
C	-1.601000000	4.239620000	-2.834730000
H	-2.286566000	5.045557000	-3.114384000
C	-3.279938000	4.266904000	-0.542323000
H	-2.467437000	4.647167000	0.081525000
H	-3.675264000	5.113525000	-1.111836000
H	-4.471834000	1.829842000	-2.070313000
C	-3.891438000	2.477104000	-2.732814000
H	-0.807576000	4.684071000	-2.228660000
H	-3.500981000	2.202319000	2.998660000
H	-4.509216000	0.932379000	2.356553000
C	-3.925852000	1.223651000	3.234352000
C	-3.248191000	-1.539730000	3.743146000
H	-3.660266000	-1.458326000	4.753666000
H	-2.415277000	-2.246218000	3.789581000
C	-1.609287000	0.518354000	4.814786000
H	-0.806177000	-0.216111000	4.914882000
H	-2.290591000	0.372286000	5.658525000
H	2.972740000	3.879400000	-0.274689000
C	1.115049000	4.535852000	2.138646000
H	0.298562000	4.222956000	2.794124000
H	1.786232000	5.162186000	2.734515000
C	3.420154000	3.581815000	0.676668000

H	4.015052000	2.690588000	0.461264000
H	1.973580000	2.204069000	3.942687000
C	2.789093000	2.567983000	3.313058000
H	3.170976000	3.484100000	3.773639000
C	-4.768180000	3.527682000	-3.392803000
H	-1.793220000	3.149762000	-4.705911000
C	-1.016247000	3.573961000	-4.066749000
H	-0.456611000	4.299388000	-4.660663000
H	-0.338461000	2.767164000	-3.784247000
C	-4.358045000	3.630045000	0.315807000
H	-4.695083000	4.325732000	1.086725000
H	-3.980155000	2.732965000	0.806924000
H	-5.229458000	3.345835000	-0.277182000
H	-5.567049000	3.047724000	-3.961982000
H	-5.240681000	4.185772000	-2.660966000
H	-4.203778000	4.151572000	-4.088576000
C	-4.791931000	1.284332000	4.480897000
H	-5.614049000	1.988259000	4.335102000
H	-4.226607000	1.620871000	5.352066000
H	-5.232927000	0.315033000	4.721884000
H	-5.179019000	-1.374227000	2.761448000
H	-3.899291000	-2.037164000	1.745224000
C	-4.299549000	-2.021346000	2.759549000
H	-4.630520000	-3.030255000	3.013724000
C	-1.039905000	1.925327000	4.811268000
H	-1.825757000	2.681426000	4.754497000
H	-0.468953000	2.107358000	5.724083000
H	-0.378109000	2.067871000	3.955864000
C	4.273855000	4.694259000	1.261500000
C	0.574441000	5.304064000	0.946155000
H	-0.017829000	6.157923000	1.281481000
H	1.378407000	5.684891000	0.313042000
H	-0.058949000	4.664704000	0.329889000
H	4.726173000	4.405619000	2.212280000
H	3.696087000	5.605206000	1.428842000
H	5.086145000	4.944989000	0.576183000
C	3.875086000	1.514893000	3.192691000
H	4.205954000	1.188596000	4.180631000
H	4.748144000	1.892966000	2.657524000
H	3.502912000	0.645885000	2.650875000

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C	-1.555309000	-4.368240000	-2.453166000
C	-1.007874000	-5.118741000	-1.250192000
H	-0.375466000	-5.947749000	-1.574190000
C	1.220206000	-0.242686000	-5.070511000

C	0.646138000	-1.648309000	-5.049915000
C	3.552154000	-0.933195000	-3.504561000
C	4.416554000	-0.984171000	-4.752816000
H	5.242839000	-1.684045000	-4.611306000
C	2.998928000	-3.906325000	0.349817000
C	4.040487000	-3.270351000	-0.552580000
H	4.357060000	-3.972001000	-1.326680000
C	4.572442000	-3.105779000	3.136062000
H	-2.179855000	-5.018400000	-3.073627000
H	-0.734132000	-4.011745000	-3.081508000
H	-0.412168000	-4.457047000	-0.619168000
H	-1.809078000	-5.534317000	-0.635550000
H	-4.160543000	-5.489855000	-1.765662000
H	-2.458006000	-2.038158000	-4.231171000
H	-3.678160000	-3.300386000	-4.095489000
H	1.430940000	-2.405393000	-4.990477000
H	-0.011870000	-1.781869000	-4.189975000
H	4.135004000	-0.641103000	-2.626630000
H	3.134269000	-1.915639000	-3.271637000
H	3.851437000	-1.320243000	-5.624317000
H	4.851579000	-0.011413000	-4.990485000
H	2.168895000	-4.304639000	-0.239156000
H	3.423044000	-4.738952000	0.919173000
H	3.638541000	-2.381785000	-1.040490000
H	4.928988000	-2.971670000	0.006915000
H	4.038222000	-3.727254000	3.857093000
H	5.029771000	-3.766920000	2.397423000
H	2.116524000	-4.642528000	2.975098000
H	0.605701000	-4.342113000	2.123775000
P	-2.519526000	-2.877082000	-2.014495000
H	0.419324000	0.494247000	-5.172633000
H	0.070505000	-1.838200000	-5.958174000
H	1.895213000	-0.106129000	-5.920849000
P	2.130630000	0.211808000	-3.552043000
P	2.254304000	-2.737683000	1.538142000
C	3.660750000	-2.074815000	2.492492000
H	3.221255000	-1.413726000	3.243161000
H	4.210096000	-1.425712000	1.806085000
H	5.382378000	-2.607799000	3.673057000
H	-5.546260000	-4.870025000	-0.874270000
C	-3.897334000	-3.479846000	-0.979247000
C	-4.749044000	-4.591923000	-1.567005000
C	-3.279379000	-2.404883000	-3.609011000
C	-4.345636000	-1.331740000	-3.462902000
C	1.401436000	-3.861492000	2.698584000
C	0.831838000	-3.186607000	3.933198000

H	-3.438597000	-3.783091000	-0.033862000
H	-4.498719000	-2.597106000	-0.743506000
Fe	-1.272677000	-1.151862000	-0.928812000
Fe	0.978543000	0.239972000	-1.715302000
H	2.024557000	2.532925000	-4.037590000
C	2.858483000	1.827112000	-4.004990000
H	3.257778000	1.750754000	-5.021129000
Co	1.017436000	-1.225421000	0.649690000
H	-5.220499000	-4.288578000	-2.503999000
H	-4.691507000	-0.998274000	-4.443321000
H	-5.214409000	-1.699089000	-2.913036000
H	-3.952009000	-0.467155000	-2.926459000
H	0.116838000	-2.411446000	3.654189000
H	0.318573000	-3.918341000	4.560430000
H	1.612528000	-2.720868000	4.538164000
S	-1.053920000	0.347319000	-2.644570000
S	-2.903682000	0.248336000	-0.150833000
S	0.817297000	-1.965442000	-1.441411000
S	-0.975160000	-2.148786000	1.090813000
S	0.749640000	2.424586000	-1.221089000
S	2.528031000	0.227289000	-0.076190000
C	3.921501000	2.307726000	-3.033276000
H	4.246265000	3.318119000	-3.289446000
H	4.802741000	1.663250000	-3.048316000
H	3.534389000	2.320905000	-2.013898000
S	0.768337000	0.061269000	2.440358000
Co	-1.275250000	1.622113000	-0.838213000
Fe	-1.288403000	0.098916000	1.497679000
Co	0.951731000	1.533929000	0.786200000
P	-2.471795000	3.168302000	-1.710876000
S	-1.071336000	2.328320000	1.259268000
P	-2.686452000	-0.013288000	3.460620000
P	2.123973000	3.091266000	1.673705000
H	-3.401594000	1.860301000	-3.451484000
C	-1.576302000	4.298698000	-2.831432000
H	-2.266202000	5.100901000	-3.111494000
C	-3.239147000	4.325840000	-0.526423000
H	-2.418399000	4.738223000	0.065856000
H	-3.668948000	5.151430000	-1.102035000
H	-4.422331000	1.864109000	-2.039233000
C	-3.856201000	2.518480000	-2.706870000
H	-0.781616000	4.749281000	-2.231449000
H	-3.571662000	2.171752000	3.264062000
H	-4.580466000	1.000098000	2.463796000
C	-4.051162000	1.198326000	3.400535000
C	-3.473106000	-1.629965000	3.777132000

H	-3.974752000	-1.607537000	4.749416000
H	-2.649895000	-2.346670000	3.854177000
C	-1.788239000	0.334351000	5.014229000
H	-0.990409000	-0.412242000	5.068818000
H	-2.456024000	0.155189000	5.862612000
H	3.067042000	3.907967000	-0.333962000
C	1.221835000	4.628430000	2.077471000
H	0.421431000	4.335256000	2.761628000
H	1.908838000	5.268893000	2.639455000
C	3.514669000	3.626246000	0.622204000
H	4.100438000	2.725053000	0.423697000
H	2.053368000	2.313570000	3.910974000
C	2.875791000	2.662976000	3.281352000
H	3.262586000	3.582257000	3.731438000
C	-4.750429000	3.558987000	-3.359006000
H	-1.774631000	3.203483000	-4.698676000
C	-0.995456000	3.628288000	-4.062741000
H	-0.435759000	4.350757000	-4.660108000
H	-0.318722000	2.820804000	-3.779100000
C	-4.278546000	3.685370000	0.375661000
H	-4.629569000	4.401944000	1.120750000
H	-3.858710000	2.825249000	0.898254000
H	-5.147217000	3.343001000	-0.190132000
H	-5.541244000	3.069031000	-3.930766000
H	-5.233707000	4.203285000	-2.621970000
H	-4.197288000	4.197102000	-4.051001000
C	-5.001996000	1.207605000	4.584457000
H	-5.770196000	1.972576000	4.451678000
H	-4.482838000	1.424464000	5.520336000
H	-5.512604000	0.249517000	4.700895000
H	-5.286918000	-1.375445000	2.605505000
H	-3.920404000	-2.028212000	1.700164000
C	-4.425635000	-2.043843000	2.667731000
H	-4.802236000	-3.054011000	2.839937000
C	-1.198512000	1.734454000	5.062491000
H	-1.976822000	2.500196000	5.060370000
H	-0.605097000	1.868268000	5.969091000
H	-0.553259000	1.910666000	4.199696000
C	4.379732000	4.742573000	1.182313000
C	0.654315000	5.364550000	0.877355000
H	0.073823000	6.230192000	1.202662000
H	1.443484000	5.723143000	0.213451000
H	0.002925000	4.709883000	0.296624000
H	4.825865000	4.472145000	2.141350000
H	3.812262000	5.664077000	1.325098000
H	5.196761000	4.966543000	0.493480000

C	3.955715000	1.601740000	3.177619000
H	4.276299000	1.280498000	4.170501000
H	4.835446000	1.971309000	2.647477000
H	3.583740000	0.730457000	2.638624000

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C	1.299339000	-0.059789000	-4.997400000
C	0.783901000	-1.483997000	-5.096516000
C	3.565072000	-0.803265000	-3.361645000
C	4.478643000	-0.803752000	-4.575870000
H	5.299675000	-1.507904000	-4.426089000
C	2.888234000	-4.028998000	0.213763000
C	3.964117000	-3.380461000	-0.637885000
H	4.276430000	-4.053457000	-1.438467000
C	4.439401000	-3.355152000	3.054586000
H	1.594408000	-2.213323000	-5.039184000
H	0.077252000	-1.704699000	-4.296043000
H	4.111612000	-0.547339000	-2.450135000
H	3.136049000	-1.792870000	-3.188996000
H	3.950744000	-1.107984000	-5.481410000
H	4.920882000	0.177563000	-4.758771000
H	2.058003000	-4.374004000	-0.407168000
H	3.278282000	-4.899445000	0.750014000
H	3.594028000	-2.460650000	-1.090953000
H	4.849764000	-3.132881000	-0.049455000
H	3.884975000	-3.991204000	3.747149000
H	4.894754000	-3.999040000	2.299853000
H	1.935473000	-4.854250000	2.795840000
H	0.445799000	-4.461978000	1.942807000
H	0.476180000	0.653323000	-5.087551000
H	0.273540000	-1.631607000	-6.049975000
H	2.005386000	0.158203000	-5.805089000
P	2.146877000	0.340268000	-3.431545000
P	2.152820000	-2.896322000	1.439108000
C	3.554434000	-2.286772000	2.434227000
H	3.116927000	-1.643588000	3.201696000
H	4.125068000	-1.625174000	1.777338000
H	5.250795000	-2.890783000	3.618759000
C	1.252733000	-4.036630000	2.544547000
C	0.697025000	-3.391172000	3.800445000
Co	-1.241431000	-1.085454000	-0.934368000
Co	0.917310000	0.257631000	-1.675517000
H	2.053889000	2.685683000	-3.796325000
C	2.881615000	1.972603000	-3.791303000
H	3.287966000	1.941464000	-4.806747000
Co	0.951870000	-1.336967000	0.604833000

H	0.011698000	-2.581697000	3.546235000
H	0.149884000	-4.126101000	4.393905000
H	1.487450000	-2.977558000	4.430130000
S	-1.083391000	0.302911000	-2.635587000
S	-2.875028000	0.115690000	-0.099785000
S	0.710729000	-1.943833000	-1.500476000
S	-1.097134000	-2.086107000	0.994880000
S	0.638168000	2.402662000	-1.205075000
S	2.446931000	0.159676000	-0.069392000
C	3.940509000	2.390487000	-2.788129000
H	4.237837000	3.428282000	-2.950438000
H	4.837041000	1.772880000	-2.867870000
H	3.561327000	2.296682000	-1.771241000
S	0.718930000	-0.105692000	2.415748000
Co	-1.395304000	1.584814000	-0.880610000
Fe	-1.201782000	0.141351000	1.439421000
Co	0.788025000	1.399198000	0.764704000
P	-2.600761000	3.078439000	-1.808839000
S	-1.212476000	2.293603000	1.196860000
P	-2.374092000	0.195669000	3.297303000
P	1.972319000	2.945849000	1.716555000
H	-3.496987000	1.669304000	-3.487623000
C	-1.716161000	4.193751000	-2.951385000
H	-2.427497000	4.962295000	-3.269683000
C	-3.392601000	4.257737000	-0.662749000
H	-2.584798000	4.686568000	-0.063781000
H	-3.815939000	5.070263000	-1.260958000
H	-4.524830000	1.727321000	-2.084962000
C	-3.965883000	2.358364000	-2.780860000
H	-0.951176000	4.693449000	-2.350758000
H	-3.421640000	2.303952000	2.983855000
H	-4.386912000	0.996863000	2.347328000
C	-3.815289000	1.313371000	3.223688000
C	-3.077896000	-1.428694000	3.754170000
H	-3.468420000	-1.337072000	4.772981000
H	-2.235593000	-2.123542000	3.793576000
C	-1.492108000	0.674312000	4.822286000
H	-0.688277000	-0.055775000	4.946739000
H	-2.180527000	0.542399000	5.661980000
H	2.911426000	3.854874000	-0.253220000
C	1.066883000	4.469513000	2.163137000
H	0.228361000	4.160708000	2.791118000
H	1.739583000	5.060401000	2.792602000
C	3.359389000	3.526419000	0.686949000
H	3.948196000	2.638027000	0.447343000
H	1.940975000	2.083626000	3.934681000

C	2.743691000	2.466603000	3.301301000
H	3.116097000	3.381852000	3.771376000
C	-4.870529000	3.353579000	-3.487948000
H	-1.836415000	3.022800000	-4.778748000
C	-1.087626000	3.509855000	-4.151256000
H	-0.558814000	4.238664000	-4.768761000
H	-0.376001000	2.746553000	-3.833967000
C	-4.447438000	3.628125000	0.229168000
H	-4.791720000	4.342705000	0.979113000
H	-4.049165000	2.754137000	0.745801000
H	-5.317777000	3.305626000	-0.345018000
H	-5.657315000	2.824801000	-4.029347000
H	-5.358286000	4.034874000	-2.787895000
H	-4.323238000	3.955836000	-4.215788000
C	-4.686900000	1.356774000	4.467537000
H	-5.527460000	2.035890000	4.310931000
H	-4.136312000	1.716763000	5.338701000
H	-5.102119000	0.377643000	4.712974000
H	-5.019555000	-1.284446000	2.788186000
H	-3.765900000	-2.022803000	1.787460000
C	-4.147525000	-1.940908000	2.805975000
H	-4.485011000	-2.930071000	3.120408000
C	-0.931127000	2.083353000	4.789464000
H	-1.721416000	2.834076000	4.724505000
H	-0.351377000	2.288477000	5.691536000
H	-0.280759000	2.211151000	3.923720000
C	4.222099000	4.616923000	1.300848000
C	0.576509000	5.290795000	0.983676000
H	0.003788000	6.150024000	1.338092000
H	1.404876000	5.669616000	0.382086000
H	-0.064637000	4.698418000	0.329459000
H	4.682829000	4.297685000	2.237354000
H	3.651583000	5.525758000	1.499977000
H	5.028618000	4.882821000	0.614619000
C	3.847507000	1.434282000	3.159988000
H	4.198028000	1.116887000	4.143864000
H	4.705488000	1.829164000	2.613219000
H	3.488537000	0.555106000	2.625772000

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C	-1.549250000	-4.294456000	-2.477450000
C	-1.022325000	-5.092789000	-1.298321000
H	-0.444093000	-5.949467000	-1.649853000
C	1.258032000	-0.199193000	-4.991913000
C	0.708966000	-1.613315000	-5.027392000
C	3.562637000	-0.917502000	-3.400258000

C	4.438483000	-0.949264000	-4.641763000
H	5.265105000	-1.648276000	-4.499240000
C	2.869094000	-3.948096000	0.368182000
C	3.930155000	-3.339348000	-0.529462000
H	4.243484000	-4.055756000	-1.291174000
C	4.433874000	-3.124563000	3.145582000
H	-2.221616000	-4.903452000	-3.089768000
H	-0.727755000	-3.973944000	-3.123303000
H	-0.376748000	-4.479105000	-0.668326000
H	-1.833166000	-5.473736000	-0.674427000
H	-4.177906000	-5.326681000	-1.780946000
H	-2.397232000	-1.922340000	-4.237165000
H	-3.622875000	-3.178403000	-4.084245000
H	1.504122000	-2.360031000	-4.978671000
H	0.036128000	-1.783775000	-4.185551000
H	4.135842000	-0.639026000	-2.512059000
H	3.139703000	-1.902339000	-3.188693000
H	3.883460000	-1.277344000	-5.522540000
H	4.873134000	0.027299000	-4.863673000
H	2.043104000	-4.347524000	-0.224804000
H	3.275662000	-4.775502000	0.957750000
H	3.546707000	-2.451458000	-1.032178000
H	4.816976000	-3.047445000	0.035963000
H	3.893564000	-3.721125000	3.882618000
H	4.880176000	-3.808083000	2.420843000
H	1.975816000	-4.629878000	2.997481000
H	0.471763000	-4.354993000	2.128017000
P	-2.456977000	-2.775462000	-2.025254000
H	0.447330000	0.527626000	-5.085005000
H	0.152312000	-1.780868000	-5.951545000
H	1.947230000	-0.025267000	-5.823951000
P	2.146321000	0.229417000	-3.455154000
P	2.126973000	-2.758619000	1.536452000
C	3.537004000	-2.092151000	2.483326000
H	3.106187000	-1.412643000	3.222156000
H	4.096086000	-1.463450000	1.786043000
H	5.252034000	-2.625402000	3.668658000
H	-5.534251000	-4.658878000	-0.881115000
C	-3.839995000	-3.332322000	-0.975093000
C	-4.730417000	-4.407785000	-1.575725000
C	-3.215881000	-2.281116000	-3.608382000
C	-4.277103000	-1.207432000	-3.452040000
C	1.256636000	-3.858413000	2.703948000
C	0.671624000	-3.173376000	3.925259000
H	-3.387260000	-3.664722000	-0.037670000
H	-4.406196000	-2.431933000	-0.723621000

Co	-1.295696000	-1.274507000	-1.049334000
Co	0.975629000	0.183024000	-1.666201000
H	2.045169000	2.563000000	-3.877662000
C	2.874229000	1.851514000	-3.867121000
H	3.265804000	1.792978000	-4.887314000
Co	0.894195000	-1.226246000	0.624639000
H	-5.194587000	-4.080386000	-2.507959000
H	-4.608982000	-0.849719000	-4.428449000
H	-5.153542000	-1.579704000	-2.918679000
H	-3.881222000	-0.359845000	-2.893079000
H	-0.073899000	-2.430155000	3.642712000
H	0.187926000	-3.909686000	4.569771000
H	1.439747000	-2.670058000	4.515711000
S	-1.036672000	0.240631000	-2.620620000
S	-2.814549000	0.080431000	-0.117721000
S	0.749920000	-1.995914000	-1.460111000
S	-1.075154000	-2.201838000	0.949916000
S	0.733259000	2.352870000	-1.232177000
S	2.516680000	0.136669000	-0.077332000
C	3.947537000	2.297396000	-2.891767000
H	4.258113000	3.321877000	-3.105411000
H	4.834695000	1.663887000	-2.949850000
H	3.575116000	2.260233000	-1.868285000
S	0.760588000	0.048146000	2.431698000
Co	-1.276182000	1.497335000	-0.809262000
Fe	-1.091560000	-0.064101000	1.305182000
Co	0.997170000	1.511512000	0.774760000
P	-2.491501000	3.046362000	-1.654880000
S	-1.070681000	2.167516000	1.274512000
P	2.140313000	3.106196000	1.613328000
H	-3.408359000	1.801136000	-3.445392000
C	-1.617325000	4.223105000	-2.744048000
H	-2.314556000	5.031269000	-2.985072000
C	-3.273198000	4.147729000	-0.427516000
H	-2.458069000	4.567979000	0.166616000
H	-3.729481000	4.976143000	-0.978621000
H	-4.426411000	1.730626000	-2.028528000
C	-3.869570000	2.417735000	-2.670274000
H	-0.816480000	4.656184000	-2.139862000
H	3.049513000	3.945214000	-0.400025000
C	1.189927000	4.611245000	2.016492000
H	0.416878000	4.295270000	2.721398000
H	1.864131000	5.284616000	2.555003000
C	3.509205000	3.674602000	0.553302000
H	4.118549000	2.789187000	0.353812000
H	2.096427000	2.348131000	3.857706000

C	2.909936000	2.697183000	3.216582000
H	3.289292000	3.626002000	3.653424000
C	-4.782097000	3.471616000	-3.274610000
H	-1.838547000	3.205944000	-4.652734000
C	-1.051035000	3.597638000	-4.006007000
H	-0.488702000	4.338102000	-4.578252000
H	-0.381595000	2.772251000	-3.759347000
C	-4.290075000	3.465005000	0.469935000
H	-4.681081000	4.173753000	1.202111000
H	-3.840835000	2.631960000	1.012773000
H	-5.136699000	3.077850000	-0.100325000
H	-5.565875000	2.993745000	-3.865897000
H	-5.274415000	4.073526000	-2.508660000
H	-4.241136000	4.148390000	-3.938761000
C	4.349412000	4.813366000	1.106531000
C	0.568338000	5.307054000	0.819667000
H	-0.021140000	6.166529000	1.144540000
H	1.325854000	5.667818000	0.120780000
H	-0.087462000	4.623887000	0.278548000
H	4.812153000	4.554791000	2.060847000
H	3.757770000	5.718548000	1.254748000
H	5.153038000	5.059950000	0.409775000
C	4.003701000	1.649456000	3.117305000
H	4.347803000	1.359433000	4.111735000
H	4.868103000	2.019357000	2.562393000
H	3.637141000	0.758127000	2.607993000

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C	1.209353000	-0.147147000	-4.994270000
C	0.664187000	-1.563455000	-5.027397000
C	3.524316000	-0.869463000	-3.416718000
C	4.390509000	-0.915484000	-4.664499000
H	5.213006000	-1.619820000	-4.523781000
C	2.921172000	-3.929318000	0.261396000
C	3.979977000	-3.279095000	-0.609907000
H	4.283027000	-3.954418000	-1.412137000
C	4.512334000	-3.219539000	3.071712000
H	1.462369000	-2.306135000	-4.967899000
H	-0.022203000	-1.741810000	-4.198703000
H	4.106399000	-0.587211000	-2.535565000
H	3.095178000	-1.849207000	-3.195029000
H	3.826051000	-1.245142000	-5.538540000
H	4.830757000	0.056558000	-4.895537000
H	2.084628000	-4.282994000	-0.345871000
H	3.324384000	-4.792769000	0.799297000
H	3.597304000	-2.363463000	-1.060702000

H	4.873381000	-3.023842000	-0.036757000
H	3.973680000	-3.847405000	3.783787000
H	4.955662000	-3.872375000	2.317486000
H	2.035179000	-4.724971000	2.882472000
H	0.530321000	-4.389313000	2.036121000
H	0.396892000	0.578564000	-5.080536000
H	0.122109000	-1.734728000	-5.959173000
H	1.891536000	0.030155000	-5.831880000
P	2.114375000	0.284123000	-3.469679000
P	2.197252000	-2.790865000	1.487853000
C	3.611887000	-2.162792000	2.453843000
H	3.183807000	-1.512199000	3.220315000
H	4.167722000	-1.506522000	1.779503000
H	5.332562000	-2.743908000	3.613305000
C	1.330107000	-3.929536000	2.622066000
C	0.769114000	-3.274096000	3.870973000
Co	-1.350615000	-1.178549000	-0.943397000
Co	0.964609000	0.281585000	-1.676473000
H	2.023772000	2.615991000	-3.910635000
C	2.850551000	1.902111000	-3.889473000
H	3.247642000	1.836610000	-4.907172000
Co	0.973078000	-1.232643000	0.668556000
H	0.063397000	-2.484908000	3.608390000
H	0.247308000	-4.012189000	4.483297000
H	1.555625000	-2.830234000	4.484760000
S	-1.072067000	0.320436000	-2.558262000
S	-2.899666000	0.199895000	-0.109264000
S	0.698949000	-1.911726000	-1.435051000
S	-1.045851000	-2.128237000	1.045562000
S	0.701245000	2.422194000	-1.195354000
S	2.484706000	0.200777000	-0.071505000
C	3.919667000	2.352131000	-2.911195000
H	4.236512000	3.373498000	-3.130971000
H	4.804254000	1.714037000	-2.958758000
H	3.541660000	2.322987000	-1.889379000
S	0.775394000	0.047571000	2.473004000
Co	-1.314139000	1.632704000	-0.784978000
Fe	-1.243012000	0.093654000	1.436620000
Co	0.924102000	1.523946000	0.810863000
P	-2.520690000	3.108344000	-1.754560000
S	-1.085043000	2.353023000	1.310167000
P	-2.624553000	0.007805000	3.358267000
P	2.139531000	3.072200000	1.676437000
H	-3.444143000	1.688691000	-3.410274000
C	-1.637570000	4.200585000	-2.919875000
H	-2.343539000	4.975445000	-3.235124000

C	-3.294640000	4.311893000	-0.620465000
H	-2.475772000	4.758464000	-0.050430000
H	-3.734728000	5.106930000	-1.230190000
H	-4.468735000	1.781632000	-2.006392000
C	-3.900744000	2.393871000	-2.711436000
H	-0.856532000	4.694234000	-2.335617000
H	-3.493271000	2.196365000	3.162176000
H	-4.488859000	1.030528000	2.328362000
C	-3.977317000	1.222994000	3.274990000
C	-3.404329000	-1.617337000	3.623389000
H	-3.897435000	-1.589195000	4.600731000
H	-2.581335000	-2.333506000	3.694551000
C	-1.738882000	0.329026000	4.919326000
H	-0.940156000	-0.416054000	4.967150000
H	-2.430008000	0.118515000	5.741936000
H	3.055120000	3.918460000	-0.328909000
C	1.251478000	4.610698000	2.107873000
H	0.461461000	4.317646000	2.804211000
H	1.951072000	5.242813000	2.663670000
C	3.516867000	3.613556000	0.613124000
H	4.091594000	2.711672000	0.387627000
H	2.097178000	2.285828000	3.913556000
C	2.912674000	2.624659000	3.269209000
H	3.320146000	3.536821000	3.715515000
C	-4.794637000	3.391849000	-3.427886000
H	-1.803457000	3.024807000	-4.740629000
C	-1.037153000	3.494813000	-4.121358000
H	-0.494205000	4.206902000	-4.746119000
H	-0.343749000	2.714721000	-3.804597000
C	-4.325350000	3.700603000	0.311070000
H	-4.670116000	4.438638000	1.037748000
H	-3.899222000	2.856813000	0.854397000
H	-5.198806000	3.341244000	-0.236248000
H	-5.589451000	2.865960000	-3.960399000
H	-5.271874000	4.087339000	-2.734557000
H	-4.242781000	3.978347000	-4.165003000
C	-4.944241000	1.207535000	4.446715000
H	-5.710346000	1.973184000	4.308875000
H	-4.442349000	1.414118000	5.394005000
H	-5.455855000	0.247726000	4.538760000
H	-5.216542000	-1.337703000	2.453927000
H	-3.876794000	-2.057848000	1.556098000
C	-4.372789000	-2.026445000	2.527416000
H	-4.773060000	-3.020327000	2.734328000
C	-1.165839000	1.731131000	5.027262000
H	-1.950365000	2.490115000	5.024551000

H	-0.604419000	1.837370000	5.957234000
H	-0.492685000	1.939673000	4.193965000
C	4.401381000	4.711546000	1.179292000
C	0.667905000	5.361336000	0.924149000
H	0.098709000	6.227225000	1.267949000
H	1.447936000	5.721932000	0.250780000
H	0.001869000	4.718445000	0.346267000
H	4.863947000	4.418379000	2.123653000
H	3.844563000	5.634556000	1.350780000
H	5.206656000	4.942546000	0.479151000
C	3.976925000	1.549658000	3.144999000
H	4.314315000	1.227135000	4.131803000
H	4.849802000	1.908310000	2.596376000
H	3.586012000	0.680598000	2.615210000

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C	-1.515687000	-4.317786000	-2.284225000
C	-0.938724000	-5.046252000	-1.084541000
H	-0.375821000	-5.923226000	-1.409876000
C	3.006187000	-3.893253000	0.230895000
C	4.003065000	-3.174666000	-0.661338000
H	4.420404000	-3.869047000	-1.392629000
C	4.481570000	-3.204588000	3.105951000
H	-2.197628000	-4.965422000	-2.844287000
H	-0.719907000	-4.016063000	-2.969697000
H	-0.265747000	-4.392804000	-0.527597000
H	-1.719555000	-5.385905000	-0.400993000
H	-4.134198000	-5.361954000	-1.586042000
H	-2.315271000	-2.008668000	-4.118696000
H	-3.545162000	-3.260578000	-3.960667000
H	2.201114000	-4.328614000	-0.366321000
H	3.485329000	-4.713558000	0.774894000
H	3.528088000	-2.356933000	-1.205263000
H	4.834049000	-2.760099000	-0.087271000
H	3.947627000	-3.890686000	3.766182000
H	4.990440000	-3.797168000	2.343600000
H	2.045503000	-4.816553000	2.787854000
H	0.552419000	-4.470964000	1.921215000
P	-2.436553000	-2.792491000	-1.888440000
P	2.198065000	-2.824628000	1.467594000
C	3.554725000	-2.167319000	2.494753000
H	3.076812000	-1.559021000	3.266456000
H	4.102443000	-1.469682000	1.856641000
H	5.251746000	-2.711997000	3.702899000
H	-5.528540000	-4.669400000	-0.766944000
C	-3.841817000	-3.331911000	-0.859847000

C	-4.701945000	-4.440867000	-1.442660000
C	-3.154340000	-2.345598000	-3.504772000
C	-4.223330000	-1.271795000	-3.423185000
C	1.334071000	-4.022918000	2.539711000
C	0.736102000	-3.413069000	3.795179000
H	-3.408764000	-3.624896000	0.099598000
H	-4.428469000	-2.431102000	-0.661991000
Co	-1.296997000	-1.233330000	-0.980509000
Co	0.967416000	0.240574000	-1.657596000
Co	0.946441000	-1.298255000	0.648226000
H	-5.134553000	-4.159916000	-2.404777000
H	-4.539746000	-0.971562000	-4.423753000
H	-5.107446000	-1.620451000	-2.885863000
H	-3.841913000	-0.390290000	-2.907225000
H	0.047833000	-2.605341000	3.541151000
H	0.186211000	-4.168604000	4.359537000
H	1.505859000	-3.003139000	4.451954000
S	-1.032935000	0.267758000	-2.611080000
S	-2.881818000	0.132422000	-0.163317000
S	0.742398000	-1.952746000	-1.464522000
S	-1.062910000	-2.162186000	1.013859000
S	0.715308000	2.398417000	-1.221208000
S	2.481112000	0.163458000	-0.039571000
S	0.712285000	0.007836000	2.442284000
Co	-1.318626000	1.590912000	-0.842222000
Fe	-1.325716000	0.056957000	1.481685000
Co	0.916067000	1.519778000	0.800311000
P	-2.515320000	3.125718000	-1.730174000
S	-1.107986000	2.314513000	1.241740000
P	-2.617557000	0.018516000	3.395047000
P	2.104221000	3.073189000	1.653164000
H	-3.413952000	1.817762000	-3.484024000
C	-1.610229000	4.257490000	-2.838086000
H	-2.303952000	5.057550000	-3.116004000
C	-3.305679000	4.269463000	-0.548646000
H	-2.498042000	4.681242000	0.061478000
H	-3.730841000	5.097354000	-1.124114000
H	-4.453940000	1.805815000	-2.082287000
C	-3.883557000	2.465930000	-2.740480000
H	-0.822692000	4.709879000	-2.230172000
H	-3.573024000	2.156383000	3.079405000
H	-4.576092000	0.901684000	2.400110000
C	-4.017789000	1.181878000	3.297623000
C	-3.341673000	-1.608211000	3.788046000
H	-3.779552000	-1.564883000	4.790145000
H	-2.499785000	-2.304759000	3.831472000

C	-1.713383000	0.459354000	4.918299000
H	-0.901504000	-0.268025000	5.003095000
H	-2.384654000	0.297973000	5.767545000
H	3.077926000	3.796876000	-0.380073000
C	1.224521000	4.630545000	2.020719000
H	0.429514000	4.367148000	2.723442000
H	1.927396000	5.276586000	2.556281000
C	3.509143000	3.542130000	0.591064000
H	4.076264000	2.622350000	0.427805000
H	1.997072000	2.340096000	3.905391000
C	2.832353000	2.654682000	3.274360000
H	3.236494000	3.574993000	3.707125000
C	-4.778008000	3.502215000	-3.399666000
H	-1.792455000	3.153813000	-4.702290000
C	-1.019860000	3.597451000	-4.071199000
H	-0.485729000	4.335921000	-4.671769000
H	-0.316019000	2.810234000	-3.799010000
C	-4.356879000	3.611461000	0.326879000
H	-4.710776000	4.308334000	1.089028000
H	-3.947560000	2.733887000	0.828319000
H	-5.222671000	3.290833000	-0.255696000
H	-5.559310000	3.006729000	-3.979582000
H	-5.273061000	4.142705000	-2.667222000
H	-4.221674000	4.143287000	-4.085948000
C	-4.918365000	1.240827000	4.519729000
H	-5.727806000	1.955527000	4.357342000
H	-4.373934000	1.561193000	5.410083000
H	-5.376166000	0.273575000	4.736318000
H	-5.250028000	-1.439061000	2.762391000
H	-3.930196000	-2.036652000	1.754662000
C	-4.357914000	-2.068407000	2.757546000
H	-4.674319000	-3.092751000	2.962556000
C	-1.158131000	1.872758000	4.915800000
H	-1.952538000	2.620702000	4.879004000
H	-0.575070000	2.051896000	5.821127000
H	-0.511143000	2.029767000	4.051301000
C	4.391632000	4.658346000	1.124345000
C	0.650889000	5.341924000	0.808963000
H	0.110238000	6.238790000	1.117583000
H	1.432667000	5.646453000	0.110678000
H	-0.039439000	4.690230000	0.271344000
H	4.819586000	4.413003000	2.098402000
H	3.844711000	5.597693000	1.224969000
H	5.222048000	4.837209000	0.438722000
C	3.890622000	1.568967000	3.208687000
H	4.204314000	1.279473000	4.213359000

H	4.777545000	1.902592000	2.667012000
H	3.503308000	0.684060000	2.703078000

1Fe_1_3_M5

C	-1.529247000	-4.291619000	-2.335733000
C	-0.958326000	-5.035878000	-1.142325000
H	-0.389430000	-5.905872000	-1.476068000
C	1.231132000	-0.176680000	-5.017787000
C	0.672736000	-1.588058000	-5.029328000
C	3.546898000	-0.889827000	-3.435656000
C	4.414141000	-0.938277000	-4.682432000
H	5.239253000	-1.638859000	-4.538698000
C	2.977260000	-3.941278000	0.285335000
C	4.031050000	-3.265207000	-0.572050000
H	4.376795000	-3.939505000	-1.357890000
C	4.472351000	-3.205850000	3.140481000
H	-2.210266000	-4.931634000	-2.905584000
H	-0.730079000	-3.984291000	-3.015106000
H	-0.293279000	-4.390074000	-0.567182000
H	-1.744279000	-5.389290000	-0.472125000
H	-4.139764000	-5.334928000	-1.593661000
H	-2.375153000	-1.977085000	-4.156477000
H	-3.594888000	-3.234195000	-3.975126000
H	1.464567000	-2.338571000	-4.985611000
H	0.015264000	-1.747084000	-4.173120000
H	4.126946000	-0.602496000	-2.554698000
H	3.122069000	-1.870535000	-3.208930000
H	3.851441000	-1.273149000	-5.555802000
H	4.850626000	0.034519000	-4.917073000
H	2.165849000	-4.329613000	-0.334930000
H	3.397652000	-4.787730000	0.836824000
H	3.628099000	-2.368339000	-1.042800000
H	4.901308000	-2.970433000	0.017340000
H	3.925247000	-3.852017000	3.829312000
H	4.958261000	-3.840964000	2.397290000
H	2.022268000	-4.776363000	2.854936000
H	0.528778000	-4.439006000	1.987889000
P	-2.447224000	-2.768553000	-1.921319000
H	0.423460000	0.553850000	-5.109435000
H	0.099682000	-1.762415000	-5.942116000
H	1.911014000	-0.016076000	-5.860134000
P	2.133414000	0.259631000	-3.491645000
P	2.194733000	-2.823176000	1.495717000
C	3.567736000	-2.166343000	2.500269000
H	3.102147000	-1.529161000	3.255933000
H	4.127603000	-1.495497000	1.843903000

H	5.260637000	-2.713628000	3.713631000
H	-5.518326000	-4.642174000	-0.748664000
C	-3.834293000	-3.305767000	-0.866664000
C	-4.703831000	-4.413304000	-1.438514000
C	-3.197383000	-2.320017000	-3.523585000
C	-4.267045000	-1.248940000	-3.414817000
C	1.314126000	-3.982680000	2.596069000
C	0.725676000	-3.351878000	3.845379000
H	-3.388760000	-3.595403000	0.088022000
H	-4.415493000	-2.404360000	-0.656766000
Co	-1.306834000	-1.213335000	-0.996119000
Co	0.972614000	0.248331000	-1.695803000
H	2.026700000	2.589370000	-3.926811000
C	2.859303000	1.882028000	-3.906794000
H	3.260904000	1.824472000	-4.923243000
Co	0.957497000	-1.286138000	0.655787000
H	-5.153374000	-4.129991000	-2.392256000
H	-4.603629000	-0.942281000	-4.406925000
H	-5.139553000	-1.603084000	-2.862868000
H	-3.877736000	-0.371115000	-2.899094000
H	0.006653000	-2.571921000	3.593131000
H	0.209823000	-4.108184000	4.439689000
H	1.497693000	-2.906064000	4.475654000
S	-1.054832000	0.289289000	-2.596905000
S	-2.901863000	0.132026000	-0.158529000
S	0.736585000	-1.938667000	-1.447807000
S	-1.078523000	-2.151679000	1.022717000
S	0.692274000	2.391777000	-1.206038000
S	2.476703000	0.169241000	-0.060032000
C	3.920291000	2.334425000	-2.920240000
H	4.226100000	3.361222000	-3.129406000
H	4.812147000	1.706863000	-2.971421000
H	3.539017000	2.291341000	-1.899910000
S	0.700681000	0.015274000	2.458010000
Co	-1.336633000	1.588710000	-0.834308000
Fe	-1.322053000	0.045654000	1.452231000
Co	0.930854000	1.510508000	0.806610000
P	-2.529960000	3.115325000	-1.744448000
S	-1.117103000	2.279338000	1.284779000
P	2.107987000	3.080124000	1.663686000
H	-3.430881000	1.818255000	-3.505903000
C	-1.623707000	4.249997000	-2.849525000
H	-2.311095000	5.051711000	-3.136899000
C	-3.313192000	4.249541000	-0.549895000
H	-2.499527000	4.675266000	0.042786000
H	-3.756612000	5.069257000	-1.124132000

H	-4.466742000	1.798029000	-2.101276000
C	-3.898446000	2.462142000	-2.757138000
H	-0.837401000	4.700613000	-2.238913000
H	3.049115000	3.904457000	-0.339881000
C	1.192572000	4.608668000	2.063864000
H	0.402198000	4.311227000	2.757499000
H	1.879300000	5.257256000	2.616933000
C	3.497103000	3.617455000	0.614315000
H	4.083873000	2.717545000	0.413297000
H	2.019332000	2.304886000	3.899248000
C	2.849030000	2.640081000	3.271695000
H	3.245869000	3.556351000	3.719662000
C	-4.796968000	3.502093000	-3.404902000
H	-1.800079000	3.159374000	-4.721773000
C	-1.028122000	3.579412000	-4.074091000
H	-0.457249000	4.300582000	-4.662239000
H	-0.359847000	2.767503000	-3.782764000
C	-4.344339000	3.591205000	0.350415000
H	-4.732375000	4.314387000	1.069697000
H	-3.908502000	2.760681000	0.907709000
H	-5.191424000	3.206586000	-0.220838000
H	-5.575383000	3.010196000	-3.991668000
H	-5.296027000	4.129333000	-2.664024000
H	-4.243784000	4.155675000	-4.082166000
C	4.361021000	4.731958000	1.180435000
C	0.608957000	5.335354000	0.865712000
H	0.036319000	6.205110000	1.193383000
H	1.388062000	5.686238000	0.185961000
H	-0.054693000	4.678188000	0.301878000
H	4.807247000	4.457013000	2.138017000
H	3.792344000	5.651992000	1.326952000
H	5.177710000	4.959727000	0.492579000
C	3.917660000	1.566615000	3.175927000
H	4.242279000	1.260904000	4.172178000
H	4.797040000	1.919202000	2.633504000
H	3.534047000	0.688323000	2.656210000

1Fe_1_5_M1

C	1.234607000	-0.128362000	-5.013869000
C	0.701559000	-1.547902000	-5.083613000
C	3.520635000	-0.883150000	-3.411609000
C	4.406627000	-0.919352000	-4.645600000
H	5.222354000	-1.630707000	-4.500776000
C	2.908880000	-3.950561000	0.280521000
C	3.970922000	-3.320518000	-0.601946000
H	4.265587000	-4.007826000	-1.397051000

C	4.511917000	-3.211328000	3.074771000
H	1.505496000	-2.284987000	-5.033038000
H	0.009171000	-1.750782000	-4.265802000
H	4.090549000	-0.615113000	-2.518155000
H	3.083913000	-1.863920000	-3.209172000
H	3.854789000	-1.233618000	-5.533262000
H	4.856654000	0.052777000	-4.856482000
H	2.068588000	-4.308998000	-0.319074000
H	3.307478000	-4.809432000	0.828973000
H	3.597928000	-2.405380000	-1.062127000
H	4.868144000	-3.067318000	-0.033924000
H	3.973297000	-3.829322000	3.795476000
H	4.950390000	-3.874316000	2.326538000
H	2.022692000	-4.705418000	2.914077000
H	0.520386000	-4.374667000	2.060283000
H	0.417911000	0.593115000	-5.098109000
H	0.169876000	-1.703421000	-6.024074000
H	1.925255000	0.070731000	-5.839469000
P	2.118285000	0.280293000	-3.469682000
P	2.193817000	-2.791205000	1.493417000
C	3.613235000	-2.158290000	2.448126000
H	3.189528000	-1.498257000	3.208904000
H	4.169533000	-1.510944000	1.765491000
H	5.335617000	-2.732805000	3.608445000
C	1.321191000	-3.910843000	2.641600000
C	0.759706000	-3.237302000	3.880567000
Co	-1.339999000	-1.178522000	-0.963841000
Co	0.934903000	0.257857000	-1.682571000
H	2.053022000	2.617313000	-3.889850000
C	2.872670000	1.895229000	-3.868129000
H	3.278461000	1.834961000	-4.882633000
Co	0.972892000	-1.243037000	0.641601000
H	0.055807000	-2.450024000	3.607154000
H	0.235073000	-3.966061000	4.501573000
H	1.545788000	-2.786664000	4.489939000
S	-1.089976000	0.307759000	-2.604933000
S	-2.912252000	0.204054000	-0.117199000
S	0.698041000	-1.946717000	-1.466326000
S	-1.050080000	-2.130128000	1.049612000
S	0.696463000	2.406260000	-1.229603000
S	2.478731000	0.187689000	-0.099128000
C	3.936758000	2.327255000	-2.876454000
H	4.265210000	3.347276000	-3.085143000
H	4.815624000	1.681109000	-2.920554000
H	3.549150000	2.293759000	-1.858560000
S	0.764197000	0.029722000	2.426564000

Co	-1.317754000	1.623939000	-0.822313000
Fe	-1.261600000	0.110791000	1.467444000
Co	0.919520000	1.512990000	0.775293000
P	-2.529140000	3.126888000	-1.748860000
S	-1.094874000	2.334625000	1.256505000
P	-2.591212000	-0.006007000	3.343853000
P	2.113518000	3.062721000	1.666670000
H	-3.470726000	1.727492000	-3.413999000
C	-1.648226000	4.221427000	-2.914043000
H	-2.351295000	5.001065000	-3.223721000
C	-3.289172000	4.321578000	-0.597362000
H	-2.465179000	4.753518000	-0.023549000
H	-3.724259000	5.128275000	-1.195198000
H	-4.479510000	1.804405000	-1.998769000
C	-3.918136000	2.425182000	-2.701672000
H	-0.860684000	4.709073000	-2.333447000
H	-3.477169000	2.178228000	3.147756000
H	-4.473621000	1.003388000	2.328742000
C	-3.953777000	1.202313000	3.269675000
C	-3.372174000	-1.626091000	3.639224000
H	-3.846092000	-1.593629000	4.625598000
H	-2.552317000	-2.347138000	3.698490000
C	-1.705068000	0.335221000	4.901777000
H	-0.911074000	-0.413653000	4.966149000
H	-2.394376000	0.148228000	5.731209000
H	3.050977000	3.908638000	-0.328992000
C	1.216998000	4.599721000	2.085740000
H	0.416037000	4.306131000	2.769035000
H	1.906562000	5.233807000	2.651614000
C	3.502042000	3.608682000	0.619849000
H	4.084371000	2.709317000	0.403958000
H	2.053439000	2.267318000	3.901142000
C	2.872185000	2.616821000	3.266904000
H	3.267126000	3.530086000	3.721972000
C	-4.816460000	3.433247000	-3.398350000
H	-1.830967000	3.046815000	-4.734482000
C	-1.058956000	3.515420000	-4.121165000
H	-0.520579000	4.226754000	-4.750659000
H	-0.360866000	2.736401000	-3.811074000
C	-4.322413000	3.706292000	0.328991000
H	-4.658770000	4.437872000	1.066023000
H	-3.902718000	2.852205000	0.861329000
H	-5.200299000	3.361250000	-0.220288000
H	-5.617487000	2.915664000	-3.929654000
H	-5.285600000	4.121635000	-2.692557000
H	-4.269912000	4.027314000	-4.133381000

C	-4.911063000	1.188968000	4.449017000
H	-5.683556000	1.948631000	4.313374000
H	-4.402323000	1.404908000	5.390569000
H	-5.415234000	0.226379000	4.552353000
H	-5.210208000	-1.350985000	2.509590000
H	-3.887353000	-2.063048000	1.582001000
C	-4.362920000	-2.037251000	2.563684000
H	-4.755978000	-3.033073000	2.775180000
C	-1.120994000	1.735090000	4.976173000
H	-1.900471000	2.499289000	4.967470000
H	-0.545943000	1.857822000	5.895791000
H	-0.458724000	1.921543000	4.128877000
C	4.374130000	4.712472000	1.194054000
C	0.651473000	5.347659000	0.891495000
H	0.071076000	6.210343000	1.224481000
H	1.442159000	5.712998000	0.233222000
H	-0.000143000	4.701459000	0.301064000
H	4.826920000	4.423300000	2.144372000
H	3.810295000	5.632624000	1.357891000
H	5.186437000	4.946997000	0.503233000
C	3.946701000	1.551216000	3.148447000
H	4.274481000	1.224023000	4.136964000
H	4.823457000	1.920229000	2.613107000
H	3.568700000	0.683084000	2.608005000

1Fe_1_5_M2_trans

C	-1.503559000	-4.291683000	-2.294614000
C	-0.954941000	-5.032944000	-1.089010000
H	-0.377384000	-5.902160000	-1.409537000
C	3.003225000	-3.878359000	0.250990000
C	3.997180000	-3.160507000	-0.645135000
H	4.408692000	-3.853861000	-1.380718000
C	4.488934000	-3.197211000	3.120624000
H	-2.177241000	-4.932260000	-2.872212000
H	-0.693200000	-3.990665000	-2.963119000
H	-0.302774000	-4.385193000	-0.501301000
H	-1.753311000	-5.387334000	-0.433735000
H	-4.104345000	-5.346500000	-1.604225000
H	-2.304130000	-1.972858000	-4.131182000
H	-3.520226000	-3.238683000	-3.981714000
H	2.195662000	-4.313736000	-0.343111000
H	3.484013000	-4.699608000	0.791922000
H	3.521996000	-2.339501000	-1.184213000
H	4.832483000	-2.749904000	-0.074527000
H	3.956331000	-3.885747000	3.779401000
H	4.995764000	-3.787066000	2.354788000

H	2.046896000	-4.803718000	2.807406000
H	0.552469000	-4.453288000	1.945179000
P	-2.423549000	-2.763588000	-1.901314000
P	2.200033000	-2.808785000	1.490414000
C	3.560640000	-2.157738000	2.515475000
H	3.085411000	-1.551467000	3.290526000
H	4.107747000	-1.458229000	1.878632000
H	5.260657000	-2.707190000	3.717688000
H	-5.508912000	-4.665050000	-0.793232000
C	-3.833920000	-3.311709000	-0.882006000
C	-4.681070000	-4.430241000	-1.465361000
C	-3.140322000	-2.322178000	-3.520180000
C	-4.220892000	-1.259801000	-3.436070000
C	1.336723000	-4.008009000	2.562474000
C	0.743176000	-3.399580000	3.820762000
H	-3.406391000	-3.596644000	0.082507000
H	-4.430019000	-2.415293000	-0.692407000
Co	-1.295295000	-1.204439000	-0.951489000
Co	0.970830000	0.238838000	-1.660591000
Co	0.940753000	-1.277676000	0.676739000
H	-5.111571000	-4.155870000	-2.430293000
H	-4.532263000	-0.950457000	-4.435494000
H	-5.105731000	-1.623060000	-2.909861000
H	-3.853487000	-0.380905000	-2.905959000
H	0.056011000	-2.589804000	3.570348000
H	0.193046000	-4.155049000	4.384968000
H	1.515420000	-2.992552000	4.476390000
S	-1.048564000	0.263781000	-2.613022000
S	-2.894646000	0.137124000	-0.157105000
S	0.737975000	-1.961452000	-1.437375000
S	-1.064556000	-2.144192000	1.043353000
S	0.696610000	2.402587000	-1.212712000
S	2.490848000	0.165950000	-0.024513000
S	0.712171000	0.010495000	2.456523000
Co	-1.336887000	1.572322000	-0.829014000
Fe	-1.328888000	0.064244000	1.483047000
Co	0.894863000	1.493064000	0.804770000
P	-2.534358000	3.110072000	-1.727420000
S	-1.127780000	2.305159000	1.248050000
P	-2.611121000	0.016863000	3.396737000
P	2.113725000	3.047532000	1.637974000
H	-3.430099000	1.805835000	-3.485073000
C	-1.625808000	4.243040000	-2.831889000
H	-2.318831000	5.042100000	-3.114060000
C	-3.325843000	4.256135000	-0.548396000
H	-2.519415000	4.664367000	0.065839000

H	-3.744970000	5.086413000	-1.124822000
H	-4.475187000	1.796296000	-2.087084000
C	-3.900534000	2.455227000	-2.742885000
H	-0.842632000	4.698402000	-2.220366000
H	-3.559214000	2.160254000	3.085887000
H	-4.561653000	0.910507000	2.395970000
C	-4.007149000	1.185839000	3.297274000
C	-3.347178000	-1.607133000	3.779917000
H	-3.785305000	-1.564551000	4.781937000
H	-2.511176000	-2.310734000	3.821159000
C	-1.713392000	0.447207000	4.926091000
H	-0.904349000	-0.283298000	5.012267000
H	-2.387739000	0.285990000	5.772876000
H	3.072325000	3.784781000	-0.398577000
C	1.238343000	4.606208000	2.018591000
H	0.449048000	4.340705000	2.727141000
H	1.945463000	5.249690000	2.551563000
C	3.510627000	3.525749000	0.568314000
H	4.078617000	2.608043000	0.396034000
H	2.029019000	2.332470000	3.897445000
C	2.858467000	2.640150000	3.255274000
H	3.269925000	3.561936000	3.677727000
C	-4.790273000	3.493138000	-3.405800000
H	-1.797012000	3.143114000	-4.698959000
C	-1.027814000	3.583775000	-4.061755000
H	-0.487330000	4.321582000	-4.657477000
H	-0.327823000	2.794083000	-3.786121000
C	-4.383981000	3.602557000	0.322065000
H	-4.739016000	4.301083000	1.082186000
H	-3.981031000	2.723505000	0.825887000
H	-5.248037000	3.285014000	-0.264755000
H	-5.570801000	2.999405000	-3.988248000
H	-5.286294000	4.134995000	-2.675213000
H	-4.230246000	4.132935000	-4.090323000
C	-4.913058000	1.240848000	4.515586000
H	-5.719913000	1.958341000	4.352515000
H	-4.372054000	1.555809000	5.409904000
H	-5.374315000	0.273770000	4.725434000
H	-5.254934000	-1.419931000	2.756451000
H	-3.939336000	-2.017696000	1.743722000
C	-4.366386000	-2.054202000	2.746667000
H	-4.688450000	-3.078183000	2.944564000
C	-1.151839000	1.858255000	4.929071000
H	-1.942921000	2.609817000	4.892515000
H	-0.569557000	2.032659000	5.835802000
H	-0.502103000	2.014471000	4.066439000

C	4.396041000	4.640591000	1.099007000
C	0.654195000	5.325735000	0.816701000
H	0.126525000	6.227101000	1.134726000
H	1.428651000	5.624628000	0.107811000
H	-0.051396000	4.683195000	0.287848000
H	4.832832000	4.390805000	2.067997000
H	3.848305000	5.578326000	1.209895000
H	5.220266000	4.825095000	0.407388000
C	3.911992000	1.550270000	3.187624000
H	4.236340000	1.268056000	4.191052000
H	4.793876000	1.875524000	2.632668000
H	3.515365000	0.662634000	2.694707000

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C	-1.508909000	-4.264108000	-2.383678000
C	-0.928820000	-5.031700000	-1.209248000
H	-0.374411000	-5.901366000	-1.566547000
C	1.279841000	-0.212096000	-5.003016000
C	0.699892000	-1.614240000	-5.007838000
C	3.557894000	-0.897337000	-3.336457000
C	4.453165000	-0.983934000	-4.561003000
H	5.270666000	-1.684210000	-4.378634000
H	-2.188825000	-4.894609000	-2.965583000
H	-0.715204000	-3.938899000	-3.061227000
H	-0.244753000	-4.409826000	-0.630534000
H	-1.709553000	-5.390736000	-0.535743000
H	-4.076831000	-5.365580000	-1.643037000
H	-2.407674000	-1.935572000	-4.159542000
H	-3.609726000	-3.209012000	-3.979771000
H	1.477599000	-2.375882000	-4.922765000
H	0.008941000	-1.746556000	-4.173836000
H	4.116717000	-0.586093000	-2.450102000
H	3.128737000	-1.870319000	-3.084907000
H	3.909617000	-1.339929000	-5.438322000
H	4.900674000	-0.020071000	-4.811863000
P	-2.439368000	-2.759272000	-1.934910000
H	0.486916000	0.529457000	-5.132195000
H	0.156373000	-1.796561000	-5.937110000
H	1.985487000	-0.077625000	-5.828709000
P	2.147291000	0.252335000	-3.464147000
H	-5.462224000	-4.721965000	-0.770708000
C	-3.809648000	-3.344175000	-0.883779000
C	-4.660836000	-4.460986000	-1.464789000
C	-3.217027000	-2.296857000	-3.520315000
C	-4.297194000	-1.240307000	-3.381247000
H	-3.347456000	-3.643769000	0.059922000

H	-4.410730000	-2.460175000	-0.656039000
Co	-1.297686000	-1.202880000	-0.998297000
Co	0.930181000	0.278542000	-1.706893000
H	2.041525000	2.562375000	-3.990420000
C	2.878258000	1.863018000	-3.916323000
H	3.309154000	1.766479000	-4.917788000
Co	0.999859000	-1.245566000	0.614006000
H	-5.127328000	-4.170534000	-2.408133000
H	-4.650009000	-0.920564000	-4.363593000
H	-5.158920000	-1.613301000	-2.824471000
H	-3.911568000	-0.366609000	-2.855899000
S	-1.082620000	0.284022000	-2.605315000
S	-2.893708000	0.090436000	-0.159460000
S	0.757716000	-1.925636000	-1.490582000
S	-1.024745000	-2.155207000	1.021013000
S	0.651568000	2.418081000	-1.250415000
S	2.497241000	0.239368000	-0.125064000
C	3.908401000	2.365130000	-2.922653000
H	4.238618000	3.371468000	-3.187135000
H	4.790231000	1.722205000	-2.896432000
H	3.487766000	2.396118000	-1.917739000
S	0.761017000	0.062401000	2.419173000
Co	-1.345918000	1.559458000	-0.826293000
Fe	-1.298072000	0.081396000	1.423505000
Co	0.915938000	1.557679000	0.750564000
P	-2.543560000	3.099617000	-1.730305000
S	-1.099804000	2.308215000	1.257519000
P	-2.586310000	0.036730000	3.338752000
P	2.119264000	3.079167000	1.659895000
H	-3.488824000	1.788975000	-3.457429000
C	-1.655471000	4.218063000	-2.867984000
H	-2.349537000	5.014733000	-3.153057000
C	-3.304209000	4.267576000	-0.551035000
H	-2.483784000	4.667095000	0.050309000
H	-3.721771000	5.101225000	-1.123587000
H	-4.508200000	1.809528000	-2.041961000
C	-3.937216000	2.453873000	-2.715296000
H	-0.858348000	4.678634000	-2.279102000
H	-3.568649000	2.170405000	3.061732000
H	-4.559729000	0.911638000	2.370090000
C	-3.998074000	1.186482000	3.267137000
C	-3.295091000	-1.601574000	3.713787000
H	-3.715197000	-1.567002000	4.723904000
H	-2.447802000	-2.291854000	3.735673000
C	-1.678112000	0.457694000	4.864573000
H	-0.861539000	-0.265867000	4.932332000

H	-2.348037000	0.272605000	5.710147000
H	3.006277000	3.985319000	-0.333470000
C	1.216794000	4.596871000	2.128150000
H	0.424950000	4.278876000	2.811220000
H	1.905518000	5.223306000	2.703466000
C	3.480554000	3.654699000	0.593759000
H	4.055821000	2.762003000	0.335629000
H	2.096104000	2.262328000	3.885929000
C	2.907846000	2.587543000	3.229895000
H	3.341964000	3.487691000	3.676391000
C	-4.826491000	3.494419000	-3.374409000
H	-1.862713000	3.098788000	-4.720594000
C	-1.080936000	3.535421000	-4.095978000
H	-0.530703000	4.254191000	-4.706432000
H	-0.397745000	2.734357000	-3.809819000
C	-4.356614000	3.628331000	0.337045000
H	-4.688319000	4.329655000	1.105066000
H	-3.957500000	2.742277000	0.831478000
H	-5.235302000	3.324905000	-0.235291000
H	-5.627286000	3.004804000	-3.932392000
H	-5.296464000	4.154892000	-2.643168000
H	-4.272422000	4.116169000	-4.080154000
C	-4.891345000	1.215892000	4.496011000
H	-5.709224000	1.924445000	4.349902000
H	-4.345018000	1.527850000	5.388136000
H	-5.337731000	0.240621000	4.699825000
H	-5.222384000	-1.429155000	2.723424000
H	-3.922720000	-2.027313000	1.690846000
C	-4.330391000	-2.058362000	2.701539000
H	-4.642479000	-3.082672000	2.913126000
C	-1.135554000	1.875403000	4.896767000
H	-1.935361000	2.617900000	4.861922000
H	-0.568464000	2.040776000	5.814702000
H	-0.474920000	2.054701000	4.047239000
C	4.370156000	4.737888000	1.180626000
C	0.634338000	5.366118000	0.955578000
H	0.043691000	6.212255000	1.311971000
H	1.416276000	5.758991000	0.302707000
H	-0.011482000	4.725490000	0.352541000
H	4.856317000	4.411245000	2.101642000
H	3.811387000	5.649594000	1.400060000
H	5.157453000	5.000928000	0.471437000
C	3.949549000	1.491748000	3.085088000
H	4.333650000	1.204260000	4.065318000
H	4.797297000	1.820052000	2.480597000
H	3.524838000	0.603528000	2.614773000

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C	-1.525089000	-4.296890000	-2.390216000
C	-0.965543000	-5.079981000	-1.216031000
H	-0.375834000	-5.927154000	-1.571445000
C	1.214639000	-0.190152000	-4.986870000
C	0.682912000	-1.611337000	-5.004716000
C	3.551053000	-0.853700000	-3.414930000
C	4.414411000	-0.877593000	-4.665230000
H	5.254650000	-1.561361000	-4.528055000
C	2.955106000	-3.966052000	0.306426000
C	4.012134000	-3.325108000	-0.574522000
H	4.327757000	-4.015554000	-1.358962000
C	4.524713000	-3.199406000	3.105683000
H	-2.199549000	-4.917038000	-2.988819000
H	-0.719081000	-3.966351000	-3.050052000
H	-0.322154000	-4.448905000	-0.600574000
H	-1.759259000	-5.473215000	-0.577614000
H	-4.127642000	-5.365398000	-1.707015000
H	-2.388051000	-1.947932000	-4.139400000
H	-3.634720000	-3.176001000	-3.957813000
H	1.487935000	-2.347871000	-4.962170000
H	0.026383000	-1.786333000	-4.150878000
H	4.128518000	-0.557741000	-2.535098000
H	3.150544000	-1.845498000	-3.191710000
H	3.855753000	-1.219836000	-5.538323000
H	4.829361000	0.105261000	-4.896852000
H	2.127704000	-4.343928000	-0.299001000
H	3.364161000	-4.814006000	0.863984000
H	3.625016000	-2.422906000	-1.048483000
H	4.898954000	-3.047391000	-0.001842000
H	3.987455000	-3.821630000	3.823797000
H	4.977549000	-3.859267000	2.363220000
H	2.059398000	-4.718689000	2.940148000
H	0.560149000	-4.418959000	2.069406000
P	-2.440662000	-2.788389000	-1.920922000
H	0.395090000	0.527143000	-5.077369000
H	0.114585000	-1.792488000	-5.919148000
H	1.891496000	-0.014407000	-5.828577000
P	2.110311000	0.263932000	-3.461681000
P	2.211612000	-2.808545000	1.505533000
C	3.618638000	-2.159510000	2.468628000
H	3.182163000	-1.500932000	3.223448000
H	4.172198000	-1.508282000	1.787437000
H	5.338047000	-2.709378000	3.644784000
H	-5.492329000	-4.729783000	-0.796390000

C	-3.819473000	-3.374571000	-0.881410000
C	-4.694255000	-4.457945000	-1.490100000
C	-3.207328000	-2.279956000	-3.496681000
C	-4.251281000	-1.185827000	-3.356649000
C	1.348616000	-3.937508000	2.653589000
C	0.763217000	-3.261885000	3.880676000
H	-3.362792000	-3.707145000	0.054102000
H	-4.402238000	-2.484665000	-0.630448000
Co	-1.271018000	-1.277209000	-0.955479000
Co	0.947221000	0.214265000	-1.664510000
H	1.945450000	2.586235000	-3.902994000
C	2.795948000	1.900180000	-3.887953000
H	3.189136000	1.847202000	-4.907826000
Co	0.967745000	-1.275481000	0.655076000
H	-5.166409000	-4.126654000	-2.416764000
H	-4.627565000	-0.895980000	-4.339271000
H	-5.103942000	-1.515961000	-2.760067000
H	-3.829653000	-0.298586000	-2.882048000
H	0.054438000	-2.483614000	3.593949000
H	0.239384000	-3.991917000	4.501031000
H	1.536758000	-2.798105000	4.496066000
S	-1.073087000	0.239338000	-2.582837000
S	-2.900325000	0.024678000	-0.113461000
S	0.761625000	-1.968068000	-1.435678000
S	-1.028168000	-2.198815000	1.032796000
S	0.652796000	2.380665000	-1.233347000
S	2.487011000	0.169658000	-0.080800000
C	3.857279000	2.379520000	-2.915065000
H	4.128830000	3.416168000	-3.122728000
H	4.766503000	1.778874000	-2.982477000
H	3.493679000	2.320027000	-1.889282000
S	0.772553000	0.024160000	2.443464000
Co	-1.366227000	1.527964000	-0.797146000
Fe	-1.256169000	-0.013857000	1.483260000
Co	0.940600000	1.485200000	0.793855000
S	-1.103973000	2.263088000	1.308612000
P	-2.605972000	0.024571000	3.352925000
P	2.118793000	3.047057000	1.677452000
H	-3.530190000	2.165202000	2.962705000
H	-4.530139000	0.906321000	2.295726000
C	-3.988480000	1.201235000	3.198558000
C	-3.354537000	-1.589567000	3.758057000
H	-3.811680000	-1.508723000	4.749506000
H	-2.520551000	-2.291689000	3.841302000
C	-1.729326000	0.464735000	4.892876000
H	-0.934890000	-0.278581000	5.002760000

H	-2.428440000	0.318016000	5.722465000
H	2.996261000	3.919337000	-0.334124000
C	1.206144000	4.562941000	2.127955000
H	0.421446000	4.250466000	2.821946000
H	1.899883000	5.194459000	2.692159000
C	3.473939000	3.618544000	0.601273000
H	4.064479000	2.729633000	0.365434000
H	2.116649000	2.242170000	3.908287000
C	2.918681000	2.594889000	3.254734000
H	3.321421000	3.508721000	3.701832000
C	-4.911615000	1.297936000	4.401410000
H	-5.706777000	2.020222000	4.206671000
H	-4.381225000	1.630425000	5.295926000
H	-5.388259000	0.342332000	4.629229000
H	-5.229478000	-1.415427000	2.674834000
H	-3.907220000	-2.108979000	1.735793000
C	-4.358991000	-2.072001000	2.727430000
H	-4.712896000	-3.073040000	2.980601000
C	-1.148703000	1.867370000	4.909806000
H	-1.927028000	2.629723000	4.840136000
H	-0.600271000	2.036208000	5.838495000
H	-0.462840000	2.011425000	4.073744000
C	4.342360000	4.732115000	1.162284000
C	0.613053000	5.323004000	0.954844000
H	0.061140000	6.194289000	1.312068000
H	1.386816000	5.678512000	0.271599000
H	-0.074921000	4.696811000	0.385242000
H	4.823495000	4.443488000	2.098787000
H	3.767773000	5.641692000	1.345734000
H	5.133088000	4.983916000	0.452771000
C	3.993667000	1.534072000	3.105697000
H	4.349611000	1.206838000	4.084413000
H	4.854120000	1.907799000	2.547504000
H	3.604852000	0.665481000	2.573981000

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C	-1.541190000	-4.290877000	-2.322418000
C	-0.967923000	-5.032952000	-1.128911000
H	-0.411898000	-5.911753000	-1.461261000
C	1.244125000	-0.165645000	-5.015762000
C	0.691998000	-1.579236000	-5.039960000
C	3.552285000	-0.881774000	-3.427363000
C	4.427097000	-0.920111000	-4.669063000
H	5.252439000	-1.620471000	-4.525396000
C	2.968646000	-3.936173000	0.282647000
C	4.027048000	-3.271608000	-0.577977000

H	4.369189000	-3.952521000	-1.359671000
C	4.470205000	-3.187833000	3.127242000
H	-2.229860000	-4.929378000	-2.884654000
H	-0.743833000	-3.993491000	-3.008380000
H	-0.289516000	-4.390998000	-0.565147000
H	-1.751346000	-5.372436000	-0.448607000
H	-4.147999000	-5.320045000	-1.569775000
H	-2.374476000	-1.979034000	-4.151515000
H	-3.594514000	-3.234608000	-3.962854000
H	1.486933000	-2.326519000	-4.997237000
H	0.030688000	-1.747527000	-4.188520000
H	4.126913000	-0.600128000	-2.541019000
H	3.128157000	-1.865031000	-3.210564000
H	3.870334000	-1.249551000	-5.548287000
H	4.863529000	0.054934000	-4.894332000
H	2.156958000	-4.325840000	-0.336395000
H	3.384383000	-4.780143000	0.841314000
H	3.630059000	-2.375214000	-1.054391000
H	4.898642000	-2.978559000	0.010293000
H	3.923218000	-3.827611000	3.822102000
H	4.951618000	-3.829635000	2.386898000
H	2.024313000	-4.750910000	2.855123000
H	0.526508000	-4.421676000	1.993889000
P	-2.446577000	-2.758637000	-1.911702000
H	0.433836000	0.561929000	-5.108079000
H	0.124375000	-1.749912000	-5.956834000
H	1.927936000	0.003017000	-5.853295000
P	2.136650000	0.265705000	-3.481736000
P	2.189142000	-2.805549000	1.483949000
C	3.567163000	-2.149667000	2.482836000
H	3.105932000	-1.507139000	3.236667000
H	4.128246000	-1.484142000	1.822085000
H	5.261989000	-2.694487000	3.694604000
H	-5.526446000	-4.616897000	-0.733266000
C	-3.837856000	-3.286605000	-0.856938000
C	-4.709428000	-4.395526000	-1.422611000
C	-3.196729000	-2.318103000	-3.516524000
C	-4.266186000	-1.246390000	-3.414784000
C	1.313937000	-3.959729000	2.595137000
C	0.730595000	-3.324111000	3.844285000
H	-3.396134000	-3.571300000	0.101038000
H	-4.417881000	-2.382680000	-0.654623000
Co	-1.286190000	-1.209518000	-0.992187000
Co	0.957262000	0.233549000	-1.697132000
H	2.034384000	2.597435000	-3.911972000
C	2.865222000	1.888042000	-3.893440000

H	3.267027000	1.831966000	-4.909793000
Co	0.952710000	-1.269520000	0.631368000
H	-5.155730000	-4.117800000	-2.379492000
H	-4.602314000	-0.945400000	-4.408811000
H	-5.139078000	-1.596906000	-2.861072000
H	-3.876946000	-0.365265000	-2.904919000
H	0.009818000	-2.545771000	3.592069000
H	0.218054000	-4.078036000	4.444538000
H	1.504945000	-2.874560000	4.469027000
S	-1.057857000	0.269339000	-2.611164000
S	-2.900398000	0.118067000	-0.167042000
S	0.740239000	-1.950137000	-1.458197000
S	-1.071332000	-2.158197000	1.019654000
S	0.688629000	2.380329000	-1.231560000
S	2.479814000	0.167129000	-0.080283000
C	3.926804000	2.336429000	-2.905857000
H	4.231590000	3.364682000	-3.109441000
H	4.819130000	1.709897000	-2.960917000
H	3.546889000	2.287169000	-1.885455000
S	0.703216000	0.018569000	2.443862000
Co	-1.322501000	1.556809000	-0.847776000
Fe	-1.289645000	0.041764000	1.400814000
Co	0.918323000	1.491612000	0.767474000
P	-2.518009000	3.099427000	-1.735364000
S	-1.120342000	2.271303000	1.266091000
P	2.091082000	3.056191000	1.650987000
H	-3.432671000	1.812138000	-3.497322000
C	-1.618191000	4.236848000	-2.843640000
H	-2.306624000	5.040543000	-3.122540000
C	-3.295553000	4.235179000	-0.537898000
H	-2.480125000	4.655441000	0.056231000
H	-3.734629000	5.059188000	-1.109104000
H	-4.464109000	1.793741000	-2.089311000
C	-3.894092000	2.456479000	-2.745134000
H	-0.825742000	4.684458000	-2.238842000
H	3.037424000	3.892282000	-0.345610000
C	1.175498000	4.584691000	2.054213000
H	0.378290000	4.285834000	2.739388000
H	1.858768000	5.228008000	2.617426000
C	3.482785000	3.602792000	0.609079000
H	4.073468000	2.705856000	0.406255000
H	2.004585000	2.278230000	3.886911000
C	2.832279000	2.619855000	3.260159000
H	3.222560000	3.537758000	3.710196000
C	-4.789819000	3.501992000	-3.387729000
H	-1.812309000	3.154162000	-4.718825000

C	-1.034197000	3.569804000	-4.075685000
H	-0.466326000	4.291939000	-4.665557000
H	-0.365169000	2.755321000	-3.793416000
C	-4.330588000	3.580210000	0.360306000
H	-4.710281000	4.301473000	1.085990000
H	-3.901421000	2.741484000	0.910520000
H	-5.182540000	3.207643000	-0.211670000
H	-5.573752000	3.015205000	-3.971425000
H	-5.281889000	4.131628000	-2.644191000
H	-4.236078000	4.153024000	-4.066951000
C	4.341749000	4.717861000	1.181500000
C	0.604900000	5.321198000	0.855830000
H	0.025926000	6.186647000	1.183844000
H	1.391836000	5.680246000	0.189469000
H	-0.049268000	4.668307000	0.276314000
H	4.786623000	4.440862000	2.139124000
H	3.770016000	5.635638000	1.330293000
H	5.159425000	4.950885000	0.496536000
C	3.908045000	1.553670000	3.163297000
H	4.229132000	1.242046000	4.158886000
H	4.788146000	1.915341000	2.628194000
H	3.533393000	0.677237000	2.634272000

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C	-1.567337000	-4.304422000	-2.328077000
C	-0.990376000	-5.054282000	-1.141016000
H	-0.415628000	-5.917853000	-1.481437000
C	1.270917000	-0.050426000	-5.033913000
C	0.714734000	-1.458972000	-5.140759000
C	3.524488000	-0.906461000	-3.436555000
C	4.447438000	-0.888288000	-4.642957000
H	5.231865000	-1.638911000	-4.526734000
C	2.942228000	-4.007262000	0.314739000
C	3.959462000	-3.386785000	-0.624449000
H	4.277800000	-4.111134000	-1.376463000
C	4.538911000	-3.110452000	3.071813000
H	-2.252826000	-4.940708000	-2.896425000
H	-0.770574000	-3.997402000	-3.010219000
H	-0.328491000	-4.408938000	-0.561297000
H	-1.773375000	-5.418949000	-0.473089000
H	-4.156069000	-5.362721000	-1.601342000
H	-2.418637000	-1.972024000	-4.127723000
H	-3.628888000	-3.239504000	-3.953486000
H	1.508595000	-2.208366000	-5.139910000
H	0.050586000	-1.675178000	-4.302171000
H	4.072501000	-0.699841000	-2.513732000

H	3.063890000	-1.887940000	-3.300416000
H	3.914849000	-1.114473000	-5.568728000
H	4.938430000	0.078791000	-4.765796000
H	2.106425000	-4.430367000	-0.248245000
H	3.385319000	-4.819832000	0.898582000
H	3.532303000	-2.526227000	-1.139395000
H	4.849734000	-3.050972000	-0.089566000
H	4.018847000	-3.707979000	3.822965000
H	4.989823000	-3.795645000	2.351175000
H	2.094138000	-4.691475000	2.965320000
H	0.580057000	-4.433207000	2.108352000
P	-2.476525000	-2.779049000	-1.898172000
H	0.464448000	0.684402000	-5.096443000
H	0.148688000	-1.575777000	-6.066869000
H	1.964910000	0.160818000	-5.853322000
P	2.145858000	0.286134000	-3.466513000
P	2.205562000	-2.818960000	1.487073000
C	3.612753000	-2.107345000	2.404928000
H	3.178704000	-1.418523000	3.134042000
H	4.147675000	-1.476782000	1.690259000
H	5.352973000	-2.588238000	3.578136000
H	-5.537445000	-4.692342000	-0.742712000
C	-3.862720000	-3.340356000	-0.853943000
C	-4.727184000	-4.447976000	-1.432582000
C	-3.236391000	-2.326693000	-3.495334000
C	-4.312752000	-1.263780000	-3.374407000
C	1.367592000	-3.926822000	2.672993000
C	0.787847000	-3.238985000	3.895365000
H	-3.411203000	-3.640886000	0.094703000
H	-4.451706000	-2.445910000	-0.634807000
Co	-1.319023000	-1.231123000	-0.962078000
Co	0.919894000	0.187460000	-1.719921000
H	2.115552000	2.629781000	-3.845704000
C	2.929408000	1.902871000	-3.785392000
H	3.388914000	1.852109000	-4.777697000
Co	0.947994000	-1.327896000	0.602497000
H	-5.182424000	-4.157247000	-2.381230000
H	-4.651403000	-0.946314000	-4.362456000
H	-5.183355000	-1.629876000	-2.826913000
H	-3.929331000	-0.389762000	-2.847900000
H	0.056974000	-2.483039000	3.605093000
H	0.291216000	-3.968389000	4.538504000
H	1.560195000	-2.745196000	4.488216000
S	-1.096876000	0.225201000	-2.610052000
S	-2.902506000	0.125333000	-0.150790000
S	0.694640000	-1.989697000	-1.481691000

S	-1.048322000	-2.172503000	1.032694000
S	0.687990000	2.351564000	-1.269986000
S	2.490311000	0.106637000	-0.146098000
C	3.943033000	2.323975000	-2.735949000
H	4.340622000	3.312776000	-2.971373000
H	4.785767000	1.631615000	-2.686867000
H	3.488179000	2.369625000	-1.745479000
S	0.769117000	-0.027861000	2.418708000
Co	-1.346925000	1.529222000	-0.864534000
Fe	-1.301795000	0.027185000	1.430045000
Co	0.958701000	1.467330000	0.751945000
P	-2.525043000	3.079118000	-1.766640000
S	-1.082746000	2.299752000	1.231699000
P	-2.576713000	0.003804000	3.360634000
H	-3.485374000	1.775599000	-3.492672000
C	-1.611921000	4.180093000	-2.899657000
H	-2.291330000	4.987285000	-3.190568000
C	-3.264729000	4.255348000	-0.584259000
H	-2.434308000	4.640589000	0.012646000
H	-3.669729000	5.095168000	-1.157073000
H	-4.504842000	1.813668000	-2.077233000
C	-3.924425000	2.448183000	-2.751851000
H	-0.813226000	4.629240000	-2.304200000
H	-3.513386000	2.149850000	3.038080000
H	-4.522473000	0.901255000	2.353066000
C	-3.966471000	1.178557000	3.252566000
C	-3.322676000	-1.616925000	3.741135000
H	-3.763151000	-1.563883000	4.741733000
H	-2.491938000	-2.325779000	3.790327000
C	-1.684536000	0.426615000	4.893912000
H	-0.868462000	-0.296792000	4.975213000
H	-2.363858000	0.242234000	5.732366000
C	-4.799551000	3.500523000	-3.411781000
H	-1.824975000	3.059212000	-4.750612000
C	-1.040629000	3.486532000	-4.122656000
H	-0.476412000	4.195634000	-4.731513000
H	-0.369970000	2.677237000	-3.829825000
C	-4.326348000	3.635690000	0.306803000
H	-4.646797000	4.346968000	1.070308000
H	-3.940068000	2.747176000	0.807180000
H	-5.209752000	3.342108000	-0.263566000
H	-5.607713000	3.021425000	-3.968253000
H	-5.259319000	4.168263000	-2.680716000
H	-4.237795000	4.113773000	-4.118890000
C	-4.871097000	1.243090000	4.471633000
H	-5.674143000	1.963991000	4.304960000

H	-4.328304000	1.559797000	5.364071000
H	-5.337457000	0.279348000	4.685715000
H	-5.224216000	-1.418417000	2.709353000
H	-3.911356000	-2.039805000	1.707959000
C	-4.342679000	-2.062391000	2.709114000
H	-4.676426000	-3.080969000	2.915652000
C	-1.141801000	1.844344000	4.927145000
H	-1.942087000	2.585671000	4.882400000
H	-0.586529000	2.012369000	5.851469000
H	-0.468270000	2.025862000	4.088607000

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C	1.304305000	-0.111865000	-5.070042000
C	0.763443000	-1.528056000	-5.147368000
C	3.572170000	-0.881598000	-3.448667000
C	4.468856000	-0.920975000	-4.674639000
H	5.279510000	-1.637080000	-4.524499000
C	2.909511000	-3.955500000	0.253982000
C	3.987860000	-3.327566000	-0.610696000
H	4.298253000	-4.017733000	-1.397347000
C	4.454690000	-3.232852000	3.083370000
H	1.563017000	-2.269772000	-5.095038000
H	0.065981000	-1.729888000	-4.333513000
H	4.136416000	-0.617085000	-2.550412000
H	3.130348000	-1.861005000	-3.249761000
H	3.923303000	-1.229921000	-5.568111000
H	4.925906000	0.049176000	-4.879574000
H	2.080747000	-4.315045000	-0.361012000
H	3.298153000	-4.814175000	0.809793000
H	3.623765000	-2.414428000	-1.081983000
H	4.873978000	-3.071490000	-0.026762000
H	3.896948000	-3.850805000	3.789586000
H	4.906890000	-3.895681000	2.343168000
H	1.948574000	-4.724375000	2.846553000
H	0.465713000	-4.354891000	1.976570000
H	0.492042000	0.614305000	-5.159184000
H	0.235213000	-1.678120000	-6.090653000
H	2.002396000	0.085286000	-5.889740000
P	2.174039000	0.287586000	-3.515294000
P	2.172910000	-2.793579000	1.452656000
C	3.576186000	-2.173457000	2.439286000
H	3.141806000	-1.509554000	3.190857000
H	4.151987000	-1.530164000	1.768834000
H	5.268489000	-2.760398000	3.637350000
C	1.266352000	-3.912807000	2.575240000
C	0.700295000	-3.246583000	3.816190000

Co	-1.292961000	-1.157339000	-1.062408000
Co	0.968278000	0.265942000	-1.730408000
H	2.122755000	2.625163000	-3.933396000
C	2.939700000	1.900029000	-3.904112000
H	3.357237000	1.841554000	-4.913921000
Co	0.977201000	-1.222241000	0.577682000
H	0.020099000	-2.437014000	3.547515000
H	0.149400000	-3.973204000	4.416742000
H	1.487565000	-2.825367000	4.444716000
S	-1.047568000	0.341106000	-2.681045000
S	-2.882596000	0.183101000	-0.181713000
S	0.740294000	-1.941094000	-1.514137000
S	-1.081736000	-2.102062000	0.963193000
S	0.729752000	2.410981000	-1.290311000
S	2.501539000	0.184007000	-0.146399000
C	3.993333000	2.326372000	-2.898800000
H	4.329638000	3.344958000	-3.101969000
H	4.869377000	1.675752000	-2.932092000
H	3.593177000	2.294193000	-1.885538000
S	0.792763000	0.049625000	2.393614000
Co	-1.274657000	1.621174000	-0.888757000
Fe	-1.290721000	0.118821000	1.479337000
Co	0.957015000	1.516534000	0.698599000
P	-2.522249000	3.120804000	-1.788120000
S	-1.067909000	2.355472000	1.198480000
P	-2.700332000	0.000742000	3.521916000
P	2.146766000	3.069574000	1.626678000
H	-3.417288000	1.750087000	-3.501059000
C	-1.653148000	4.259624000	-2.919893000
H	-2.365045000	5.037580000	-3.213191000
C	-3.316204000	4.271442000	-0.615180000
H	-2.504137000	4.723605000	-0.039482000
H	-3.780605000	5.071105000	-1.200354000
H	-4.436517000	1.754996000	-2.090935000
C	-3.887540000	2.412670000	-2.770100000
H	-0.875973000	4.742749000	-2.321601000
H	-3.656400000	2.155331000	3.296983000
H	-4.634623000	0.936371000	2.527701000
C	-4.100738000	1.168260000	3.454111000
C	-3.420799000	-1.645820000	3.837937000
H	-3.888273000	-1.644026000	4.827711000
H	-2.573169000	-2.336168000	3.884606000
C	-1.780241000	0.388146000	5.050859000
H	-0.979042000	-0.354785000	5.108642000
H	-2.434215000	0.224128000	5.912874000
H	3.094046000	3.933802000	-0.358867000

C	1.246628000	4.603328000	2.052164000
H	0.435865000	4.303257000	2.721134000
H	1.927673000	5.231427000	2.634650000
C	3.540013000	3.627856000	0.590658000
H	4.125687000	2.731377000	0.371073000
H	2.081069000	2.259097000	3.854995000
C	2.901695000	2.615778000	3.226887000
H	3.293625000	3.525481000	3.691500000
C	-4.808478000	3.417334000	-3.441335000
H	-1.805256000	3.126666000	-4.769870000
C	-1.045097000	3.593421000	-4.140621000
H	-0.516046000	4.329372000	-4.749256000
H	-0.334239000	2.819797000	-3.846177000
C	-4.324990000	3.613629000	0.309346000
H	-4.701410000	4.335353000	1.036736000
H	-3.869019000	2.785869000	0.854377000
H	-5.181636000	3.222116000	-0.242532000
H	-5.583660000	2.895665000	-4.005937000
H	-5.310817000	4.061145000	-2.716668000
H	-4.270191000	4.057440000	-4.143085000
C	-5.037661000	1.161900000	4.649817000
H	-5.836391000	1.893473000	4.511059000
H	-4.516963000	1.417108000	5.574920000
H	-5.508594000	0.186828000	4.788827000
H	-5.276133000	-1.432635000	2.723292000
H	-3.931753000	-2.076485000	1.775803000
C	-4.400926000	-2.084172000	2.761343000
H	-4.753109000	-3.097963000	2.959148000
C	-1.195996000	1.791568000	5.057542000
H	-1.976686000	2.554571000	5.040386000
H	-0.597934000	1.950774000	5.956681000
H	-0.555000000	1.948264000	4.187644000
C	4.408594000	4.728951000	1.175249000
C	0.698255000	5.364692000	0.858034000
H	0.117326000	6.226812000	1.191676000
H	1.498407000	5.733233000	0.213014000
H	0.050988000	4.727464000	0.253115000
H	4.858170000	4.433541000	2.125197000
H	3.842370000	5.646727000	1.344164000
H	5.223192000	4.970346000	0.489377000
C	3.978274000	1.552183000	3.103545000
H	4.304921000	1.219156000	4.090547000
H	4.855589000	1.926103000	2.572474000
H	3.602574000	0.686430000	2.557556000

1Fe_1_7_M2_trans

C	-1.480016000	-4.270618000	-2.358772000
C	-0.945886000	-5.063333000	-1.180339000
H	-0.364216000	-5.916929000	-1.534162000
C	2.944009000	-3.928474000	0.308876000
C	3.955522000	-3.261513000	-0.607093000
H	4.321143000	-3.975599000	-1.346956000
C	4.520316000	-3.185172000	3.109107000
H	-2.149410000	-4.886230000	-2.967948000
H	-0.663558000	-3.946112000	-3.008710000
H	-0.306079000	-4.443375000	-0.551103000
H	-1.752800000	-5.447423000	-0.552941000
H	-4.090945000	-5.332106000	-1.707922000
H	-2.276607000	-1.949057000	-4.155250000
H	-3.495302000	-3.212149000	-4.014599000
H	2.114616000	-4.343226000	-0.269231000
H	3.399327000	-4.757247000	0.860319000
H	3.511078000	-2.420497000	-1.141752000
H	4.818875000	-2.889955000	-0.051869000
H	3.996475000	-3.844089000	3.803964000
H	4.994148000	-3.806577000	2.347023000
H	2.051613000	-4.728102000	2.951903000
H	0.554099000	-4.433258000	2.071142000
P	-2.407024000	-2.755230000	-1.931618000
P	2.192780000	-2.807351000	1.535459000
C	3.591291000	-2.147183000	2.502177000
H	3.145901000	-1.512288000	3.271494000
H	4.129773000	-1.473643000	1.831053000
H	5.317637000	-2.691085000	3.667940000
H	-5.489301000	-4.677700000	-0.864764000
C	-3.816231000	-3.321004000	-0.922177000
C	-4.666878000	-4.421053000	-1.535529000
C	-3.117530000	-2.296386000	-3.549524000
C	-4.197912000	-1.234329000	-3.474207000
C	1.334231000	-3.952454000	2.666418000
C	0.734255000	-3.286647000	3.891858000
H	-3.386093000	-3.634239000	0.032159000
H	-4.407736000	-2.426983000	-0.709286000
Co	-1.281857000	-1.199734000	-0.978000000
Co	0.985349000	0.241329000	-1.667696000
Co	0.950653000	-1.291507000	0.681313000
H	-5.105365000	-4.115967000	-2.487525000
H	-4.506917000	-0.933275000	-4.477001000
H	-5.083406000	-1.594740000	-2.947086000
H	-3.833506000	-0.352924000	-2.946905000
H	0.025937000	-2.509982000	3.599430000
H	0.207558000	-4.022817000	4.502341000

H	1.499304000	-2.822426000	4.517389000
S	-1.025555000	0.281369000	-2.624987000
S	-2.939811000	0.126599000	-0.257941000
S	0.757490000	-1.954835000	-1.441786000
S	-1.049143000	-2.242728000	0.986603000
S	0.693785000	2.397513000	-1.225942000
S	2.492490000	0.150664000	-0.030416000
S	0.783690000	0.022218000	2.468976000
Co	-1.347735000	1.581628000	-0.844498000
Fe	-1.354907000	0.048797000	1.484587000
Co	0.903833000	1.490676000	0.792187000
P	-2.562780000	3.116881000	-1.712004000
S	-1.104625000	2.381881000	1.227393000
P	-2.681642000	0.008501000	3.484378000
P	2.136462000	3.051306000	1.595121000
H	-3.376765000	1.855039000	-3.540013000
C	-1.642595000	4.303471000	-2.748686000
H	-2.333914000	5.113707000	-3.001817000
C	-3.410152000	4.204190000	-0.518667000
H	-2.624143000	4.644333000	0.099981000
H	-3.871495000	5.016971000	-1.087844000
H	-4.459365000	1.774618000	-2.173983000
C	-3.882296000	2.468176000	-2.790103000
H	-0.869852000	4.730284000	-2.104483000
H	-3.648075000	2.142343000	3.177099000
H	-4.643559000	0.884431000	2.493637000
C	-4.086821000	1.164391000	3.392244000
C	-3.381012000	-1.635256000	3.847009000
H	-3.834711000	-1.609906000	4.842810000
H	-2.525932000	-2.315179000	3.895294000
C	-1.747709000	0.445309000	4.988592000
H	-0.934877000	-0.283345000	5.052372000
H	-2.399095000	0.285755000	5.853681000
H	3.126421000	3.711599000	-0.457999000
C	1.296835000	4.638215000	1.931955000
H	0.500200000	4.412387000	2.645644000
H	2.023313000	5.273359000	2.448758000
C	3.549249000	3.475089000	0.521371000
H	4.106470000	2.545203000	0.384071000
H	2.038924000	2.362987000	3.862571000
C	2.870800000	2.669843000	3.223661000
H	3.269614000	3.602501000	3.634489000
C	-4.775510000	3.510468000	-3.441239000
H	-1.787655000	3.303024000	-4.672755000
C	-1.026868000	3.703664000	-4.000162000
H	-0.470256000	4.466533000	-4.547392000

H	-0.337308000	2.895356000	-3.753349000
C	-4.432134000	3.488626000	0.345458000
H	-4.842731000	4.169929000	1.093254000
H	-3.974215000	2.645196000	0.862780000
H	-5.265336000	3.105139000	-0.246898000
H	-5.523187000	3.020433000	-4.068214000
H	-5.312373000	4.108465000	-2.702425000
H	-4.211620000	4.191791000	-4.081229000
C	-4.985320000	1.209690000	4.616622000
H	-5.796752000	1.923723000	4.462001000
H	-4.439927000	1.523100000	5.508871000
H	-5.440077000	0.238988000	4.824031000
H	-5.266879000	-1.477929000	2.776854000
H	-3.919640000	-2.072141000	1.800853000
C	-4.371225000	-2.101901000	2.793719000
H	-4.685602000	-3.127415000	2.995434000
C	-1.188879000	1.857884000	4.968845000
H	-1.981874000	2.607822000	4.943579000
H	-0.589452000	2.038311000	5.863022000
H	-0.556371000	2.009264000	4.092367000
C	4.446028000	4.592923000	1.026977000
C	0.733103000	5.344294000	0.713330000
H	0.258507000	6.282700000	1.007322000
H	1.509607000	5.577621000	-0.017795000
H	-0.015560000	4.719186000	0.224972000
H	4.861521000	4.371893000	2.012211000
H	3.914519000	5.543983000	1.093094000
H	5.285346000	4.736208000	0.343731000
C	3.937018000	1.591174000	3.181631000
H	4.252458000	1.327258000	4.192853000
H	4.821770000	1.919488000	2.633157000
H	3.553328000	0.691951000	2.699424000

1Fe_1_7_M5

C	-1.578361000	-4.273378000	-2.398324000
C	-1.017992000	-5.072933000	-1.236746000
H	-0.467762000	-5.940106000	-1.607707000
C	1.241587000	-0.173735000	-5.037691000
C	0.681224000	-1.583808000	-5.057708000
C	3.552899000	-0.892214000	-3.449389000
C	4.424328000	-0.935767000	-4.693526000
H	5.250304000	-1.635117000	-4.549049000
C	2.962517000	-3.952540000	0.388207000
C	3.989168000	-3.331918000	-0.540922000
H	4.299684000	-4.051755000	-1.300514000
C	4.573891000	-3.113080000	3.152337000

H	-2.270983000	-4.881588000	-2.988765000
H	-0.777009000	-3.959029000	-3.072330000
H	-0.342374000	-4.465037000	-0.634050000
H	-1.809504000	-5.437913000	-0.579391000
H	-4.188789000	-5.304179000	-1.672029000
H	-2.390129000	-1.942260000	-4.174388000
H	-3.615297000	-3.194414000	-4.003257000
H	1.471223000	-2.336050000	-5.009121000
H	0.013489000	-1.742576000	-4.209214000
H	4.130470000	-0.607805000	-2.565786000
H	3.128730000	-1.874449000	-3.227408000
H	3.865119000	-1.269251000	-5.569611000
H	4.859727000	0.038453000	-4.924157000
H	2.118964000	-4.352205000	-0.180300000
H	3.391907000	-4.782145000	0.958600000
H	3.574695000	-2.459310000	-1.046229000
H	4.882737000	-3.014421000	-0.000332000
H	4.049377000	-3.727387000	3.886094000
H	5.025787000	-3.779716000	2.415360000
H	2.097347000	-4.636431000	3.054240000
H	0.603061000	-4.381070000	2.158701000
P	-2.476921000	-2.747129000	-1.945045000
H	0.435820000	0.558702000	-5.130946000
H	0.115967000	-1.754904000	-5.975861000
H	1.926764000	-0.011406000	-5.875431000
P	2.138460000	0.257391000	-3.507129000
P	2.244347000	-2.775026000	1.582794000
C	3.652922000	-2.088972000	2.510135000
H	3.215237000	-1.423379000	3.257297000
H	4.191543000	-1.446102000	1.809512000
H	5.387034000	-2.605381000	3.674965000
H	-5.560369000	-4.621000000	-0.808061000
C	-3.868641000	-3.292573000	-0.901748000
C	-4.746223000	-4.382414000	-1.495043000
C	-3.218672000	-2.281840000	-3.547656000
C	-4.285322000	-1.208125000	-3.449943000
C	1.373154000	-3.874880000	2.746478000
C	0.757128000	-3.190497000	3.952742000
H	-3.425615000	-3.605983000	0.046736000
H	-4.442393000	-2.390263000	-0.676623000
Co	-1.294551000	-1.224177000	-1.011986000
Co	0.970335000	0.219389000	-1.721407000
H	2.033224000	2.588726000	-3.934221000
C	2.864863000	1.880173000	-3.918292000
H	3.262717000	1.823791000	-4.936212000
Co	0.918586000	-1.243993000	0.613195000

H	-5.196855000	-4.075345000	-2.440802000
H	-4.616727000	-0.907804000	-4.445904000
H	-5.160625000	-1.556661000	-2.898766000
H	-3.897070000	-0.329945000	-2.935731000
H	-0.004014000	-2.471201000	3.649651000
H	0.284608000	-3.932443000	4.599172000
H	1.503483000	-2.659263000	4.546581000
S	-1.047535000	0.270652000	-2.618839000
S	-2.961155000	0.103127000	-0.257821000
S	0.722546000	-1.962424000	-1.493674000
S	-1.065797000	-2.261813000	0.958818000
S	0.691482000	2.347020000	-1.232117000
S	2.503708000	0.153687000	-0.118629000
C	3.930483000	2.329139000	-2.935726000
H	4.236688000	3.355977000	-3.143853000
H	4.821471000	1.700727000	-2.991434000
H	3.553443000	2.285722000	-1.914026000
S	0.740333000	0.003504000	2.488109000
Co	-1.322781000	1.539936000	-0.844040000
Fe	-1.381838000	0.028027000	1.433922000
Co	0.911410000	1.431705000	0.761982000
P	-2.536435000	3.082142000	-1.693900000
S	-1.092674000	2.312533000	1.243207000
P	2.079525000	3.014411000	1.647166000
H	-3.371142000	1.843279000	-3.528985000
C	-1.620252000	4.273112000	-2.732196000
H	-2.304387000	5.090427000	-2.980405000
C	-3.369844000	4.165242000	-0.487030000
H	-2.577247000	4.612326000	0.118228000
H	-3.841114000	4.974599000	-1.053613000
H	-4.445743000	1.761793000	-2.156714000
C	-3.866826000	2.454945000	-2.771311000
H	-0.837286000	4.689076000	-2.093697000
H	3.040956000	3.813483000	-0.359862000
C	1.187586000	4.563773000	2.023725000
H	0.376592000	4.292012000	2.703180000
H	1.882945000	5.195205000	2.585823000
C	3.479792000	3.538687000	0.601901000
H	4.070763000	2.637797000	0.418798000
H	2.005301000	2.251464000	3.891582000
C	2.824981000	2.607015000	3.262720000
H	3.193771000	3.537792000	3.704110000
C	-4.757364000	3.508763000	-3.407132000
H	-1.789221000	3.305122000	-4.670971000
C	-1.018996000	3.668080000	-3.987759000
H	-0.425648000	4.412508000	-4.522321000

H	-0.370110000	2.826519000	-3.739136000
C	-4.380687000	3.456388000	0.396967000
H	-4.819756000	4.160752000	1.105740000
H	-3.910038000	2.652666000	0.964819000
H	-5.194867000	3.022392000	-0.186732000
H	-5.511157000	3.029594000	-4.035256000
H	-5.287407000	4.100817000	-2.658933000
H	-4.193850000	4.194877000	-4.042649000
C	4.339027000	4.661516000	1.158584000
C	0.646198000	5.301910000	0.813540000
H	0.099570000	6.192861000	1.128673000
H	1.445076000	5.621564000	0.141334000
H	-0.034757000	4.663073000	0.249887000
H	4.772626000	4.404210000	2.126763000
H	3.771367000	5.585546000	1.280727000
H	5.164932000	4.874324000	0.476805000
C	3.924983000	1.565629000	3.174336000
H	4.243170000	1.258480000	4.172348000
H	4.802315000	1.947272000	2.648675000
H	3.570209000	0.683867000	2.641896000

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C	-1.514902000	-4.280424000	-2.309432000
C	-0.921959000	-5.004832000	-1.114398000
H	-0.328534000	-5.860450000	-1.442999000
C	1.254592000	-0.114767000	-4.984746000
C	0.720980000	-1.534547000	-5.037632000
C	3.549181000	-0.818568000	-3.375972000
C	4.433486000	-0.845976000	-4.610983000
H	5.263659000	-1.539998000	-4.463432000
C	2.949746000	-3.986166000	0.213985000
C	4.034651000	-3.303694000	-0.599172000
H	4.383286000	-3.957222000	-1.401194000
C	4.412917000	-3.335398000	3.094903000
H	-2.194364000	-4.933082000	-2.866299000
H	-0.725109000	-3.970402000	-2.998334000
H	-0.276378000	-4.335735000	-0.543751000
H	-1.697345000	-5.376440000	-0.441282000
H	-4.083869000	-5.362030000	-1.553712000
H	-2.405969000	-1.972614000	-4.123064000
H	-3.605311000	-3.248774000	-3.930180000
H	1.523835000	-2.273063000	-4.989176000
H	0.045207000	-1.721822000	-4.202075000
H	4.115811000	-0.535000000	-2.485003000
H	3.132578000	-1.806255000	-3.165183000
H	3.885770000	-1.177650000	-5.495063000

H	4.863467000	0.133206000	-4.831028000
H	2.148490000	-4.341835000	-0.437848000
H	3.343185000	-4.854697000	0.750691000
H	3.658136000	-2.384173000	-1.047538000
H	4.898596000	-3.046452000	0.016682000
H	3.851863000	-3.994191000	3.760612000
H	4.899285000	-3.957232000	2.340894000
H	1.934515000	-4.879255000	2.734176000
H	0.450110000	-4.465550000	1.881265000
P	-2.435937000	-2.759713000	-1.886999000
H	0.435387000	0.602309000	-5.079150000
H	0.173686000	-1.698928000	-5.968112000
H	1.948343000	0.074599000	-5.809671000
P	2.120435000	0.314563000	-3.434395000
P	2.155962000	-2.879374000	1.429426000
C	3.526271000	-2.271164000	2.470852000
H	3.060961000	-1.646722000	3.237475000
H	4.102043000	-1.589545000	1.839249000
H	5.201118000	-2.868326000	3.689166000
H	-5.467343000	-4.699099000	-0.692654000
C	-3.809310000	-3.329238000	-0.828611000
C	-4.664435000	-4.452096000	-1.390311000
C	-3.215008000	-2.330414000	-3.481294000
C	-4.296673000	-1.273641000	-3.352599000
C	1.253777000	-4.055640000	2.498046000
C	0.686724000	-3.440643000	3.764455000
H	-3.347488000	-3.614188000	0.119828000
H	-4.406304000	-2.439480000	-0.612393000
Co	-1.286903000	-1.203503000	-0.986699000
Co	0.934178000	0.273466000	-1.653225000
H	2.008900000	2.648893000	-3.858398000
C	2.842788000	1.943077000	-3.840028000
H	3.246723000	1.892958000	-4.855814000
Co	0.965798000	-1.302566000	0.611155000
H	-5.129339000	-4.176779000	-2.339034000
H	-4.642559000	-0.953776000	-4.337465000
H	-5.162152000	-1.645908000	-2.801072000
H	-3.913796000	-0.400857000	-2.823921000
H	0.018587000	-2.612774000	3.523953000
H	0.118991000	-4.183996000	4.327589000
H	1.473265000	-3.058416000	4.418189000
S	-1.072235000	0.276531000	-2.618702000
S	-2.858775000	0.082833000	-0.108242000
S	0.748294000	-1.928751000	-1.487648000
S	-1.072199000	-2.077238000	1.009052000
S	0.645220000	2.402790000	-1.191443000

S	2.456836000	0.189335000	-0.054672000
C	3.900511000	2.394262000	-2.849823000
H	4.197709000	3.426171000	-3.046610000
H	4.797457000	1.774575000	-2.908255000
H	3.520262000	2.335180000	-1.830328000
S	0.722792000	-0.083710000	2.426580000
Co	-1.367876000	1.562712000	-0.864837000
Fe	-1.192775000	0.148484000	1.430109000
Co	0.788104000	1.413687000	0.786543000
P	-2.569939000	3.067605000	-1.791608000
S	-1.207178000	2.301694000	1.203116000
P	-2.386278000	0.176198000	3.272591000
P	1.982760000	2.968178000	1.730169000
H	-3.465880000	1.742281000	-3.531750000
C	-1.666277000	4.193843000	-2.910691000
H	-2.358649000	4.984570000	-3.215853000
C	-3.368902000	4.239415000	-0.640941000
H	-2.567108000	4.653923000	-0.024488000
H	-3.780496000	5.063231000	-1.231794000
H	-4.508792000	1.752320000	-2.133916000
C	-3.936961000	2.403257000	-2.800385000
H	-0.890016000	4.662400000	-2.300039000
H	-3.458491000	2.268887000	2.951374000
H	-4.409609000	0.950630000	2.319010000
C	-3.842667000	1.275661000	3.195518000
C	-3.076290000	-1.449608000	3.747921000
H	-3.459754000	-1.364128000	4.769585000
H	-2.229635000	-2.139623000	3.776573000
C	-1.518698000	0.670431000	4.802506000
H	-0.714055000	-0.057066000	4.937493000
H	-2.213146000	0.542084000	5.637885000
H	2.912088000	3.870387000	-0.247028000
C	1.083483000	4.497399000	2.176652000
H	0.248687000	4.190244000	2.810840000
H	1.756831000	5.095686000	2.798328000
C	3.366492000	3.547956000	0.692502000
H	3.953889000	2.658547000	0.452225000
H	1.961102000	2.131805000	3.957151000
C	2.763365000	2.504720000	3.316581000
H	3.145542000	3.420156000	3.778288000
C	-4.830417000	3.428325000	-3.477270000
H	-1.811871000	3.073740000	-4.767540000
C	-1.051211000	3.515903000	-4.121101000
H	-0.487162000	4.237268000	-4.715870000
H	-0.374526000	2.716984000	-3.814885000
C	-4.437536000	3.600546000	0.227967000

H	-4.784779000	4.301692000	0.989315000
H	-4.050657000	2.713088000	0.730002000
H	-5.304548000	3.295811000	-0.361209000
H	-5.611485000	2.925357000	-4.051240000
H	-5.326090000	4.080726000	-2.755763000
H	-4.272711000	4.059746000	-4.171721000
C	-4.716257000	1.318088000	4.437823000
H	-5.566096000	1.984577000	4.276191000
H	-4.170517000	1.692630000	5.305902000
H	-5.117897000	0.335581000	4.693095000
H	-5.044768000	-1.342265000	2.834989000
H	-3.783850000	-1.977311000	1.776689000
C	-4.147778000	-1.963822000	2.804221000
H	-4.439504000	-2.979936000	3.076972000
C	-0.958187000	2.079646000	4.768444000
H	-1.747616000	2.829632000	4.685482000
H	-0.393196000	2.290838000	5.678602000
H	-0.293667000	2.201800000	3.912786000
C	4.233117000	4.642131000	1.292976000
C	0.582214000	5.308102000	0.994292000
H	0.004498000	6.166039000	1.344085000
H	1.405739000	5.687973000	0.386548000
H	-0.056754000	4.705922000	0.346788000
H	4.700527000	4.327866000	2.227992000
H	3.662876000	5.551205000	1.492568000
H	5.034742000	4.906298000	0.600174000
C	3.857952000	1.462047000	3.178149000
H	4.215390000	1.152174000	4.162099000
H	4.713770000	1.844487000	2.618979000
H	3.487360000	0.580061000	2.656404000

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C	-1.514902000	-4.280424000	-2.309432000
C	-0.921959000	-5.004832000	-1.114398000
H	-0.328534000	-5.860450000	-1.442999000
C	1.254592000	-0.114767000	-4.984746000
C	0.720980000	-1.534547000	-5.037632000
C	3.549181000	-0.818568000	-3.375972000
C	4.433486000	-0.845976000	-4.610983000
H	5.263659000	-1.539998000	-4.463432000
C	2.949746000	-3.986166000	0.213985000
C	4.034651000	-3.303694000	-0.599172000
H	4.383286000	-3.957222000	-1.401194000
C	4.412917000	-3.335398000	3.094903000
H	-2.194364000	-4.933082000	-2.866299000
H	-0.725109000	-3.970402000	-2.998334000

H	-0.276378000	-4.335735000	-0.543751000
H	-1.697345000	-5.376440000	-0.441282000
H	-4.083869000	-5.362030000	-1.553712000
H	-2.405969000	-1.972614000	-4.123064000
H	-3.605311000	-3.248774000	-3.930180000
H	1.523835000	-2.273063000	-4.989176000
H	0.045207000	-1.721822000	-4.202075000
H	4.115811000	-0.535000000	-2.485003000
H	3.132578000	-1.806255000	-3.165183000
H	3.885770000	-1.177650000	-5.495063000
H	4.863467000	0.133206000	-4.831028000
H	2.148490000	-4.341835000	-0.437848000
H	3.343185000	-4.854697000	0.750691000
H	3.658136000	-2.384173000	-1.047538000
H	4.898596000	-3.046452000	0.016682000
H	3.851863000	-3.994191000	3.760612000
H	4.899285000	-3.957232000	2.340894000
H	1.934515000	-4.879255000	2.734176000
H	0.450110000	-4.465550000	1.881265000
P	-2.435937000	-2.759713000	-1.886999000
H	0.435387000	0.602309000	-5.079150000
H	0.173686000	-1.698928000	-5.968112000
H	1.948343000	0.074599000	-5.809671000
P	2.120435000	0.314563000	-3.434395000
P	2.155962000	-2.879374000	1.429426000
C	3.526271000	-2.271164000	2.470852000
H	3.060961000	-1.646722000	3.237475000
H	4.102043000	-1.589545000	1.839249000
H	5.201118000	-2.868326000	3.689166000
H	-5.467343000	-4.699099000	-0.692654000
C	-3.809310000	-3.329238000	-0.828611000
C	-4.664435000	-4.452096000	-1.390311000
C	-3.215008000	-2.330414000	-3.481294000
C	-4.296673000	-1.273641000	-3.352599000
C	1.253777000	-4.055640000	2.498046000
C	0.686724000	-3.440643000	3.764455000
H	-3.347488000	-3.614188000	0.119828000
H	-4.406304000	-2.439480000	-0.612393000
Co	-1.286903000	-1.203503000	-0.986699000
Co	0.934178000	0.273466000	-1.653225000
H	2.008900000	2.648893000	-3.858398000
C	2.842788000	1.943077000	-3.840028000
H	3.246723000	1.892958000	-4.855814000
Co	0.965798000	-1.302566000	0.611155000
H	-5.129339000	-4.176779000	-2.339034000
H	-4.642559000	-0.953776000	-4.337465000

H	-5.162152000	-1.645908000	-2.801072000
H	-3.913796000	-0.400857000	-2.823921000
H	0.018587000	-2.612774000	3.523953000
H	0.118991000	-4.183996000	4.327589000
H	1.473265000	-3.058416000	4.418189000
S	-1.072235000	0.276531000	-2.618702000
S	-2.858775000	0.082833000	-0.108242000
S	0.748294000	-1.928751000	-1.487648000
S	-1.072199000	-2.077238000	1.009052000
S	0.645220000	2.402790000	-1.191443000
S	2.456836000	0.189335000	-0.054672000
C	3.900511000	2.394262000	-2.849823000
H	4.197709000	3.426171000	-3.046610000
H	4.797457000	1.774575000	-2.908255000
H	3.520262000	2.335180000	-1.830328000
S	0.722792000	-0.083710000	2.426580000
Co	-1.367876000	1.562712000	-0.864837000
Fe	-1.192775000	0.148484000	1.430109000
Co	0.788104000	1.413687000	0.786543000
P	-2.569939000	3.067605000	-1.791608000
S	-1.207178000	2.301694000	1.203116000
P	-2.386278000	0.176198000	3.272591000
P	1.982760000	2.968178000	1.730169000
H	-3.465880000	1.742281000	-3.531750000
C	-1.666277000	4.193843000	-2.910691000
H	-2.358649000	4.984570000	-3.215853000
C	-3.368902000	4.239415000	-0.640941000
H	-2.567108000	4.653923000	-0.024488000
H	-3.780496000	5.063231000	-1.231794000
H	-4.508792000	1.752320000	-2.133916000
C	-3.936961000	2.403257000	-2.800385000
H	-0.890016000	4.662400000	-2.300039000
H	-3.458491000	2.268887000	2.951374000
H	-4.409609000	0.950630000	2.319010000
C	-3.842667000	1.275661000	3.195518000
C	-3.076290000	-1.449608000	3.747921000
H	-3.459754000	-1.364128000	4.769585000
H	-2.229635000	-2.139623000	3.776573000
C	-1.518698000	0.670431000	4.802506000
H	-0.714055000	-0.057066000	4.937493000
H	-2.213146000	0.542084000	5.637885000
H	2.912088000	3.870387000	-0.247028000
C	1.083483000	4.497399000	2.176652000
H	0.248687000	4.190244000	2.810840000
H	1.756831000	5.095686000	2.798328000
C	3.366492000	3.547956000	0.692502000

H	3.953889000	2.658547000	0.452225000
H	1.961102000	2.131805000	3.957151000
C	2.763365000	2.504720000	3.316581000
H	3.145542000	3.420156000	3.778288000
C	-4.830417000	3.428325000	-3.477270000
H	-1.811871000	3.073740000	-4.767540000
C	-1.051211000	3.515903000	-4.121101000
H	-0.487162000	4.237268000	-4.715870000
H	-0.374526000	2.716984000	-3.814885000
C	-4.437536000	3.600546000	0.227967000
H	-4.784779000	4.301692000	0.989315000
H	-4.050657000	2.713088000	0.730002000
H	-5.304548000	3.295811000	-0.361209000
H	-5.611485000	2.925357000	-4.051240000
H	-5.326090000	4.080726000	-2.755763000
H	-4.272711000	4.059746000	-4.171721000
C	-4.716257000	1.318088000	4.437823000
H	-5.566096000	1.984577000	4.276191000
H	-4.170517000	1.692630000	5.305902000
H	-5.117897000	0.335581000	4.693095000
H	-5.044768000	-1.342265000	2.834989000
H	-3.783850000	-1.977311000	1.776689000
C	-4.147778000	-1.963822000	2.804221000
H	-4.439504000	-2.979936000	3.076972000
C	-0.958187000	2.079646000	4.768444000
H	-1.747616000	2.829632000	4.685482000
H	-0.393196000	2.290838000	5.678602000
H	-0.293667000	2.201800000	3.912786000
C	4.233117000	4.642131000	1.292976000
C	0.582214000	5.308102000	0.994292000
H	0.004498000	6.166039000	1.344085000
H	1.405739000	5.687973000	0.386548000
H	-0.056754000	4.705922000	0.346788000
H	4.700527000	4.327866000	2.227992000
H	3.662876000	5.551205000	1.492568000
H	5.034742000	4.906298000	0.600174000
C	3.857952000	1.462047000	3.178149000
H	4.215390000	1.152174000	4.162099000
H	4.713770000	1.844487000	2.618979000
H	3.487360000	0.580061000	2.656404000

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C	-1.514235000	-4.284331000	-2.336051000
C	-0.949725000	-5.032987000	-1.142166000
H	-0.355757000	-5.886517000	-1.475089000
C	1.231544000	-0.154697000	-5.005360000

C	0.681289000	-1.568717000	-5.036428000
C	3.535856000	-0.879974000	-3.418028000
C	4.406991000	-0.922689000	-4.661976000
H	5.230237000	-1.626195000	-4.520804000
C	2.927648000	-3.949049000	0.289993000
C	3.990407000	-3.301754000	-0.578772000
H	4.313636000	-3.986541000	-1.365215000
C	4.472570000	-3.198554000	3.104215000
H	-2.185819000	-4.923598000	-2.917513000
H	-0.709150000	-3.967411000	-3.003645000
H	-0.310400000	-4.380164000	-0.546054000
H	-1.740637000	-5.412051000	-0.491663000
H	-4.106408000	-5.358186000	-1.641097000
H	-2.372751000	-1.959759000	-4.139725000
H	-3.583629000	-3.228076000	-3.970795000
H	1.477284000	-2.315159000	-4.996731000
H	0.020751000	-1.740162000	-4.185153000
H	4.113311000	-0.598005000	-2.533644000
H	3.109947000	-1.861676000	-3.197786000
H	3.846356000	-1.250059000	-5.539632000
H	4.846476000	0.050612000	-4.889102000
H	2.106317000	-4.325711000	-0.324252000
H	3.333588000	-4.798263000	0.847981000
H	3.604253000	-2.397382000	-1.049092000
H	4.872099000	-3.025389000	0.002606000
H	3.929576000	-3.829508000	3.810494000
H	4.935173000	-3.850072000	2.360307000
H	2.008485000	-4.729002000	2.893145000
H	0.508168000	-4.401331000	2.032220000
P	-2.437296000	-2.766027000	-1.910327000
H	0.419574000	0.571502000	-5.093109000
H	0.113569000	-1.736242000	-5.953975000
H	1.914958000	0.019466000	-5.842160000
P	2.121606000	0.270686000	-3.467411000
P	2.171243000	-2.797114000	1.487004000
C	3.570608000	-2.155255000	2.467208000
H	3.126669000	-1.502765000	3.222915000
H	4.128527000	-1.498074000	1.795438000
H	5.278935000	-2.711836000	3.656824000
H	-5.494271000	-4.703968000	-0.780164000
C	-3.827559000	-3.340086000	-0.877202000
C	-4.683859000	-4.448508000	-1.465992000
C	-3.192303000	-2.315699000	-3.510613000
C	-4.267865000	-1.251723000	-3.390784000
C	1.303525000	-3.937427000	2.621073000
C	0.728598000	-3.274811000	3.859698000

H	-3.379091000	-3.642630000	0.072248000
H	-4.421281000	-2.449248000	-0.656388000
Co	-1.303124000	-1.220905000	-0.967992000
Co	0.947105000	0.238927000	-1.690521000
H	2.029677000	2.602358000	-3.900598000
C	2.857789000	1.889891000	-3.881767000
H	3.259817000	1.831330000	-4.897936000
Co	0.947499000	-1.259491000	0.635857000
H	-5.138718000	-4.153192000	-2.413497000
H	-4.604810000	-0.932734000	-4.379015000
H	-5.139662000	-1.616982000	-2.844493000
H	-3.882800000	-0.379289000	-2.862831000
H	0.035011000	-2.479247000	3.583811000
H	0.191020000	-4.006091000	4.466808000
H	1.509357000	-2.834833000	4.483449000
S	-1.073124000	0.262165000	-2.589829000
S	-2.891763000	0.121977000	-0.132587000
S	0.729309000	-1.940833000	-1.454182000
S	-1.052526000	-2.151825000	1.030941000
S	0.683941000	2.382770000	-1.225618000
S	2.474405000	0.181517000	-0.081843000
C	3.920299000	2.335575000	-2.894155000
H	4.231016000	3.361793000	-3.099747000
H	4.809252000	1.703800000	-2.945794000
H	3.537764000	2.290439000	-1.874628000
S	0.732274000	0.017678000	2.435169000
Co	-1.326019000	1.559433000	-0.824836000
Fe	-1.297597000	0.056716000	1.464542000
Co	0.908908000	1.504999000	0.780816000
P	-2.506552000	3.096064000	-1.732581000
S	-1.118408000	2.299360000	1.254087000
P	-2.561421000	0.007883000	3.352970000
P	2.087889000	3.054795000	1.664688000
H	-3.434557000	1.793964000	-3.474997000
C	-1.603804000	4.213999000	-2.859866000
H	-2.286490000	5.021129000	-3.143155000
C	-3.280290000	4.268190000	-0.565375000
H	-2.466547000	4.667537000	0.044900000
H	-3.689472000	5.100604000	-1.145889000
H	-4.465057000	1.804459000	-2.067983000
C	-3.891000000	2.454089000	-2.733582000
H	-0.803125000	4.659865000	-2.264501000
H	-3.511706000	2.147711000	3.037703000
H	-4.511004000	0.894869000	2.348134000
C	-3.959068000	1.173466000	3.249639000
C	-3.294152000	-1.615874000	3.740928000

H	-3.729296000	-1.563528000	4.743979000
H	-2.457836000	-2.318360000	3.785019000
C	-1.668303000	0.441406000	4.883638000
H	-0.861054000	-0.289998000	4.975130000
H	-2.351643000	0.279333000	5.723285000
H	3.000968000	3.918069000	-0.334269000
C	1.181144000	4.581801000	2.098850000
H	0.384576000	4.274526000	2.781272000
H	1.866167000	5.218691000	2.667177000
C	3.463244000	3.619204000	0.609466000
H	4.050985000	2.725465000	0.385112000
H	2.055228000	2.253075000	3.897066000
C	2.865382000	2.612131000	3.257266000
H	3.255760000	3.527903000	3.711400000
C	-4.778094000	3.495826000	-3.393454000
H	-1.818385000	3.114872000	-4.722981000
C	-1.032868000	3.530818000	-4.088924000
H	-0.462659000	4.242645000	-4.689300000
H	-0.369733000	2.713346000	-3.802177000
C	-4.344437000	3.634233000	0.312434000
H	-4.681256000	4.337934000	1.076190000
H	-3.952780000	2.747251000	0.811405000
H	-5.218207000	3.333124000	-0.268689000
H	-5.572511000	3.007621000	-3.961869000
H	-5.256522000	4.149919000	-2.661863000
H	-4.220119000	4.124528000	-4.090081000
C	-4.864577000	1.226108000	4.468372000
H	-5.673168000	1.941220000	4.303419000
H	-4.325175000	1.544295000	5.362535000
H	-5.323695000	0.258233000	4.679278000
H	-5.203140000	-1.433733000	2.718947000
H	-3.889722000	-2.046458000	1.712019000
C	-4.316478000	-2.070696000	2.715075000
H	-4.640338000	-3.091643000	2.925512000
C	-1.108262000	1.852349000	4.893091000
H	-1.899545000	2.603424000	4.852104000
H	-0.532523000	2.024442000	5.804475000
H	-0.453320000	2.009262000	4.034824000
C	4.330170000	4.728608000	1.180126000
C	0.604087000	5.330964000	0.911056000
H	0.013570000	6.184467000	1.250173000
H	1.388926000	5.709665000	0.253181000
H	-0.039689000	4.678821000	0.318951000
H	4.795551000	4.439144000	2.124330000
H	3.758763000	5.642189000	1.354757000
H	5.133085000	4.975076000	0.482368000

C	3.948074000	1.556366000	3.126856000
H	4.289640000	1.231548000	4.111596000
H	4.815522000	1.933567000	2.581940000
H	3.571362000	0.685889000	2.589542000

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C	-1.508886000	-4.277204000	-2.365685000
C	-0.941560000	-5.033540000	-1.178118000
H	-0.358926000	-5.892070000	-1.518211000
C	1.268777000	-0.153995000	-5.042944000
C	0.715335000	-1.566991000	-5.071736000
C	3.570329000	-0.878513000	-3.451875000
C	4.444654000	-0.921087000	-4.693482000
H	5.268096000	-1.624140000	-4.550958000
C	2.953365000	-3.948347000	0.275077000
C	4.012641000	-3.302392000	-0.599100000
H	4.341045000	-3.992707000	-1.378518000
C	4.482346000	-3.189708000	3.097831000
H	-2.187289000	-4.911259000	-2.945080000
H	-0.705952000	-3.963956000	-3.037855000
H	-0.290309000	-4.389006000	-0.586024000
H	-1.730573000	-5.406387000	-0.521765000
H	-4.102260000	-5.336219000	-1.644391000
H	-2.366706000	-1.960259000	-4.169654000
H	-3.578968000	-3.224607000	-3.987074000
H	1.509798000	-2.314952000	-5.030247000
H	0.054099000	-1.736421000	-4.220468000
H	4.146232000	-0.597109000	-2.566138000
H	3.144672000	-1.860730000	-3.232542000
H	3.886090000	-1.248233000	-5.572561000
H	4.883936000	0.052613000	-4.919430000
H	2.133917000	-4.333924000	-0.336323000
H	3.363973000	-4.791694000	0.838513000
H	3.621543000	-2.405254000	-1.079249000
H	4.892015000	-3.014662000	-0.019740000
H	3.934144000	-3.816459000	3.803816000
H	4.948732000	-3.845482000	2.360020000
H	2.020880000	-4.722201000	2.870558000
H	0.525326000	-4.395740000	2.002759000
P	-2.421853000	-2.753392000	-1.935019000
H	0.458029000	0.573449000	-5.133694000
H	0.147463000	-1.735477000	-5.989003000
H	1.953000000	0.016990000	-5.879653000
P	2.154974000	0.271517000	-3.502266000
P	2.191181000	-2.792087000	1.464850000
C	3.585836000	-2.148380000	2.450062000

H	3.138443000	-1.491021000	3.199628000
H	4.149498000	-1.495653000	1.778649000
H	5.285886000	-2.701289000	3.653063000
H	-5.481458000	-4.670140000	-0.778668000
C	-3.807446000	-3.316891000	-0.889462000
C	-4.673193000	-4.422333000	-1.469761000
C	-3.184248000	-2.309982000	-3.534239000
C	-4.257461000	-1.243457000	-3.418305000
C	1.316896000	-3.930564000	2.595996000
C	0.735429000	-3.270896000	3.833355000
H	-3.354663000	-3.618767000	0.058181000
H	-4.394367000	-2.422082000	-0.666537000
Co	-1.265628000	-1.205589000	-1.007733000
Co	0.968250000	0.234025000	-1.721030000
H	2.063263000	2.603574000	-3.933901000
C	2.891479000	1.890929000	-3.916705000
H	3.293707000	1.835336000	-4.932894000
Co	0.968584000	-1.253536000	0.597053000
H	-5.131339000	-4.127929000	-2.415966000
H	-4.598749000	-0.932691000	-4.407687000
H	-5.127014000	-1.602806000	-2.864592000
H	-3.868920000	-0.367108000	-2.899798000
H	0.037473000	-2.478958000	3.558041000
H	0.200822000	-4.006035000	4.438503000
H	1.512831000	-2.828086000	4.459318000
S	-1.044428000	0.263144000	-2.631007000
S	-2.888287000	0.118655000	-0.188154000
S	0.754484000	-1.945479000	-1.481766000
S	-1.044648000	-2.160683000	0.999216000
S	0.704099000	2.378066000	-1.266915000
S	2.496546000	0.172808000	-0.118027000
C	3.953407000	2.335561000	-2.927797000
H	4.263457000	3.362575000	-3.130498000
H	4.842958000	1.704721000	-2.980553000
H	3.571037000	2.287732000	-1.908301000
S	0.761988000	0.029138000	2.413717000
Co	-1.297925000	1.549111000	-0.870901000
Fe	-1.299945000	0.053776000	1.445391000
Co	0.934430000	1.492169000	0.728711000
P	-2.496793000	3.090434000	-1.757940000
S	-1.094523000	2.304596000	1.224972000
P	-2.688634000	0.009143000	3.511312000
P	2.107934000	3.049376000	1.628325000
H	-3.418428000	1.801315000	-3.513215000
C	-1.601432000	4.224790000	-2.874907000
H	-2.289144000	5.028464000	-3.155758000

C	-3.274289000	4.242683000	-0.574155000
H	-2.458576000	4.654473000	0.025518000
H	-3.705120000	5.070079000	-1.146121000
H	-4.447802000	1.790537000	-2.105233000
C	-3.878079000	2.450718000	-2.764205000
H	-0.806075000	4.673234000	-2.274336000
H	-3.648138000	2.149321000	3.208343000
H	-4.645863000	0.899180000	2.520470000
C	-4.091499000	1.172782000	3.423163000
C	-3.407827000	-1.624276000	3.895988000
H	-3.863214000	-1.595414000	4.890874000
H	-2.559258000	-2.312959000	3.948680000
C	-1.766384000	0.442582000	5.027533000
H	-0.955719000	-0.288937000	5.096356000
H	-2.414589000	0.289502000	5.896082000
H	3.044213000	3.901363000	-0.365881000
C	1.201934000	4.581586000	2.046482000
H	0.396394000	4.281250000	2.721440000
H	1.883607000	5.216695000	2.620733000
C	3.495425000	3.606769000	0.584599000
H	4.085036000	2.711477000	0.371432000
H	2.049105000	2.258687000	3.862793000
C	2.867677000	2.612974000	3.230881000
H	3.255920000	3.529396000	3.685433000
C	-4.772286000	3.493696000	-3.412210000
H	-1.800074000	3.133836000	-4.744923000
C	-1.020391000	3.552634000	-4.105597000
H	-0.453805000	4.272112000	-4.700131000
H	-0.350774000	2.739435000	-3.821329000
C	-4.315475000	3.590452000	0.318077000
H	-4.666034000	4.295212000	1.074639000
H	-3.897559000	2.720786000	0.826983000
H	-5.184698000	3.259082000	-0.253472000
H	-5.559536000	3.006498000	-3.991351000
H	-5.260074000	4.131465000	-2.672504000
H	-4.217454000	4.138249000	-4.096783000
C	-4.999842000	1.228928000	4.639309000
H	-5.804823000	1.950056000	4.481682000
H	-4.457103000	1.535460000	5.535780000
H	-5.463477000	0.261694000	4.843911000
H	-5.287281000	-1.455260000	2.816563000
H	-3.945580000	-2.074160000	1.850882000
C	-4.399675000	-2.090569000	2.843040000
H	-4.729173000	-3.110319000	3.051053000
C	-1.197810000	1.852042000	5.003756000
H	-1.986996000	2.606123000	4.975005000

H	-0.597324000	2.035293000	5.896891000
H	-0.564165000	1.997603000	4.126927000
C	4.358124000	4.718147000	1.157969000
C	0.642754000	5.330632000	0.850051000
H	0.056280000	6.190511000	1.179975000
H	1.437104000	5.700133000	0.198363000
H	-0.000869000	4.681648000	0.254456000
H	4.810693000	4.434249000	2.110055000
H	3.786715000	5.634178000	1.319046000
H	5.170358000	4.957841000	0.468656000
C	3.948478000	1.553340000	3.115573000
H	4.277643000	1.229788000	4.104935000
H	4.823418000	1.926278000	2.579778000
H	3.574597000	0.682640000	2.576699000

Co6_0_1

C	1.270505000	-0.114927000	-5.026732000
C	0.721397000	-1.528672000	-5.090242000
C	3.540904000	-0.885431000	-3.415627000
C	4.437336000	-0.918725000	-4.641134000
H	5.249349000	-1.635869000	-4.498161000
C	2.908374000	-3.958141000	0.333569000
C	3.956985000	-3.330546000	-0.566182000
H	4.270936000	-4.032176000	-1.342305000
C	4.471443000	-3.177166000	3.128823000
H	1.518496000	-2.274144000	-5.044493000
H	0.041414000	-1.717047000	-4.258618000
H	4.101507000	-0.625534000	-2.513886000
H	3.096062000	-1.863746000	-3.218828000
H	3.889532000	-1.220718000	-5.536288000
H	4.892965000	0.053705000	-4.841310000
H	2.073899000	-4.337934000	-0.261267000
H	3.320340000	-4.797841000	0.902449000
H	3.556267000	-2.439499000	-1.049716000
H	4.845992000	-3.035437000	-0.004275000
H	3.923465000	-3.797351000	3.841458000
H	4.927634000	-3.841414000	2.391508000
H	1.992062000	-4.690917000	2.946407000
H	0.495578000	-4.355514000	2.073627000
H	0.456519000	0.610432000	-5.104550000
H	0.174672000	-1.682045000	-6.023344000
H	1.963028000	0.078301000	-5.852792000
P	2.137547000	0.281449000	-3.466684000
P	2.163567000	-2.773043000	1.508971000
C	3.574989000	-2.137660000	2.479289000
H	3.135474000	-1.469638000	3.223941000

H	4.134885000	-1.493764000	1.796270000
H	5.282683000	-2.691276000	3.676439000
C	1.294714000	-3.896467000	2.661039000
C	0.716951000	-3.211345000	3.885576000
Co	-1.322491000	-1.169196000	-0.952884000
Co	0.941569000	0.238246000	-1.717799000
H	2.084029000	2.614432000	-3.881670000
C	2.904571000	1.892991000	-3.865791000
H	3.317807000	1.840416000	-4.878195000
Co	0.962383000	-1.267415000	0.625966000
H	0.029781000	-2.418565000	3.586840000
H	0.170883000	-3.928944000	4.502602000
H	1.495798000	-2.761106000	4.505147000
S	-1.099925000	0.294264000	-2.607344000
S	-2.871743000	0.169668000	-0.068072000
S	0.691248000	-1.964569000	-1.475878000
S	-1.062666000	-2.084807000	1.048264000
S	0.695959000	2.403852000	-1.252012000
S	2.498557000	0.167756000	-0.119301000
C	3.957398000	2.317198000	-2.858609000
H	4.279817000	3.344638000	-3.042668000
H	4.841238000	1.677093000	-2.905218000
H	3.556902000	2.257384000	-1.846848000
S	0.727753000	0.033494000	2.406467000
Co	-1.330766000	1.592925000	-0.821022000
Co	-1.311818000	0.076580000	1.519383000
Co	0.943827000	1.511522000	0.761770000
P	-2.537974000	3.080866000	-1.716417000
S	-1.080335000	2.272477000	1.283452000
P	-2.511208000	0.017668000	3.258153000
P	2.095362000	3.046351000	1.651977000
H	-3.485727000	1.695470000	-3.383020000
C	-1.689131000	4.199104000	-2.889194000
H	-2.401784000	4.975218000	-3.187082000
C	-3.304636000	4.280757000	-0.569318000
H	-2.478633000	4.700711000	0.010504000
H	-3.738685000	5.093379000	-1.160573000
H	-4.483873000	1.756376000	-1.961578000
C	-3.936341000	2.387110000	-2.666643000
H	-0.898714000	4.685239000	-2.310994000
H	-3.430069000	2.188707000	3.080259000
H	-4.436937000	0.995941000	2.304202000
C	-3.893547000	1.210225000	3.227977000
C	-3.303760000	-1.592956000	3.602082000
H	-3.767102000	-1.539684000	4.592997000
H	-2.487158000	-2.317036000	3.660149000

C	-1.646504000	0.360341000	4.832680000
H	-0.844703000	-0.379766000	4.896019000
H	-2.341369000	0.164195000	5.655712000
H	3.026609000	3.910534000	-0.336416000
C	1.197255000	4.580851000	2.084013000
H	0.401627000	4.272624000	2.766902000
H	1.883468000	5.223035000	2.645797000
C	3.483061000	3.615474000	0.611307000
H	4.070262000	2.720187000	0.391997000
H	2.051871000	2.251907000	3.882521000
C	2.867957000	2.612392000	3.251369000
H	3.261317000	3.525683000	3.708975000
C	-4.847014000	3.390115000	-3.352823000
H	-1.869541000	3.033801000	-4.715674000
C	-1.098659000	3.506889000	-4.103650000
H	-0.566164000	4.225535000	-4.731440000
H	-0.398256000	2.729462000	-3.795683000
C	-4.333851000	3.657158000	0.355068000
H	-4.661825000	4.375473000	1.109908000
H	-3.909650000	2.791725000	0.864420000
H	-5.216928000	3.322730000	-0.193546000
H	-5.650826000	2.872953000	-3.882041000
H	-5.313055000	4.074483000	-2.640172000
H	-4.307580000	3.991679000	-4.087857000
C	-4.818485000	1.205248000	4.431990000
H	-5.605125000	1.953743000	4.309735000
H	-4.285955000	1.439374000	5.356477000
H	-5.307302000	0.237668000	4.564689000
H	-5.153437000	-1.329982000	2.490147000
H	-3.840097000	-2.053887000	1.560655000
C	-4.307990000	-2.019324000	2.545631000
H	-4.701464000	-3.012588000	2.772827000
C	-1.071745000	1.762765000	4.919694000
H	-1.856519000	2.522356000	4.911340000
H	-0.495845000	1.886035000	5.839791000
H	-0.414450000	1.954279000	4.069924000
C	4.346812000	4.725053000	1.185198000
C	0.610031000	5.315845000	0.892428000
H	0.016209000	6.170506000	1.225007000
H	1.389051000	5.689038000	0.223825000
H	-0.032760000	4.649578000	0.315381000
H	4.800147000	4.438303000	2.136651000
H	3.773513000	5.639494000	1.351462000
H	5.158651000	4.969470000	0.496026000
C	3.940952000	1.546803000	3.122083000
H	4.271221000	1.207115000	4.106323000

H	4.816569000	1.918076000	2.585215000
H	3.553403000	0.688031000	2.573845000

Co6_1_2

C	1.251090000	-0.121094000	-5.010040000
C	0.718736000	-1.540540000	-5.086057000
C	3.530779000	-0.870043000	-3.395621000
C	4.423280000	-0.900001000	-4.625065000
H	5.240892000	-1.608627000	-4.477459000
C	2.915664000	-3.968890000	0.264013000
C	3.987831000	-3.326254000	-0.597174000
H	4.295609000	-4.004026000	-1.395511000
C	4.475270000	-3.256670000	3.090501000
H	1.522186000	-2.277759000	-5.029843000
H	0.019629000	-1.744380000	-4.274291000
H	4.094949000	-0.600905000	-2.498880000
H	3.097797000	-1.853194000	-3.196839000
H	3.877406000	-1.214382000	-5.516383000
H	4.870810000	0.074256000	-4.831387000
H	2.084948000	-4.323204000	-0.351186000
H	3.309320000	-4.832478000	0.808577000
H	3.618300000	-2.407271000	-1.052466000
H	4.876445000	-3.076513000	-0.014258000
H	3.925851000	-3.886471000	3.792713000
H	4.929919000	-3.907897000	2.341609000
H	1.977940000	-4.763338000	2.864853000
H	0.485850000	-4.396520000	2.007848000
H	0.435068000	0.600467000	-5.099462000
H	0.194938000	-1.694605000	-6.031171000
H	1.948440000	0.079337000	-5.829683000
P	2.122779000	0.286517000	-3.459154000
P	2.180805000	-2.823657000	1.478202000
C	3.584402000	-2.198748000	2.461043000
H	3.147379000	-1.547373000	3.221922000
H	4.150118000	-1.543078000	1.794174000
H	5.287276000	-2.782687000	3.645735000
C	1.289773000	-3.954182000	2.601615000
C	0.730992000	-3.292756000	3.848344000
Co	-1.332847000	-1.183178000	-0.980935000
Co	0.932489000	0.257994000	-1.678816000
H	2.048109000	2.624474000	-3.871552000
C	2.871579000	1.906882000	-3.846022000
H	3.285735000	1.852679000	-4.857508000
Co	0.967571000	-1.267955000	0.635775000
H	0.048964000	-2.483385000	3.584243000
H	0.183614000	-4.020738000	4.450263000

H	1.521193000	-2.871940000	4.473463000
S	-1.089640000	0.312224000	-2.618540000
S	-2.901236000	0.154343000	-0.112022000
S	0.709901000	-1.954428000	-1.476168000
S	-1.075991000	-2.116244000	1.022552000
S	0.670927000	2.397030000	-1.216044000
S	2.460920000	0.178137000	-0.087996000
C	3.925406000	2.340518000	-2.844162000
H	4.248563000	3.363856000	-3.044565000
H	4.808850000	1.700456000	-2.885370000
H	3.530473000	2.298746000	-1.829299000
S	0.722498000	-0.005931000	2.417550000
Co	-1.342114000	1.610524000	-0.830135000
Co	-1.289450000	0.085798000	1.467566000
Co	0.878372000	1.482539000	0.785072000
P	-2.557551000	3.102869000	-1.763966000
S	-1.132857000	2.293550000	1.252713000
P	-2.504865000	0.089348000	3.334657000
P	2.066843000	3.028765000	1.701401000
H	-3.480348000	1.695018000	-3.431821000
C	-1.678439000	4.206403000	-2.922077000
H	-2.386909000	4.979768000	-3.235215000
C	-3.332742000	4.291856000	-0.616135000
H	-2.515893000	4.722687000	-0.031263000
H	-3.763297000	5.101036000	-1.213842000
H	-4.497922000	1.767293000	-2.022198000
C	-3.936717000	2.390660000	-2.723201000
H	-0.900604000	4.700850000	-2.334053000
H	-3.479131000	2.226745000	3.052824000
H	-4.461510000	0.969754000	2.344555000
C	-3.911509000	1.242671000	3.249172000
C	-3.227416000	-1.540621000	3.721682000
H	-3.656623000	-1.478100000	4.727112000
H	-2.387018000	-2.237841000	3.772453000
C	-1.598842000	0.520110000	4.856716000
H	-0.797433000	-0.217560000	4.947288000
H	-2.279099000	0.367044000	5.700355000
H	2.993909000	3.908033000	-0.285569000
C	1.162888000	4.556029000	2.140755000
H	0.356901000	4.248105000	2.811629000
H	1.844800000	5.183237000	2.723231000
C	3.449521000	3.597653000	0.657720000
H	4.036404000	2.704879000	0.427359000
H	2.026500000	2.215502000	3.931802000
C	2.838463000	2.570935000	3.292571000
H	3.236867000	3.480700000	3.751594000

C	-4.838094000	3.391218000	-3.426738000
H	-1.832411000	3.028720000	-4.743407000
C	-1.071598000	3.510234000	-4.126119000
H	-0.541981000	4.230649000	-4.752729000
H	-0.362516000	2.742786000	-3.812434000
C	-4.374779000	3.669337000	0.295502000
H	-4.713587000	4.392458000	1.039766000
H	-3.963234000	2.806034000	0.819243000
H	-5.250335000	3.335343000	-0.264189000
H	-5.633786000	2.867599000	-3.960116000
H	-5.314041000	4.079321000	-2.725228000
H	-4.291292000	3.985991000	-4.161001000
C	-4.819999000	1.265498000	4.466917000
H	-5.632581000	1.978476000	4.313681000
H	-4.285375000	1.569566000	5.368845000
H	-5.273860000	0.291040000	4.656691000
H	-5.127782000	-1.359866000	2.681622000
H	-3.834322000	-2.069264000	1.710284000
C	-4.258396000	-2.019208000	2.714339000
H	-4.609716000	-3.016954000	2.982480000
C	-1.028271000	1.926828000	4.858541000
H	-1.813607000	2.683694000	4.810903000
H	-0.453542000	2.100758000	5.770166000
H	-0.369476000	2.073747000	4.001519000
C	4.317634000	4.698293000	1.243811000
C	0.605094000	5.321875000	0.954072000
H	0.016226000	6.175236000	1.296131000
H	1.400463000	5.703569000	0.310889000
H	-0.036446000	4.683495000	0.344221000
H	4.779411000	4.396870000	2.185960000
H	3.748454000	5.611530000	1.426855000
H	5.123341000	4.950177000	0.551311000
C	3.912161000	1.506546000	3.156790000
H	4.250990000	1.174467000	4.139974000
H	4.782892000	1.878214000	2.613514000
H	3.528662000	0.640901000	2.616206000

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C	1.294264000	-0.066188000	-5.029471000
C	0.759247000	-1.484099000	-5.119523000
C	3.563121000	-0.848666000	-3.413161000
C	4.470417000	-0.861483000	-4.632092000
H	5.280303000	-1.579762000	-4.488942000
C	2.863220000	-3.981574000	0.234645000
C	3.932592000	-3.343097000	-0.632965000
H	4.233626000	-4.022375000	-1.432612000

C	4.441188000	-3.274175000	3.048035000
H	1.562288000	-2.222678000	-5.078338000
H	0.065593000	-1.696887000	-4.305135000
H	4.117789000	-0.601598000	-2.504204000
H	3.119411000	-1.831664000	-3.238674000
H	3.933065000	-1.153009000	-5.536295000
H	4.928170000	0.113078000	-4.813022000
H	2.028842000	-4.335749000	-0.375522000
H	3.258099000	-4.844594000	0.779205000
H	3.563194000	-2.423316000	-1.086867000
H	4.825206000	-3.095752000	-0.055158000
H	3.894333000	-3.901353000	3.754558000
H	4.887861000	-3.927704000	2.296371000
H	1.943721000	-4.771611000	2.838137000
H	0.443006000	-4.401461000	1.997506000
H	0.479651000	0.657889000	-5.110749000
H	0.228406000	-1.625860000	-6.062555000
H	1.992183000	0.141945000	-5.846768000
P	2.165155000	0.319099000	-3.473123000
P	2.137009000	-2.832121000	1.450615000
C	3.550178000	-2.212843000	2.424506000
H	3.121139000	-1.560212000	3.188811000
H	4.113868000	-1.559264000	1.753945000
H	5.259121000	-2.803252000	3.597193000
C	1.254312000	-3.961102000	2.582488000
C	0.710826000	-3.298669000	3.835385000
Co	-1.332801000	-1.182668000	-0.987203000
Co	0.958625000	0.263013000	-1.710462000
H	2.102621000	2.662656000	-3.845971000
C	2.922834000	1.941063000	-3.829430000
H	3.341921000	1.902465000	-4.839569000
Co	0.931134000	-1.263033000	0.618032000
H	0.030224000	-2.485829000	3.578590000
H	0.165521000	-4.024668000	4.441571000
H	1.509048000	-2.882619000	4.453485000
S	-1.075758000	0.295646000	-2.631002000
S	-2.910211000	0.146301000	-0.104733000
S	0.703389000	-1.947936000	-1.494029000
S	-1.098069000	-2.113188000	1.026998000
S	0.672405000	2.388698000	-1.220853000
S	2.453367000	0.174333000	-0.092535000
C	3.972885000	2.350719000	-2.813327000
H	4.296517000	3.378677000	-2.987317000
H	4.856648000	1.712021000	-2.866501000
H	3.573526000	2.283501000	-1.801595000
S	0.717062000	-0.009237000	2.417104000

Co	-1.339170000	1.572288000	-0.831795000
Co	-1.300317000	0.096459000	1.491695000
Co	0.871458000	1.479183000	0.784335000
P	-2.564744000	3.049050000	-1.780197000
S	-1.139083000	2.295688000	1.242853000
P	-2.495540000	0.123367000	3.381998000
P	2.055857000	3.022970000	1.707627000
H	-3.481471000	1.636337000	-3.447193000
C	-1.692758000	4.158624000	-2.938583000
H	-2.411131000	4.920045000	-3.258296000
C	-3.346725000	4.240884000	-0.639176000
H	-2.532063000	4.681073000	-0.058154000
H	-3.781728000	5.042997000	-1.243179000
H	-4.499843000	1.706754000	-2.038218000
C	-3.940991000	2.331261000	-2.740037000
H	-0.926275000	4.667380000	-2.347786000
H	-3.479555000	2.255683000	3.089374000
H	-4.461511000	0.989159000	2.398925000
C	-3.906550000	1.271585000	3.297767000
C	-3.209378000	-1.507329000	3.782404000
H	-3.629444000	-1.445715000	4.791685000
H	-2.366076000	-2.201688000	3.825932000
C	-1.578425000	0.567288000	4.893575000
H	-0.778002000	-0.171447000	4.985415000
H	-2.250510000	0.426450000	5.745758000
H	2.988447000	3.901148000	-0.277444000
C	1.150808000	4.549936000	2.144994000
H	0.340979000	4.242362000	2.811224000
H	1.830901000	5.175020000	2.731910000
C	3.440947000	3.591789000	0.667565000
H	4.029438000	2.699363000	0.440520000
H	2.012818000	2.206369000	3.937561000
C	2.824973000	2.562446000	3.299163000
H	3.222425000	3.472202000	3.759086000
C	-4.846233000	3.326850000	-3.445442000
H	-1.815731000	2.965146000	-4.752070000
C	-1.067828000	3.468845000	-4.136672000
H	-0.553807000	4.197165000	-4.767222000
H	-0.341503000	2.720872000	-3.815726000
C	-4.385359000	3.621221000	0.277984000
H	-4.729545000	4.350071000	1.014188000
H	-3.968939000	2.766111000	0.811238000
H	-5.258137000	3.275475000	-0.278900000
H	-5.639606000	2.798847000	-3.977973000
H	-5.325414000	4.014096000	-2.745287000
H	-4.301954000	3.922614000	-4.180766000

C	-4.807296000	1.302254000	4.521094000
H	-5.623628000	2.010878000	4.367517000
H	-4.267483000	1.615920000	5.416661000
H	-5.256020000	0.327748000	4.722570000
H	-5.119332000	-1.336174000	2.757665000
H	-3.831670000	-2.043347000	1.776965000
C	-4.247188000	-1.992139000	2.784601000
H	-4.592559000	-2.990606000	3.057786000
C	-1.003623000	1.972295000	4.872066000
H	-1.787253000	2.730862000	4.822808000
H	-0.418695000	2.156822000	5.775088000
H	-0.353715000	2.106407000	4.006079000
C	4.306145000	4.693266000	1.256607000
C	0.600758000	5.318570000	0.956463000
H	0.011385000	6.172147000	1.296994000
H	1.400264000	5.700198000	0.318429000
H	-0.038641000	4.682726000	0.341682000
H	4.765338000	4.392223000	2.200121000
H	3.735826000	5.606141000	1.437744000
H	5.113798000	4.945543000	0.566521000
C	3.899666000	1.498887000	3.163785000
H	4.236951000	1.166339000	4.147311000
H	4.771081000	1.871696000	2.622448000
H	3.517927000	0.633231000	2.621948000

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C	-1.552125000	-4.322080000	-2.296531000
C	-0.955440000	-5.041518000	-1.100539000
H	-0.379218000	-5.908395000	-1.429613000
C	2.943905000	-3.982702000	0.333194000
C	3.976841000	-3.334921000	-0.572280000
H	4.352126000	-4.061139000	-1.295340000
C	4.447812000	-3.218549000	3.175236000
H	-2.238327000	-4.976489000	-2.843494000
H	-0.768311000	-4.020934000	-2.996088000
H	-0.292915000	-4.378284000	-0.542341000
H	-1.727473000	-5.395622000	-0.414383000
H	-4.158389000	-5.365894000	-1.568750000
H	-2.370847000	-2.029595000	-4.131791000
H	-3.612163000	-3.266495000	-3.951347000
H	2.125312000	-4.404636000	-0.255353000
H	3.383406000	-4.803827000	0.908577000
H	3.546966000	-2.498201000	-1.124719000
H	4.831886000	-2.961549000	-0.005455000
H	3.897074000	-3.863985000	3.862203000
H	4.939054000	-3.854367000	2.436399000

H	1.956246000	-4.761806000	2.936422000
H	0.480441000	-4.419101000	2.038259000
P	-2.471102000	-2.796184000	-1.894971000
P	2.171125000	-2.838372000	1.525620000
C	3.547898000	-2.181471000	2.524775000
H	3.086960000	-1.529899000	3.271004000
H	4.113663000	-1.524448000	1.859529000
H	5.232299000	-2.724366000	3.751938000
H	-5.543097000	-4.676459000	-0.730934000
C	-3.862318000	-3.333942000	-0.849149000
C	-4.726845000	-4.446288000	-1.418523000
C	-3.205751000	-2.353452000	-3.505170000
C	-4.261806000	-1.267506000	-3.414754000
C	1.268110000	-3.962878000	2.643033000
C	0.674978000	-3.280507000	3.862294000
H	-3.415725000	-3.623048000	0.105140000
H	-4.447962000	-2.433488000	-0.647111000
Co	-1.288222000	-1.233973000	-1.045646000
Co	1.005402000	0.233659000	-1.734533000
Co	0.987296000	-1.317312000	0.605408000
H	-5.173774000	-4.167663000	-2.374730000
H	-4.584032000	-0.963517000	-4.412340000
H	-5.144594000	-1.607070000	-2.869442000
H	-3.867841000	-0.391037000	-2.899643000
H	0.005949000	-2.471774000	3.564082000
H	0.105842000	-3.996065000	4.458921000
H	1.448181000	-2.853492000	4.503951000
S	-1.018470000	0.267158000	-2.669581000
S	-2.833849000	0.111598000	-0.180532000
S	0.762396000	-1.963084000	-1.515363000
S	-1.047169000	-2.114389000	0.969409000
S	0.723799000	2.390804000	-1.262224000
S	2.518384000	0.145185000	-0.098020000
S	0.701373000	-0.009126000	2.361090000
Co	-1.321207000	1.575816000	-0.895626000
Co	-1.327198000	0.030944000	1.455985000
Co	0.954544000	1.496954000	0.763142000
P	-2.549045000	3.117719000	-1.725399000
S	-1.091606000	2.220132000	1.209029000
P	-2.483413000	0.033695000	3.254014000
P	2.089962000	3.054933000	1.677377000
H	-3.435767000	1.833317000	-3.503101000
C	-1.657314000	4.283485000	-2.810262000
H	-2.357960000	5.085638000	-3.063530000
C	-3.346036000	4.227023000	-0.516562000
H	-2.541617000	4.616158000	0.112291000

H	-3.766190000	5.074087000	-1.067324000
H	-4.475359000	1.788818000	-2.101656000
C	-3.910499000	2.464890000	-2.748313000
H	-0.870535000	4.727142000	-2.194605000
H	-3.475184000	2.161380000	2.965270000
H	-4.476768000	0.890248000	2.312003000
C	-3.898791000	1.180514000	3.193343000
C	-3.206665000	-1.587701000	3.678293000
H	-3.609227000	-1.524817000	4.694081000
H	-2.372579000	-2.293131000	3.703125000
C	-1.581247000	0.478903000	4.777614000
H	-0.774603000	-0.252067000	4.874154000
H	-2.261968000	0.324423000	5.620428000
H	3.028347000	3.867755000	-0.338766000
C	1.170499000	4.580060000	2.079682000
H	0.373714000	4.278486000	2.764323000
H	1.850862000	5.229459000	2.639595000
C	3.475414000	3.588416000	0.618180000
H	4.059444000	2.687158000	0.415714000
H	2.022441000	2.274552000	3.916357000
C	2.843195000	2.615148000	3.280314000
H	3.242261000	3.530837000	3.727436000
C	-4.811528000	3.506011000	-3.391074000
H	-1.842743000	3.229293000	-4.702087000
C	-1.069269000	3.660473000	-4.063498000
H	-0.542737000	4.417571000	-4.647435000
H	-0.359901000	2.870251000	-3.815533000
C	-4.403106000	3.541090000	0.328961000
H	-4.757035000	4.208598000	1.116967000
H	-3.999728000	2.642564000	0.796065000
H	-5.268115000	3.246809000	-0.268392000
H	-5.591869000	3.015448000	-3.976449000
H	-5.307712000	4.133661000	-2.648341000
H	-4.259405000	4.159517000	-4.068985000
C	-4.768199000	1.229962000	4.438519000
H	-5.594732000	1.928256000	4.291773000
H	-4.207677000	1.568293000	5.311961000
H	-5.202757000	0.256707000	4.674885000
H	-5.157870000	-1.420719000	2.737961000
H	-3.882511000	-2.013953000	1.673753000
C	-4.265804000	-2.048540000	2.693677000
H	-4.571706000	-3.073603000	2.911089000
C	-1.020685000	1.889482000	4.780984000
H	-1.811295000	2.640953000	4.731428000
H	-0.448804000	2.068589000	5.693627000
H	-0.361708000	2.042092000	3.924818000

C	4.341082000	4.703959000	1.179976000
C	0.594223000	5.305979000	0.877452000
H	0.018797000	6.175881000	1.200048000
H	1.377628000	5.656763000	0.202874000
H	-0.066491000	4.647780000	0.311095000
H	4.791726000	4.430789000	2.136156000
H	3.773608000	5.624824000	1.327196000
H	5.154746000	4.930018000	0.488142000
C	3.912040000	1.543042000	3.171722000
H	4.249112000	1.236529000	4.163699000
H	4.784455000	1.896336000	2.619049000
H	3.521433000	0.664967000	2.657033000

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C	-1.539452000	-4.282119000	-2.378062000
C	-0.965238000	-5.064839000	-1.210433000
H	-0.401873000	-5.925235000	-1.575946000
C	1.265335000	-0.176939000	-5.024750000
C	0.707204000	-1.588181000	-5.038122000
C	3.560165000	-0.880150000	-3.387506000
C	4.449246000	-0.944447000	-4.618298000
H	5.268974000	-1.645845000	-4.451026000
H	-2.221528000	-4.903321000	-2.967522000
H	-0.744008000	-3.951892000	-3.051061000
H	-0.291535000	-4.448565000	-0.613888000
H	-1.750738000	-5.440045000	-0.551447000
H	-4.115215000	-5.371741000	-1.640452000
H	-2.447691000	-1.927661000	-4.121366000
H	-3.661053000	-3.191898000	-3.945203000
H	1.497956000	-2.338450000	-4.975908000
H	0.031612000	-1.740938000	-4.194943000
H	4.122448000	-0.582338000	-2.498814000
H	3.132793000	-1.857073000	-3.149001000
H	3.902107000	-1.287363000	-5.498534000
H	4.893545000	0.024394000	-4.855266000
P	-2.462016000	-2.778485000	-1.908912000
H	0.459706000	0.554223000	-5.130649000
H	0.151587000	-1.767006000	-5.960749000
H	1.956813000	-0.020414000	-5.858597000
P	2.149513000	0.271169000	-3.492280000
H	-5.480307000	-4.736391000	-0.730825000
C	-3.820929000	-3.367446000	-0.846072000
C	-4.689744000	-4.467033000	-1.434012000
C	-3.253199000	-2.290336000	-3.478095000
C	-4.319938000	-1.224847000	-3.305700000
H	-3.345812000	-3.688773000	0.083900000

H	-4.409065000	-2.482057000	-0.592192000
Co	-1.286158000	-1.261455000	-0.963303000
Co	0.974786000	0.242748000	-1.710482000
H	2.041189000	2.593124000	-3.967509000
C	2.876828000	1.890996000	-3.912818000
H	3.302461000	1.815184000	-4.918407000
Co	1.008994000	-1.272595000	0.634743000
H	-5.170872000	-4.154792000	-2.362863000
H	-4.672745000	-0.873238000	-4.277061000
H	-5.183586000	-1.603343000	-2.755734000
H	-3.922086000	-0.371919000	-2.755766000
S	-1.063015000	0.238490000	-2.577310000
S	-2.834053000	0.070873000	-0.077182000
S	0.773080000	-1.964115000	-1.467955000
S	-1.003001000	-2.133249000	1.068187000
S	0.679942000	2.378509000	-1.219257000
S	2.517595000	0.202981000	-0.093789000
C	3.913638000	2.369082000	-2.913338000
H	4.238322000	3.383067000	-3.154237000
H	4.798092000	1.729297000	-2.912345000
H	3.501142000	2.372847000	-1.904276000
S	0.728000000	0.010612000	2.424436000
Co	-1.340639000	1.547040000	-0.815396000
Co	-1.315452000	0.025325000	1.541273000
Co	0.950415000	1.521729000	0.799681000
P	-2.513420000	3.087597000	-1.725822000
S	-1.099917000	2.211336000	1.285271000
P	-2.534565000	0.065324000	3.295724000
P	2.083592000	3.100282000	1.687415000
H	-3.468556000	1.771025000	-3.442453000
C	-1.612760000	4.190596000	-2.868216000
H	-2.298808000	4.991316000	-3.161356000
C	-3.261297000	4.263802000	-0.547164000
H	-2.439538000	4.636446000	0.068870000
H	-3.650433000	5.112228000	-1.118295000
H	-4.485825000	1.810783000	-2.026194000
C	-3.911090000	2.445434000	-2.705485000
H	-0.813447000	4.648029000	-2.279906000
H	-3.530763000	2.185584000	2.970071000
H	-4.513609000	0.903683000	2.307295000
C	-3.953410000	1.203847000	3.196724000
C	-3.243234000	-1.561034000	3.720891000
H	-3.675194000	-1.485669000	4.723871000
H	-2.394096000	-2.246211000	3.784036000
C	-1.651161000	0.520100000	4.826728000
H	-0.855771000	-0.221051000	4.939612000

H	-2.347011000	0.375642000	5.659165000
H	2.983733000	3.982907000	-0.311024000
C	1.144778000	4.603725000	2.121578000
H	0.355908000	4.277855000	2.803935000
H	1.814460000	5.258337000	2.687889000
C	3.449575000	3.682121000	0.630395000
H	4.047455000	2.796514000	0.400891000
H	2.043532000	2.301473000	3.920277000
C	2.858527000	2.634168000	3.272411000
H	3.272161000	3.544940000	3.717158000
C	-4.791361000	3.489538000	-3.371485000
H	-1.826249000	3.063830000	-4.715143000
C	-1.041454000	3.493206000	-4.089245000
H	-0.477959000	4.200292000	-4.701329000
H	-0.371929000	2.683967000	-3.793742000
C	-4.340697000	3.641826000	0.320236000
H	-4.656714000	4.338836000	1.098662000
H	-3.972933000	2.734795000	0.800503000
H	-5.223618000	3.376759000	-0.264364000
H	-5.601798000	3.003788000	-3.918804000
H	-5.248101000	4.164862000	-2.645434000
H	-4.233659000	4.095771000	-4.087837000
C	-4.846381000	1.256649000	4.425132000
H	-5.669282000	1.955295000	4.261046000
H	-4.302736000	1.595799000	5.308864000
H	-5.286263000	0.284093000	4.654146000
H	-5.161549000	-1.435934000	2.709591000
H	-3.850780000	-2.064572000	1.711545000
C	-4.267013000	-2.061844000	2.719247000
H	-4.576425000	-3.079165000	2.965633000
C	-1.076735000	1.924726000	4.835797000
H	-1.858679000	2.684152000	4.770498000
H	-0.520137000	2.099297000	5.758607000
H	-0.400318000	2.069267000	3.991929000
C	4.306328000	4.795560000	1.209576000
C	0.551103000	5.329900000	0.927679000
H	-0.065939000	6.167063000	1.259624000
H	1.326747000	5.728860000	0.270898000
H	-0.070765000	4.654758000	0.337761000
H	4.782475000	4.498596000	2.145833000
H	3.724751000	5.699577000	1.399506000
H	5.100689000	5.060247000	0.508911000
C	3.919234000	1.553753000	3.149852000
H	4.298726000	1.284202000	4.136934000
H	4.767654000	1.888861000	2.549998000
H	3.512314000	0.653770000	2.686745000

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C	-1.525425000	-4.287579000	-2.344891000
C	-0.927315000	-5.019398000	-1.156597000
H	-0.313857000	-5.856730000	-1.494711000
C	1.263317000	-0.186462000	-5.038977000
C	0.690928000	-1.591830000	-5.056039000
C	3.571642000	-0.882359000	-3.423155000
C	4.462511000	-0.922702000	-4.653565000
H	5.286485000	-1.621860000	-4.497209000
C	2.891810000	-3.963419000	0.306792000
C	3.970895000	-3.337247000	-0.558027000
H	4.284644000	-4.029616000	-1.341510000
C	4.428221000	-3.210143000	3.135653000
H	-2.198867000	-4.938884000	-2.910563000
H	-0.739085000	-3.960716000	-3.029698000
H	-0.300806000	-4.347815000	-0.567538000
H	-1.700445000	-5.419025000	-0.497261000
H	-4.108560000	-5.380305000	-1.622450000
H	-2.425905000	-1.975398000	-4.129941000
H	-3.655160000	-3.218535000	-3.928617000
H	1.474136000	-2.350469000	-4.997058000
H	0.016508000	-1.742862000	-4.211703000
H	4.133310000	-0.590480000	-2.531874000
H	3.149957000	-1.866451000	-3.205172000
H	3.917841000	-1.254400000	-5.539475000
H	4.900929000	0.052430000	-4.874325000
H	2.067757000	-4.328974000	-0.310407000
H	3.280161000	-4.817563000	0.869885000
H	3.604180000	-2.426371000	-1.031818000
H	4.855124000	-3.077666000	0.027063000
H	3.870391000	-3.818137000	3.850402000
H	4.881586000	-3.883313000	2.405500000
H	1.936216000	-4.707267000	2.920465000
H	0.449266000	-4.358048000	2.043901000
P	-2.459941000	-2.784424000	-1.900675000
H	0.466425000	0.554292000	-5.143333000
H	0.132713000	-1.761323000	-5.978818000
H	1.955664000	-0.034900000	-5.873070000
P	2.152908000	0.257521000	-3.508327000
P	2.148614000	-2.794851000	1.496118000
C	3.549271000	-2.160587000	2.476404000
H	3.109735000	-1.488749000	3.217499000
H	4.124353000	-1.524064000	1.799154000
H	5.241154000	-2.729161000	3.683482000
H	-5.479073000	-4.741862000	-0.722901000

C	-3.823682000	-3.368647000	-0.841970000
C	-4.686400000	-4.475539000	-1.424861000
C	-3.239314000	-2.310120000	-3.481111000
C	-4.298521000	-1.229277000	-3.350366000
C	1.249887000	-3.904579000	2.633494000
C	0.681201000	-3.214048000	3.859637000
H	-3.355328000	-3.676898000	0.095757000
H	-4.417613000	-2.482480000	-0.604449000
Co	-1.321655000	-1.211163000	-1.009697000
Co	0.941788000	0.287906000	-1.749514000
H	2.013086000	2.572243000	-3.981927000
C	2.861849000	1.886063000	-3.925151000
H	3.291565000	1.817171000	-4.929539000
Co	0.974980000	-1.248503000	0.596733000
H	-5.165028000	-4.171217000	-2.357482000
H	-4.681457000	-0.955431000	-4.334930000
H	-5.145035000	-1.565965000	-2.748686000
H	-3.889048000	-0.331690000	-2.884907000
H	0.011486000	-2.402933000	3.569805000
H	0.118559000	-3.924388000	4.468722000
H	1.467344000	-2.788503000	4.486444000
S	-1.103958000	0.309193000	-2.626101000
S	-2.885019000	0.104292000	-0.103103000
S	0.726220000	-1.900318000	-1.506201000
S	-1.045188000	-2.080176000	1.003685000
S	0.634089000	2.442621000	-1.263671000
S	2.467244000	0.230852000	-0.137878000
C	3.887939000	2.379890000	-2.922312000
H	4.194683000	3.399942000	-3.160660000
H	4.783805000	1.755797000	-2.921086000
H	3.475063000	2.372954000	-1.913262000
S	0.704587000	0.050501000	2.368254000
Co	-1.379282000	1.584358000	-0.829646000
Co	-1.336355000	0.053465000	1.509396000
Co	0.924601000	1.559746000	0.761426000
S	-1.132518000	2.261470000	1.277358000
P	-2.503073000	0.013489000	3.296956000
P	2.106390000	3.067896000	1.713358000
H	-3.486340000	2.143844000	2.968318000
H	-4.479785000	0.872671000	2.316755000
C	-3.913437000	1.166192000	3.204288000
C	-3.229700000	-1.608358000	3.710535000
H	-3.650682000	-1.538488000	4.718505000
H	-2.394591000	-2.311703000	3.757047000
C	-1.612366000	0.452367000	4.828253000
H	-0.807713000	-0.280729000	4.928071000

H	-2.301254000	0.293220000	5.663755000
H	2.985783000	3.990094000	-0.276295000
C	1.188048000	4.570282000	2.194638000
H	0.393235000	4.237250000	2.867046000
H	1.872670000	5.185864000	2.787039000
C	3.463078000	3.661116000	0.649871000
H	4.048150000	2.776099000	0.387718000
H	2.098248000	2.204812000	3.921151000
C	2.902083000	2.569777000	3.277083000
H	3.312715000	3.468296000	3.747596000
C	-4.796825000	1.225115000	4.439424000
H	-5.617178000	1.927423000	4.279172000
H	-4.245605000	1.563898000	5.318729000
H	-5.240261000	0.255288000	4.674005000
H	-5.155642000	-1.439198000	2.720065000
H	-3.863549000	-2.075906000	1.701604000
C	-4.271348000	-2.079171000	2.712558000
H	-4.595186000	-3.094738000	2.947856000
C	-1.051864000	1.862604000	4.845754000
H	-1.841638000	2.614232000	4.787967000
H	-0.493904000	2.037169000	5.767770000
H	-0.378014000	2.017409000	4.001538000
C	4.336621000	4.754480000	1.242442000
C	0.612987000	5.362301000	1.033789000
H	0.052911000	6.221758000	1.406541000
H	1.397649000	5.739971000	0.375206000
H	-0.063948000	4.751933000	0.434804000
H	4.820133000	4.434745000	2.167494000
H	3.765082000	5.659186000	1.457029000
H	5.125493000	5.026659000	0.538442000
C	3.966778000	1.503853000	3.095273000
H	4.321749000	1.145854000	4.063511000
H	4.829462000	1.884393000	2.545219000
H	3.566207000	0.654789000	2.541359000

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C	-1.514134000	-4.309631000	-2.351285000
C	-0.945859000	-5.040542000	-1.148202000
H	-0.361410000	-5.904346000	-1.470892000
C	1.225692000	-0.168318000	-5.007812000
C	0.675113000	-1.582610000	-5.028004000
C	3.540096000	-0.875457000	-3.422499000
C	4.414580000	-0.908260000	-4.664722000
H	5.243320000	-1.604771000	-4.521941000
C	2.989376000	-3.952509000	0.262123000
C	4.043836000	-3.255164000	-0.577206000

H	4.403360000	-3.915744000	-1.368505000
C	4.444249000	-3.245565000	3.146044000
H	-2.186855000	-4.958214000	-2.921221000
H	-0.712573000	-4.000227000	-3.026753000
H	-0.295634000	-4.382442000	-0.569705000
H	-1.734302000	-5.401531000	-0.484928000
H	-4.119084000	-5.368003000	-1.627384000
H	-2.362360000	-1.992734000	-4.179381000
H	-3.577782000	-3.255930000	-4.009253000
H	1.470791000	-2.329088000	-4.984826000
H	0.015674000	-1.748985000	-4.174778000
H	4.113569000	-0.591896000	-2.536051000
H	3.120209000	-1.860629000	-3.206309000
H	3.859009000	-1.239629000	-5.543966000
H	4.846188000	0.069144000	-4.889114000
H	2.188000000	-4.341778000	-0.370548000
H	3.413421000	-4.801042000	0.807610000
H	3.635859000	-2.356376000	-1.039825000
H	4.905926000	-2.959012000	0.023464000
H	3.893183000	-3.905749000	3.818317000
H	4.944924000	-3.866208000	2.400451000
H	1.999669000	-4.834885000	2.799817000
H	0.512816000	-4.476795000	1.929636000
P	-2.442955000	-2.790870000	-1.946952000
H	0.414333000	0.558068000	-5.099255000
H	0.106243000	-1.755870000	-5.943645000
H	1.908127000	-0.000062000	-5.846577000
P	2.119934000	0.265980000	-3.476406000
P	2.184561000	-2.855988000	1.477362000
C	3.540464000	-2.204013000	2.507980000
H	3.060995000	-1.579682000	3.265785000
H	4.104085000	-1.521154000	1.867374000
H	5.221040000	-2.755560000	3.736570000
H	-5.507815000	-4.686114000	-0.790220000
C	-3.834026000	-3.335795000	-0.901012000
C	-4.691624000	-4.450945000	-1.475989000
C	-3.186083000	-2.342090000	-3.552001000
C	-4.260449000	-1.275531000	-3.442326000
C	1.295701000	-4.034269000	2.551078000
C	0.701231000	-3.424055000	3.807695000
H	-3.392403000	-3.619847000	0.057126000
H	-4.422651000	-2.438018000	-0.696385000
Co	-1.321808000	-1.234601000	-1.009464000
Co	0.957120000	0.244161000	-1.682769000
H	2.003141000	2.597525000	-3.900225000
C	2.838882000	1.893915000	-3.882479000

H	3.242583000	1.843368000	-4.898472000
Co	0.949381000	-1.314756000	0.657338000
H	-5.138489000	-4.172380000	-2.432367000
H	-4.593134000	-0.963717000	-4.434118000
H	-5.134452000	-1.636265000	-2.897037000
H	-3.876562000	-0.399334000	-2.919443000
H	-0.011444000	-2.635543000	3.564057000
H	0.177008000	-4.188320000	4.384239000
H	1.470921000	-2.994118000	4.451675000
S	-1.066805000	0.283569000	-2.595158000
S	-2.893365000	0.107404000	-0.144757000
S	0.729208000	-1.946363000	-1.451695000
S	-1.095112000	-2.141937000	1.011954000
S	0.668797000	2.385296000	-1.183591000
S	2.458572000	0.158390000	-0.042150000
C	3.895859000	2.346093000	-2.891497000
H	4.193455000	3.377173000	-3.091265000
H	4.792750000	1.726208000	-2.947941000
H	3.514478000	2.290545000	-1.871816000
S	0.638584000	-0.019939000	2.441521000
Co	-1.363654000	1.580509000	-0.832563000
Co	-1.376136000	0.014051000	1.487051000
Co	0.905842000	1.493311000	0.825768000
P	-2.547723000	3.103909000	-1.748985000
S	-1.148960000	2.215572000	1.294377000
P	2.080179000	3.056172000	1.686455000
H	-3.449821000	1.805334000	-3.508653000
C	-1.642646000	4.238998000	-2.854019000
H	-2.331371000	5.038269000	-3.145015000
C	-3.330196000	4.237336000	-0.552605000
H	-2.516083000	4.658887000	0.042443000
H	-3.770258000	5.060367000	-1.124782000
H	-4.482942000	1.783790000	-2.101969000
C	-3.917113000	2.448711000	-2.759301000
H	-0.859291000	4.692767000	-2.241857000
H	3.027163000	3.899953000	-0.305308000
C	1.154788000	4.576700000	2.093712000
H	0.368991000	4.268779000	2.788072000
H	1.836855000	5.229441000	2.647698000
C	3.472434000	3.604863000	0.647745000
H	4.060971000	2.707580000	0.440203000
H	1.976201000	2.277003000	3.918814000
C	2.811765000	2.607115000	3.296318000
H	3.213871000	3.519071000	3.748521000
C	-4.818726000	3.486936000	-3.405536000
H	-1.810278000	3.143022000	-4.723898000

C	-1.041438000	3.566868000	-4.074978000
H	-0.470481000	4.287855000	-4.663258000
H	-0.372421000	2.757295000	-3.779022000
C	-4.364847000	3.579891000	0.344130000
H	-4.748891000	4.301144000	1.067526000
H	-3.933428000	2.743641000	0.896229000
H	-5.214220000	3.203507000	-0.229212000
H	-5.598107000	2.993851000	-3.990029000
H	-5.316494000	4.114328000	-2.663873000
H	-4.267771000	4.140524000	-4.084584000
C	4.332904000	4.715163000	1.227229000
C	0.561028000	5.302339000	0.899995000
H	-0.018533000	6.165717000	1.232415000
H	1.334857000	5.662780000	0.219192000
H	-0.097775000	4.641145000	0.335084000
H	4.778693000	4.430478000	2.182199000
H	3.761700000	5.632082000	1.383281000
H	5.149886000	4.952706000	0.543035000
C	3.871610000	1.525068000	3.202903000
H	4.193821000	1.218507000	4.199700000
H	4.753804000	1.869452000	2.659705000
H	3.480894000	0.649224000	2.684281000

Co6_1_4_M6

C	-1.482814000	-4.258597000	-2.297153000
C	-0.908488000	-4.981108000	-1.091692000
H	-0.299126000	-5.828877000	-1.410958000
C	1.244814000	-0.174006000	-5.060842000
C	0.666185000	-1.577301000	-5.067551000
C	3.548919000	-0.916963000	-3.465255000
C	4.437890000	-0.958573000	-4.696826000
H	5.246992000	-1.676983000	-4.550552000
C	2.931325000	-3.983758000	0.337021000
C	3.978083000	-3.361789000	-0.569014000
H	4.301965000	-4.077561000	-1.326845000
C	4.478707000	-3.142662000	3.141674000
H	-2.151966000	-4.912655000	-2.864663000
H	-0.683518000	-3.946453000	-2.973675000
H	-0.283455000	-4.308506000	-0.502327000
H	-1.694697000	-5.364298000	-0.438072000
H	-4.051898000	-5.353748000	-1.574152000
H	-2.358416000	-1.935272000	-4.118361000
H	-3.550601000	-3.221005000	-3.953184000
H	1.447856000	-2.338363000	-5.023564000
H	0.008650000	-1.724137000	-4.209170000
H	4.117277000	-0.642829000	-2.572711000

H	3.110672000	-1.895582000	-3.255476000
H	3.886466000	-1.265891000	-5.587435000
H	4.896844000	0.010270000	-4.902395000
H	2.103773000	-4.388760000	-0.250544000
H	3.351221000	-4.809976000	0.918962000
H	3.575411000	-2.484913000	-1.076790000
H	4.861510000	-3.050026000	-0.008928000
H	3.933340000	-3.740503000	3.874515000
H	4.936465000	-3.826898000	2.424486000
H	1.997463000	-4.689228000	2.964495000
H	0.504642000	-4.374976000	2.085089000
P	-2.417564000	-2.743721000	-1.888901000
H	0.447978000	0.568344000	-5.152904000
H	0.088692000	-1.746174000	-5.978478000
H	1.926961000	-0.024361000	-5.903462000
P	2.150347000	0.249323000	-3.534489000
P	2.185298000	-2.801921000	1.509893000
C	3.582610000	-2.119232000	2.464265000
H	3.143145000	-1.429427000	3.188900000
H	4.142274000	-1.491075000	1.766698000
H	5.288160000	-2.637516000	3.672182000
H	-5.455625000	-4.694983000	-0.743309000
C	-3.802727000	-3.316455000	-0.851720000
C	-4.640580000	-4.446577000	-1.426071000
C	-3.173676000	-2.303581000	-3.491018000
C	-4.265231000	-1.255764000	-3.369049000
C	1.299223000	-3.900576000	2.666867000
C	0.722426000	-3.201979000	3.884323000
H	-3.355316000	-3.596068000	0.104934000
H	-4.410133000	-2.430293000	-0.651230000
Co	-1.293826000	-1.166060000	-0.978257000
Co	0.985009000	0.271085000	-1.747332000
H	2.059070000	2.572676000	-4.002671000
C	2.891878000	1.868101000	-3.934534000
H	3.329274000	1.789642000	-4.935230000
Co	1.004518000	-1.262129000	0.619691000
H	-5.088068000	-4.177324000	-2.384784000
H	-4.593261000	-0.925492000	-4.356416000
H	-5.139129000	-1.641783000	-2.841026000
H	-3.900073000	-0.387281000	-2.820610000
H	0.024324000	-2.418805000	3.584535000
H	0.186225000	-3.916477000	4.512077000
H	1.501229000	-2.741978000	4.495610000
S	-1.058750000	0.327068000	-2.598688000
S	-2.816669000	0.194942000	-0.082331000
S	0.740005000	-1.908006000	-1.476295000

S	-1.027560000	-2.034450000	1.039818000
S	0.727492000	2.431570000	-1.259618000
S	2.535216000	0.177220000	-0.144542000
C	3.919793000	2.348675000	-2.925099000
H	4.286117000	3.338613000	-3.202234000
H	4.780983000	1.679339000	-2.876925000
H	3.488476000	2.415001000	-1.925202000
S	0.767657000	0.053157000	2.400449000
Co	-1.312273000	1.638631000	-0.837008000
Co	-1.284652000	0.111339000	1.527087000
Co	1.001008000	1.529110000	0.751486000
P	-2.552099000	3.116236000	-1.759081000
S	-1.021316000	2.312430000	1.271640000
P	-2.515058000	0.009534000	3.276559000
H	-3.525805000	1.773179000	-3.444069000
C	-1.677025000	4.212237000	-2.926671000
H	-2.382470000	4.993040000	-3.228177000
C	-3.276262000	4.300791000	-0.575727000
H	-2.433835000	4.706486000	-0.009957000
H	-3.708424000	5.124501000	-1.152360000
H	-4.509637000	1.805690000	-2.003030000
C	-3.961259000	2.444408000	-2.700024000
H	-0.888363000	4.697871000	-2.346470000
H	-3.418307000	2.187126000	3.084015000
H	-4.437830000	0.996405000	2.315019000
C	-3.885258000	1.210688000	3.233327000
C	-3.306688000	-1.602011000	3.597302000
H	-3.732605000	-1.572430000	4.604910000
H	-2.500388000	-2.339233000	3.606491000
C	-1.633604000	0.346234000	4.838597000
H	-0.825729000	-0.387578000	4.898179000
H	-2.329796000	0.124615000	5.653953000
C	-4.872962000	3.471515000	-3.350143000
H	-1.868744000	3.045349000	-4.751729000
C	-1.093976000	3.512782000	-4.140647000
H	-0.561667000	4.229076000	-4.769529000
H	-0.393469000	2.732629000	-3.838779000
C	-4.303543000	3.683659000	0.355277000
H	-4.615312000	4.405756000	1.112083000
H	-3.889378000	2.812173000	0.863150000
H	-5.196556000	3.363445000	-0.185010000
H	-5.682248000	2.969759000	-3.884435000
H	-5.331012000	4.136110000	-2.615175000
H	-4.339018000	4.089264000	-4.074551000
C	-4.800321000	1.214103000	4.446498000
H	-5.591212000	1.955721000	4.317146000

H	-4.262853000	1.467721000	5.362028000
H	-5.283098000	0.246639000	4.597779000
H	-5.228080000	-1.317890000	2.623915000
H	-3.948017000	-1.893693000	1.558054000
C	-4.356259000	-1.972294000	2.565464000
H	-4.700559000	-2.996933000	2.718048000
C	-1.086147000	1.757153000	4.960394000
H	-1.884084000	2.502157000	4.944811000
H	-0.546782000	1.871134000	5.902266000
H	-0.397591000	1.984981000	4.145731000

Co6_1_6

C	1.397300000	0.031822000	-5.145771000
C	0.847882000	-1.373754000	-5.315592000
C	3.608569000	-0.897289000	-3.520592000
C	4.553892000	-0.876490000	-4.709750000
H	5.329830000	-1.634875000	-4.586904000
C	2.943685000	-4.024564000	0.256593000
C	3.976047000	-3.385865000	-0.654129000
H	4.312405000	-4.098653000	-1.409159000
C	4.480384000	-3.210882000	3.072351000
H	1.644606000	-2.120153000	-5.315396000
H	0.151304000	-1.625370000	-4.514611000
H	4.141243000	-0.717163000	-2.583169000
H	3.127074000	-1.872151000	-3.410916000
H	4.035686000	-1.089522000	-5.646539000
H	5.054844000	0.087699000	-4.816029000
H	2.115420000	-4.437259000	-0.324929000
H	3.378203000	-4.847062000	0.833207000
H	3.555735000	-2.519178000	-1.165133000
H	4.854370000	-3.053354000	-0.097422000
H	3.937411000	-3.844167000	3.776342000
H	4.963244000	-3.860129000	2.339542000
H	2.000286000	-4.755392000	2.876971000
H	0.520656000	-4.455752000	1.973933000
H	0.591424000	0.768873000	-5.196147000
H	0.316755000	-1.458639000	-6.265172000
H	2.105102000	0.274538000	-5.944859000
P	2.252215000	0.320157000	-3.559097000
P	2.188049000	-2.859541000	1.438597000
C	3.572505000	-2.185438000	2.414490000
H	3.115583000	-1.525976000	3.156373000
H	4.129430000	-1.534045000	1.736300000
H	5.271147000	-2.706723000	3.631581000
C	1.295597000	-3.973763000	2.575458000
C	0.686702000	-3.297603000	3.790331000

Co	-1.329155000	-1.234012000	-1.102445000
Co	0.977767000	0.186955000	-1.824587000
H	2.267018000	2.675021000	-3.835812000
C	3.066733000	1.930211000	-3.829551000
H	3.511014000	1.921840000	-4.829503000
Co	0.957516000	-1.367969000	0.520267000
H	-0.027006000	-2.528646000	3.491231000
H	0.162279000	-4.031748000	4.405138000
H	1.446474000	-2.823386000	4.414911000
S	-1.055089000	0.253494000	-2.740489000
S	-2.893652000	0.110035000	-0.237469000
S	0.701813000	-2.015707000	-1.595396000
S	-1.110179000	-2.180019000	0.904557000
S	0.707888000	2.329406000	-1.326743000
S	2.475070000	0.075707000	-0.184965000
C	4.100180000	2.267479000	-2.770020000
H	4.454268000	3.293141000	-2.890279000
H	4.968677000	1.608719000	-2.829535000
H	3.675045000	2.166512000	-1.771569000
S	0.682317000	-0.087838000	2.302469000
Co	-1.322238000	1.555206000	-0.962308000
Co	-1.477901000	-0.034457000	1.538273000
Co	0.932293000	1.421344000	0.673106000
P	-2.539142000	3.082434000	-1.824075000
S	-1.123861000	2.181396000	1.143748000
P	-2.665944000	0.081617000	3.590907000
P	2.029821000	3.013934000	1.627867000
H	-3.426075000	1.745599000	-3.567658000
C	-1.655468000	4.234551000	-2.929242000
H	-2.361665000	5.019574000	-3.217682000
C	-3.334547000	4.202569000	-0.624785000
H	-2.524879000	4.641534000	-0.036159000
H	-3.798075000	5.014886000	-1.193345000
H	-4.450773000	1.721148000	-2.162156000
C	-3.899599000	2.392722000	-2.825271000
H	-0.881501000	4.704752000	-2.317075000
H	-3.590657000	2.239090000	3.281609000
H	-4.672083000	0.994291000	2.722311000
C	-4.040465000	1.283811000	3.567680000
C	-3.405571000	-1.514765000	4.084771000
H	-3.840076000	-1.426327000	5.085292000
H	-2.567515000	-2.214550000	4.161721000
C	-1.637515000	0.538025000	5.029624000
H	-0.833053000	-0.202539000	5.064006000
H	-2.224313000	0.422533000	5.945739000
H	3.024868000	3.881444000	-0.333416000

C	1.075970000	4.521881000	2.019189000
H	0.259369000	4.200124000	2.670164000
H	1.724888000	5.174404000	2.611313000
C	3.443030000	3.600000000	0.635970000
H	4.062006000	2.718462000	0.450865000
H	1.908647000	2.187688000	3.847289000
C	2.740280000	2.569066000	3.249915000
H	3.093139000	3.486234000	3.731256000
C	-4.817084000	3.412670000	-3.478514000
H	-1.798967000	3.125756000	-4.794147000
C	-1.041020000	3.580177000	-4.153332000
H	-0.503396000	4.320650000	-4.748686000
H	-0.336058000	2.800134000	-3.860966000
C	-4.345691000	3.522090000	0.280714000
H	-4.730817000	4.229483000	1.017530000
H	-3.888911000	2.688094000	0.815851000
H	-5.196808000	3.135640000	-0.283111000
H	-5.589525000	2.902945000	-4.057575000
H	-5.323064000	4.039951000	-2.742068000
H	-4.276202000	4.067757000	-4.164277000
C	-4.854497000	1.413685000	4.843474000
H	-5.653216000	2.147466000	4.716006000
H	-4.240011000	1.742306000	5.684172000
H	-5.322996000	0.467645000	5.122206000
H	-5.297705000	-1.367224000	3.024482000
H	-3.995462000	-2.094280000	2.079034000
C	-4.427317000	-2.024280000	3.079782000
H	-4.782531000	-3.016527000	3.363144000
C	-1.055421000	1.937807000	4.919193000
H	-1.836023000	2.701329000	4.930583000
H	-0.381120000	2.141747000	5.753312000
H	-0.496775000	2.048935000	3.987799000
C	4.257098000	4.732648000	1.239019000
C	0.532711000	5.252717000	0.804388000
H	-0.080151000	6.101644000	1.113961000
H	1.335293000	5.635705000	0.170793000
H	-0.081995000	4.586028000	0.197645000
H	4.679107000	4.461824000	2.208822000
H	3.658542000	5.635273000	1.374835000
H	5.089625000	4.990049000	0.581004000
C	3.846078000	1.533131000	3.156007000
H	4.145636000	1.199686000	4.151347000
H	4.732584000	1.931954000	2.659449000
H	3.508163000	0.664168000	2.590806000

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C	-1.534335000	-4.270662000	-2.325821000
C	-0.953696000	-5.013114000	-1.135554000
H	-0.349816000	-5.860528000	-1.468959000
C	1.260013000	-0.149948000	-5.018381000
C	0.700498000	-1.560403000	-5.050752000
C	3.546165000	-0.879197000	-3.414950000
C	4.430865000	-0.920488000	-4.648369000
H	5.252909000	-1.626001000	-4.503971000
C	2.929290000	-3.959508000	0.325603000
C	3.990470000	-3.318712000	-0.550195000
H	4.319491000	-4.009315000	-1.330200000
C	4.442270000	-3.187114000	3.144520000
H	-2.212486000	-4.911484000	-2.898836000
H	-0.733674000	-3.954112000	-2.999128000
H	-0.322408000	-4.347666000	-0.545047000
H	-1.737029000	-5.398005000	-0.478571000
H	-4.105695000	-5.344584000	-1.605683000
H	-2.403184000	-1.947386000	-4.117009000
H	-3.610589000	-3.222462000	-3.941148000
H	1.492201000	-2.311930000	-5.008980000
H	0.042390000	-1.724258000	-4.196155000
H	4.112579000	-0.601062000	-2.522163000
H	3.115832000	-1.860176000	-3.199258000
H	3.877446000	-1.241678000	-5.533523000
H	4.872804000	0.054130000	-4.867720000
H	2.112299000	-4.344554000	-0.289703000
H	3.336317000	-4.799645000	0.897306000
H	3.596169000	-2.421738000	-1.028271000
H	4.869208000	-3.028369000	0.029929000
H	3.887332000	-3.814958000	3.845167000
H	4.913757000	-3.844603000	2.410627000
H	1.975866000	-4.720860000	2.908829000
H	0.482766000	-4.373903000	2.034681000
P	-2.437359000	-2.740064000	-1.884653000
H	0.448649000	0.577270000	-5.106464000
H	0.129264000	-1.725852000	-5.967412000
H	1.949116000	0.022392000	-5.851530000
P	2.127216000	0.271069000	-3.462541000
P	2.153445000	-2.782214000	1.491360000
C	3.549594000	-2.149574000	2.487311000
H	3.095510000	-1.487743000	3.228850000
H	4.115833000	-1.497991000	1.816835000
H	5.242272000	-2.699858000	3.707452000
H	-5.490949000	-4.691858000	-0.736789000
C	-3.823798000	-3.325668000	-0.848852000
C	-4.683906000	-4.435355000	-1.427456000

C	-3.216520000	-2.309631000	-3.483160000
C	-4.289616000	-1.244529000	-3.350489000
C	1.281871000	-3.921966000	2.627943000
C	0.701048000	-3.245964000	3.856400000
H	-3.365126000	-3.624491000	0.096839000
H	-4.414654000	-2.434468000	-0.622155000
Co	-1.288893000	-1.204781000	-0.979319000
Co	0.947543000	0.241077000	-1.702602000
H	2.046804000	2.596796000	-3.912339000
C	2.875882000	1.885211000	-3.889420000
H	3.287955000	1.825397000	-4.902016000
Co	0.962096000	-1.262283000	0.615352000
H	-5.143763000	-4.142734000	-2.374056000
H	-4.625793000	-0.906261000	-4.333399000
H	-5.161978000	-1.615273000	-2.807817000
H	-3.899696000	-0.384920000	-2.805252000
H	0.030539000	-2.436948000	3.563064000
H	0.137596000	-3.962916000	4.458575000
H	1.480793000	-2.816508000	4.489382000
S	-1.074294000	0.271248000	-2.618322000
S	-2.865005000	0.115483000	-0.113770000
S	0.742207000	-1.950934000	-1.480676000
S	-1.051191000	-2.103879000	1.026899000
S	0.686694000	2.396535000	-1.249236000
S	2.500932000	0.177208000	-0.108288000
C	3.925160000	2.335030000	-2.889538000
H	4.236833000	3.363005000	-3.088708000
H	4.815511000	1.703313000	-2.927918000
H	3.526100000	2.286138000	-1.876454000
S	0.710712000	0.021912000	2.396705000
Co	-1.326872000	1.555418000	-0.836353000
Co	-1.310590000	0.051610000	1.479840000
Co	0.923947000	1.497001000	0.757020000
P	-2.518446000	3.075338000	-1.712326000
S	-1.106252000	2.244022000	1.259422000
P	-2.493018000	0.018003000	3.239649000
P	2.074269000	3.032487000	1.659234000
H	-3.459524000	1.780546000	-3.450023000
C	-1.647062000	4.215685000	-2.848451000
H	-2.340996000	5.014927000	-3.128495000
C	-3.294959000	4.251928000	-0.546321000
H	-2.478022000	4.638169000	0.068306000
H	-3.703516000	5.091413000	-1.117892000
H	-4.480639000	1.790856000	-2.038577000
C	-3.914095000	2.442415000	-2.708811000
H	-0.847609000	4.667039000	-2.255211000

H	-3.480506000	2.150026000	2.979208000
H	-4.476485000	0.892617000	2.297842000
C	-3.911516000	1.168743000	3.192168000
C	-3.242461000	-1.596493000	3.663474000
H	-3.655470000	-1.537886000	4.675759000
H	-2.413707000	-2.308443000	3.686136000
C	-1.626741000	0.437027000	4.796488000
H	-0.815382000	-0.290226000	4.884277000
H	-2.316253000	0.263864000	5.629139000
H	3.001448000	3.914790000	-0.323543000
C	1.172293000	4.563713000	2.100425000
H	0.372801000	4.247710000	2.775408000
H	1.851480000	5.204900000	2.671805000
C	3.460344000	3.616842000	0.622306000
H	4.051021000	2.725319000	0.396383000
H	2.040860000	2.241673000	3.892135000
C	2.854135000	2.603141000	3.257741000
H	3.248528000	3.516310000	3.714773000
C	-4.806474000	3.479796000	-3.366680000
H	-1.846968000	3.111768000	-4.710725000
C	-1.066874000	3.540399000	-4.077611000
H	-0.503308000	4.257604000	-4.679377000
H	-0.396620000	2.730870000	-3.785111000
C	-4.354600000	3.609901000	0.330441000
H	-4.684149000	4.300335000	1.110369000
H	-3.958583000	2.713743000	0.808635000
H	-5.233284000	3.317974000	-0.248974000
H	-5.606019000	2.992414000	-3.930153000
H	-5.278553000	4.137236000	-2.633125000
H	-4.251135000	4.107692000	-4.066962000
C	-4.798318000	1.207647000	4.424152000
H	-5.619870000	1.913765000	4.279898000
H	-4.246344000	1.526656000	5.310997000
H	-5.240967000	0.232687000	4.640564000
H	-5.181301000	-1.412853000	2.700644000
H	-3.891041000	-1.993899000	1.649279000
C	-4.290948000	-2.044543000	2.661943000
H	-4.602833000	-3.072842000	2.859104000
C	-1.067326000	1.847511000	4.830464000
H	-1.859118000	2.598969000	4.789278000
H	-0.496351000	2.012061000	5.747439000
H	-0.408988000	2.012371000	3.976225000
C	4.320706000	4.727057000	1.199500000
C	0.589494000	5.305376000	0.910760000
H	-0.013202000	6.153415000	1.244734000
H	1.371551000	5.689273000	0.251672000

H	-0.043433000	4.639700000	0.322284000
H	4.780717000	4.435487000	2.146346000
H	3.742635000	5.636559000	1.376789000
H	5.127622000	4.982652000	0.508351000
C	3.926970000	1.537713000	3.125839000
H	4.263482000	1.200516000	4.109006000
H	4.799186000	1.907714000	2.582412000
H	3.536724000	0.677548000	2.581733000

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C	-1.534763000	-4.287177000	-2.371318000
C	-0.946317000	-5.023373000	-1.181213000
H	-0.361708000	-5.884518000	-1.513925000
C	1.339993000	-0.137083000	-5.078623000
C	0.783935000	-1.548748000	-5.125597000
C	3.606308000	-0.874163000	-3.451107000
C	4.509576000	-0.907726000	-4.671108000
H	5.329204000	-1.614777000	-4.520136000
C	2.958149000	-3.971642000	0.280661000
C	4.024688000	-3.321786000	-0.581986000
H	4.368384000	-4.009039000	-1.358561000
C	4.430083000	-3.204212000	3.124017000
H	-2.222370000	-4.929180000	-2.931813000
H	-0.738769000	-3.982952000	-3.056201000
H	-0.294220000	-4.360894000	-0.610413000
H	-1.724238000	-5.386992000	-0.506032000
H	-4.120483000	-5.325082000	-1.614471000
H	-2.382106000	-1.989736000	-4.186773000
H	-3.602760000	-3.248771000	-3.989366000
H	1.577048000	-2.298683000	-5.081690000
H	0.117751000	-1.720711000	-4.278853000
H	4.160430000	-0.603139000	-2.548280000
H	3.173085000	-1.856824000	-3.248347000
H	3.969058000	-1.221678000	-5.566795000
H	4.954984000	0.068322000	-4.876883000
H	2.150831000	-4.361083000	-0.344710000
H	3.364576000	-4.810461000	0.854730000
H	3.629266000	-2.427757000	-1.064647000
H	4.894227000	-3.024934000	0.008632000
H	3.867944000	-3.837802000	3.813670000
H	4.915939000	-3.856083000	2.394479000
H	1.969010000	-4.750225000	2.839978000
H	0.486436000	-4.398022000	1.951359000
P	-2.423304000	-2.744203000	-1.942502000
H	0.527077000	0.588229000	-5.170520000
H	0.221712000	-1.709536000	-6.048645000

H	2.036633000	0.042306000	-5.903965000
P	2.187048000	0.275884000	-3.509384000
P	2.162541000	-2.802199000	1.440877000
C	3.542396000	-2.168124000	2.457888000
H	3.075325000	-1.510392000	3.195149000
H	4.115697000	-1.511829000	1.797962000
H	5.219052000	-2.715278000	3.700909000
H	-5.494109000	-4.641687000	-0.750834000
C	-3.810734000	-3.298498000	-0.889542000
C	-4.686545000	-4.405907000	-1.448184000
C	-3.199956000	-2.331903000	-3.547134000
C	-4.262259000	-1.253985000	-3.436863000
C	1.277045000	-3.949654000	2.558684000
C	0.679587000	-3.287277000	3.786886000
H	-3.351058000	-3.587971000	0.058775000
H	-4.388098000	-2.396177000	-0.671750000
Co	-1.253334000	-1.205572000	-1.063796000
Co	0.978732000	0.234259000	-1.754678000
H	2.111695000	2.604844000	-3.941621000
C	2.940573000	1.892721000	-3.918767000
H	3.361359000	1.843427000	-4.928289000
Co	0.977203000	-1.275416000	0.552105000
H	-5.146340000	-4.122208000	-2.397550000
H	-4.600034000	-0.938306000	-4.426749000
H	-5.135253000	-1.602713000	-2.880724000
H	-3.861794000	-0.384263000	-2.916258000
H	0.003554000	-2.482326000	3.494993000
H	0.117732000	-4.014594000	4.378083000
H	1.450459000	-2.857170000	4.430259000
S	-1.029378000	0.264970000	-2.702999000
S	-2.868423000	0.103887000	-0.229485000
S	0.774288000	-1.959980000	-1.541951000
S	-1.054485000	-2.133101000	0.947364000
S	0.707818000	2.386031000	-1.301147000
S	2.508214000	0.165961000	-0.140613000
C	3.980974000	2.333718000	-2.905420000
H	4.292374000	3.364511000	-3.089943000
H	4.872868000	1.704189000	-2.943671000
H	3.574524000	2.272614000	-1.895895000
S	0.713024000	-0.009493000	2.362960000
Co	-1.300943000	1.548446000	-0.930189000
Co	-1.383157000	0.030630000	1.477697000
Co	0.908778000	1.466471000	0.695659000
P	-2.519872000	3.066193000	-1.777630000
S	-1.128054000	2.257960000	1.173994000
P	-2.621964000	0.060752000	3.497165000

P	2.043859000	3.009203000	1.628983000
H	-3.409806000	1.798525000	-3.562031000
C	-1.651078000	4.249660000	-2.870234000
H	-2.348541000	5.050283000	-3.137182000
C	-3.333945000	4.191451000	-0.588030000
H	-2.527491000	4.606599000	0.022096000
H	-3.783146000	5.018740000	-1.146829000
H	-4.447280000	1.747670000	-2.163008000
C	-3.887769000	2.429571000	-2.808607000
H	-0.863010000	4.691233000	-2.254738000
H	-3.605321000	2.196125000	3.235251000
H	-4.647377000	0.938949000	2.639509000
C	-4.033707000	1.224731000	3.499219000
C	-3.345616000	-1.557640000	3.956651000
H	-3.780360000	-1.512447000	4.960686000
H	-2.496984000	-2.247356000	4.000120000
C	-1.653193000	0.499516000	4.986704000
H	-0.830359000	-0.221014000	5.016110000
H	-2.258281000	0.346300000	5.886218000
H	3.007089000	3.889790000	-0.339489000
C	1.139066000	4.543395000	2.055098000
H	0.319664000	4.229695000	2.706739000
H	1.807842000	5.175699000	2.648189000
C	3.448091000	3.592580000	0.615075000
H	4.043566000	2.701282000	0.401373000
H	1.977788000	2.210224000	3.858222000
C	2.799124000	2.580732000	3.239722000
H	3.177673000	3.495942000	3.705943000
C	-4.796963000	3.464067000	-3.447415000
H	-1.818646000	3.198463000	-4.765770000
C	-1.049375000	3.610170000	-4.108724000
H	-0.477769000	4.344474000	-4.681297000
H	-0.381694000	2.793918000	-3.828594000
C	-4.357499000	3.500927000	0.295762000
H	-4.726509000	4.184500000	1.064057000
H	-3.913825000	2.635211000	0.789718000
H	-5.217515000	3.152288000	-0.280529000
H	-5.571776000	2.974261000	-4.042427000
H	-5.300918000	4.080975000	-2.700102000
H	-4.247224000	4.131498000	-4.114864000
C	-4.863106000	1.308716000	4.768093000
H	-5.680262000	2.025469000	4.652016000
H	-4.262325000	1.633038000	5.620920000
H	-5.308293000	0.344424000	5.024377000
H	-5.245505000	-1.412535000	2.909133000
H	-3.917717000	-2.042510000	1.931531000

C	-4.356229000	-2.046729000	2.931354000
H	-4.680560000	-3.064933000	3.158618000
C	-1.096305000	1.912535000	4.924649000
H	-1.892113000	2.660939000	4.937115000
H	-0.440259000	2.108923000	5.776005000
H	-0.524751000	2.053544000	4.005432000
C	4.298237000	4.703829000	1.205583000
C	0.594321000	5.297965000	0.855484000
H	-0.006161000	6.151364000	1.179697000
H	1.396748000	5.676126000	0.217903000
H	-0.032475000	4.643318000	0.248412000
H	4.742596000	4.413410000	2.160198000
H	3.717100000	5.613291000	1.372572000
H	5.116474000	4.959131000	0.527689000
C	3.883668000	1.525084000	3.124088000
H	4.206550000	1.189817000	4.112489000
H	4.761609000	1.903391000	2.595883000
H	3.509759000	0.661776000	2.573526000

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C	-1.534460000	-4.344185000	-2.386585000
C	-0.935374000	-5.101561000	-1.214597000
H	-0.353396000	-5.956142000	-1.567934000
C	1.370858000	-0.248656000	-5.063448000
C	0.835670000	-1.668990000	-5.090539000
C	3.666030000	-0.921041000	-3.446171000
C	4.558881000	-0.951078000	-4.674069000
H	5.393902000	-1.639864000	-4.522888000
C	3.049507000	-4.016908000	0.320799000
C	4.101056000	-3.358138000	-0.553738000
H	4.450910000	-4.045740000	-1.327288000
C	4.520760000	-3.206559000	3.154870000
H	-2.228979000	-4.975008000	-2.951316000
H	-0.744843000	-4.029820000	-3.074329000
H	-0.277365000	-4.450710000	-0.636814000
H	-1.707482000	-5.478730000	-0.540178000
H	-4.132256000	-5.372298000	-1.634703000
H	-2.402969000	-2.047785000	-4.158473000
H	-3.663456000	-3.259449000	-3.924448000
H	1.639393000	-2.407154000	-5.039730000
H	0.174291000	-1.840052000	-4.239820000
H	4.223582000	-0.628496000	-2.552088000
H	3.256287000	-1.910583000	-3.227875000
H	4.016135000	-1.286136000	-5.560686000
H	4.982455000	0.031261000	-4.895327000
H	2.244446000	-4.422843000	-0.297538000

H	3.471605000	-4.845680000	0.898070000
H	3.689705000	-2.473904000	-1.041404000
H	4.969474000	-3.043474000	0.029316000
H	3.967417000	-3.843438000	3.848599000
H	5.014922000	-3.856623000	2.429244000
H	2.072750000	-4.786397000	2.890694000
H	0.587068000	-4.458774000	1.998247000
P	-2.410936000	-2.807193000	-1.915355000
H	0.546131000	0.463107000	-5.156943000
H	0.273187000	-1.849615000	-6.009788000
H	2.057626000	-0.067410000	-5.896538000
P	2.221462000	0.197902000	-3.505328000
P	2.242080000	-2.846210000	1.472116000
C	3.617453000	-2.188767000	2.481895000
H	3.143783000	-1.530982000	3.215257000
H	4.181031000	-1.529345000	1.816382000
H	5.303301000	-2.703105000	3.728167000
H	-5.467514000	-4.710952000	-0.696908000
C	-3.778644000	-3.376574000	-0.845016000
C	-4.683163000	-4.455434000	-1.413526000
C	-3.215678000	-2.357042000	-3.495506000
C	-4.237376000	-1.241600000	-3.366291000
C	1.372839000	-3.995693000	2.601327000
C	0.766265000	-3.328501000	3.822852000
H	-3.299201000	-3.699699000	0.082505000
H	-4.339325000	-2.474936000	-0.584875000
Co	-1.205484000	-1.297917000	-1.027803000
Co	1.017436000	0.150290000	-1.735230000
H	2.086750000	2.518921000	-3.953540000
C	2.933642000	1.827622000	-3.935937000
H	3.343782000	1.781865000	-4.949976000
Co	1.024419000	-1.326847000	0.575024000
H	-5.174064000	-4.131485000	-2.333876000
H	-4.619707000	-0.955258000	-4.348994000
H	-5.088561000	-1.543877000	-2.751907000
H	-3.785992000	-0.362972000	-2.903640000
H	0.077752000	-2.536775000	3.523516000
H	0.215427000	-4.057174000	4.422754000
H	1.531139000	-2.880098000	4.460987000
S	-1.008335000	0.158095000	-2.691897000
S	-2.870062000	-0.013436000	-0.194955000
S	0.823392000	-2.036864000	-1.509459000
S	-0.997997000	-2.211577000	0.979696000
S	0.719992000	2.322635000	-1.324304000
S	2.527379000	0.134709000	-0.124727000
C	3.975076000	2.299863000	-2.937582000

H	4.257917000	3.337252000	-3.130925000
H	4.882163000	1.692998000	-2.984751000
H	3.582673000	2.234403000	-1.922750000
S	0.736582000	-0.050274000	2.375855000
Co	-1.369410000	1.519213000	-0.942325000
Co	-1.357745000	-0.053782000	1.501491000
Co	0.891799000	1.397829000	0.689375000
P	-2.634843000	3.322234000	-1.824463000
S	-1.168909000	2.184300000	1.211640000
P	-2.621620000	0.004580000	3.502514000
P	2.007203000	2.974951000	1.609266000
H	-3.546390000	2.130869000	-3.658761000
C	-1.684565000	4.483275000	-2.872220000
H	-2.300651000	5.349190000	-3.135525000
C	-3.417758000	4.422412000	-0.590097000
H	-2.595940000	4.780477000	0.037361000
H	-3.858099000	5.296467000	-1.080674000
H	-4.597604000	2.068426000	-2.275850000
C	-4.012254000	2.757429000	-2.892259000
H	-0.870130000	4.841646000	-2.235394000
H	-3.586793000	2.134016000	3.159240000
H	-4.618171000	0.867325000	2.567732000
C	-4.027777000	1.172148000	3.437376000
C	-3.356056000	-1.601108000	3.988715000
H	-3.814662000	-1.527781000	4.980455000
H	-2.508096000	-2.288154000	4.072820000
C	-1.683209000	0.475183000	5.001962000
H	-0.864441000	-0.247973000	5.065458000
H	-2.308319000	0.342222000	5.891032000
H	2.957447000	3.840777000	-0.372367000
C	1.084326000	4.500767000	2.025504000
H	0.278409000	4.184322000	2.692622000
H	1.751469000	5.150571000	2.601185000
C	3.402053000	3.567123000	0.587580000
H	4.012770000	2.682740000	0.388621000
H	1.961224000	2.199966000	3.848749000
C	2.774521000	2.573247000	3.221441000
H	3.142696000	3.499129000	3.674830000
C	-4.889706000	3.829822000	-3.512865000
H	-1.896839000	3.514412000	-4.807987000
C	-1.110796000	3.811922000	-4.110039000
H	-0.436308000	4.488776000	-4.639696000
H	-0.551621000	2.915518000	-3.833357000
C	-4.437217000	3.686932000	0.265628000
H	-4.790330000	4.321597000	1.081874000
H	-3.994534000	2.787077000	0.697564000

H	-5.308893000	3.383562000	-0.318970000
H	-5.673031000	3.382676000	-4.130470000
H	-5.381774000	4.438593000	-2.750873000
H	-4.313472000	4.502300000	-4.152754000
C	-4.889170000	1.292593000	4.681362000
H	-5.699777000	2.009283000	4.525801000
H	-4.308640000	1.636615000	5.540545000
H	-5.345327000	0.337222000	4.951476000
H	-5.226158000	-1.482723000	2.886863000
H	-3.877232000	-2.153228000	1.967420000
C	-4.341961000	-2.120757000	2.954701000
H	-4.678223000	-3.128719000	3.208582000
C	-1.118054000	1.884139000	4.925246000
H	-1.909571000	2.636762000	4.901997000
H	-0.483314000	2.094218000	5.789429000
H	-0.521559000	2.003566000	4.019035000
C	4.233166000	4.701320000	1.160839000
C	0.513266000	5.229446000	0.822291000
H	-0.094333000	6.079786000	1.141386000
H	1.301930000	5.608065000	0.168020000
H	-0.112106000	4.556120000	0.234553000
H	4.679299000	4.434919000	2.121679000
H	3.637718000	5.604608000	1.309961000
H	5.049264000	4.957089000	0.480541000
C	3.873517000	1.531550000	3.115121000
H	4.208100000	1.218170000	4.106807000
H	4.742157000	1.913888000	2.574616000
H	3.510037000	0.652640000	2.582504000

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C	-1.513756000	-4.289407000	-2.342568000
C	-0.933987000	-5.028808000	-1.150318000
H	-0.342520000	-5.883946000	-1.483588000
C	1.243770000	-0.140704000	-5.003434000
C	0.695595000	-1.555492000	-5.038148000
C	3.546607000	-0.849787000	-3.406598000
C	4.430251000	-0.873835000	-4.642163000
H	5.258471000	-1.571046000	-4.498702000
C	2.950073000	-3.962726000	0.260497000
C	4.016816000	-3.294169000	-0.587106000
H	4.358183000	-3.966699000	-1.376463000
C	4.445198000	-3.252042000	3.112561000
H	-2.188546000	-4.934463000	-2.913854000
H	-0.716488000	-3.972269000	-3.019413000
H	-0.287755000	-4.369856000	-0.568436000
H	-1.716293000	-5.403910000	-0.487179000

H	-4.097069000	-5.370921000	-1.621456000
H	-2.390852000	-1.967768000	-4.143327000
H	-3.596232000	-3.240722000	-3.966816000
H	1.492154000	-2.300986000	-4.992536000
H	0.029199000	-1.727926000	-4.191673000
H	4.113009000	-0.570498000	-2.514263000
H	3.127559000	-1.837155000	-3.198989000
H	3.881313000	-1.198903000	-5.528013000
H	4.863079000	0.105298000	-4.856834000
H	2.139688000	-4.338440000	-0.368669000
H	3.357278000	-4.815663000	0.811905000
H	3.626208000	-2.389369000	-1.052890000
H	4.887738000	-3.013981000	0.008599000
H	3.893080000	-3.901001000	3.795173000
H	4.927256000	-3.885116000	2.365135000
H	1.978032000	-4.800315000	2.822185000
H	0.488486000	-4.435359000	1.957627000
P	-2.437461000	-2.772409000	-1.913769000
H	0.431405000	0.584218000	-5.097594000
H	0.134964000	-1.723612000	-5.959959000
H	1.933420000	0.034160000	-5.834982000
P	2.121761000	0.287964000	-3.459663000
P	2.169348000	-2.834107000	1.463700000
C	3.548493000	-2.202590000	2.478248000
H	3.087836000	-1.565713000	3.237447000
H	4.114468000	-1.530889000	1.827803000
H	5.236870000	-2.770997000	3.690825000
H	-5.482151000	-4.715159000	-0.757313000
C	-3.818694000	-3.348590000	-0.868874000
C	-4.675451000	-4.461466000	-1.448163000
C	-3.205150000	-2.326959000	-3.509185000
C	-4.283414000	-1.266713000	-3.381334000
C	1.284089000	-3.994596000	2.563686000
C	0.706228000	-3.354873000	3.812961000
H	-3.362872000	-3.646458000	0.078630000
H	-4.413412000	-2.458972000	-0.645831000
Co	-1.300165000	-1.224905000	-0.986990000
Co	0.941522000	0.243536000	-1.686711000
H	2.011164000	2.620313000	-3.885677000
C	2.845372000	1.915027000	-3.865964000
H	3.251946000	1.863724000	-4.880710000
Co	0.953792000	-1.289578000	0.627257000
H	-5.135365000	-4.171785000	-2.395009000
H	-4.627532000	-0.946992000	-4.366856000
H	-5.150615000	-1.635558000	-2.830136000
H	-3.897279000	-0.393974000	-2.854569000

H	0.029098000	-2.541190000	3.549862000
H	0.149637000	-4.091921000	4.395386000
H	1.487131000	-2.944021000	4.456033000
S	-1.074317000	0.265939000	-2.603740000
S	-2.885599000	0.078302000	-0.133500000
S	0.737849000	-1.944358000	-1.473047000
S	-1.067920000	-2.131560000	1.007420000
S	0.655678000	2.378177000	-1.207957000
S	2.462204000	0.172080000	-0.075619000
C	3.899979000	2.365969000	-2.872307000
H	4.198420000	3.397687000	-3.068297000
H	4.796816000	1.745715000	-2.927062000
H	3.515559000	2.307204000	-1.854217000
S	0.703315000	-0.031001000	2.423084000
Co	-1.356625000	1.548398000	-0.834044000
Co	-1.305964000	0.046912000	1.457845000
Co	0.866987000	1.463160000	0.789423000
P	-2.536619000	3.077589000	-1.746070000
S	-1.155913000	2.256195000	1.252109000
P	-2.485809000	0.110804000	3.321532000
P	2.042251000	3.008993000	1.694847000
H	-3.456234000	1.761595000	-3.481104000
C	-1.632114000	4.199551000	-2.867880000
H	-2.319430000	4.999238000	-3.161042000
C	-3.317572000	4.247386000	-0.580901000
H	-2.509490000	4.638434000	0.042305000
H	-3.714475000	5.086480000	-1.160249000
H	-4.498968000	1.792277000	-2.083181000
C	-3.916127000	2.431875000	-2.751036000
H	-0.842773000	4.654778000	-2.264459000
H	-3.495523000	2.223337000	2.985938000
H	-4.474623000	0.930235000	2.341997000
C	-3.910518000	1.241634000	3.225157000
C	-3.187410000	-1.515518000	3.763427000
H	-3.593310000	-1.439369000	4.777378000
H	-2.340723000	-2.205389000	3.802444000
C	-1.581181000	0.584044000	4.832122000
H	-0.779125000	-0.150206000	4.940675000
H	-2.265375000	0.447256000	5.675541000
H	2.963232000	3.887939000	-0.294119000
C	1.135060000	4.535293000	2.132892000
H	0.330860000	4.226600000	2.805296000
H	1.816919000	5.164829000	2.713059000
C	3.421835000	3.581747000	0.648945000
H	4.011034000	2.690353000	0.419723000
H	2.008371000	2.206820000	3.929365000

C	2.818322000	2.560402000	3.286818000
H	3.215777000	3.473909000	3.739407000
C	-4.792218000	3.470424000	-3.430298000
H	-1.813854000	3.091983000	-4.729352000
C	-1.040051000	3.518732000	-4.088158000
H	-0.471144000	4.234922000	-4.684554000
H	-0.371648000	2.709276000	-3.791392000
C	-4.397073000	3.613123000	0.277775000
H	-4.735030000	4.309361000	1.047893000
H	-4.021019000	2.714470000	0.767420000
H	-5.267814000	3.329181000	-0.316350000
H	-5.584174000	2.979713000	-3.999983000
H	-5.273546000	4.135408000	-2.710529000
H	-4.224845000	4.088164000	-4.129173000
C	-4.792274000	1.297763000	4.461441000
H	-5.621817000	1.988633000	4.297517000
H	-4.243424000	1.650260000	5.336756000
H	-5.222876000	0.324303000	4.704003000
H	-5.126483000	-1.382523000	2.791582000
H	-3.840994000	-2.031165000	1.770556000
C	-4.236459000	-2.014662000	2.786554000
H	-4.547420000	-3.027491000	3.049241000
C	-1.013209000	1.991073000	4.809722000
H	-1.798680000	2.746084000	4.737998000
H	-0.448243000	2.184296000	5.723773000
H	-0.346184000	2.119846000	3.956646000
C	4.286306000	4.686929000	1.231547000
C	0.572775000	5.297587000	0.946278000
H	-0.018830000	6.149404000	1.287793000
H	1.365630000	5.680693000	0.300757000
H	-0.066439000	4.654559000	0.339258000
H	4.751350000	4.389111000	2.173293000
H	3.713762000	5.598230000	1.414150000
H	5.089578000	4.940923000	0.536882000
C	3.893321000	1.497064000	3.155187000
H	4.236967000	1.173806000	4.139741000
H	4.760882000	1.865737000	2.604715000
H	3.508058000	0.627002000	2.623328000

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C	-1.501146000	-4.381734000	-2.521499000
C	-0.981506000	-5.109803000	-1.292265000
H	-0.313619000	-5.923238000	-1.582579000
C	1.248328000	-0.186650000	-5.011288000
C	0.691753000	-1.598534000	-5.028670000
C	3.549784000	-0.883600000	-3.403879000

C	4.435164000	-0.921561000	-4.637888000
H	5.260674000	-1.620192000	-4.486431000
C	2.928177000	-3.969793000	0.328100000
C	3.991434000	-3.345320000	-0.556851000
H	4.299231000	-4.042781000	-1.338231000
C	4.490155000	-3.204875000	3.133553000
H	-2.103170000	-5.044297000	-3.150781000
H	-0.665542000	-4.025308000	-3.130389000
H	-0.430180000	-4.426027000	-0.643883000
H	-1.795120000	-5.541773000	-0.706143000
H	-4.119326000	-5.506998000	-1.881580000
H	-2.403835000	-2.043214000	-4.325053000
H	-3.615826000	-3.315865000	-4.211914000
H	1.484108000	-2.347875000	-4.972666000
H	0.022708000	-1.756307000	-4.181661000
H	4.115165000	-0.596896000	-2.513293000
H	3.128260000	-1.868080000	-3.187732000
H	3.886678000	-1.253023000	-5.521616000
H	4.871814000	0.053992000	-4.860631000
H	2.096604000	-4.345470000	-0.273231000
H	3.329489000	-4.816142000	0.893802000
H	3.612645000	-2.441118000	-1.034195000
H	4.881462000	-3.074426000	0.014263000
H	3.940401000	-3.819723000	3.848703000
H	4.942566000	-3.871604000	2.396903000
H	1.997143000	-4.707565000	2.942045000
H	0.502826000	-4.363475000	2.076956000
P	-2.481925000	-2.894870000	-2.114455000
H	0.440972000	0.542607000	-5.115607000
H	0.132441000	-1.774979000	-5.949710000
H	1.940120000	-0.026045000	-5.843943000
P	2.127753000	0.256838000	-3.472821000
P	2.193006000	-2.795944000	1.516738000
C	3.600461000	-2.157626000	2.485489000
H	3.164539000	-1.490803000	3.233294000
H	4.165680000	-1.515595000	1.805167000
H	5.303889000	-2.721897000	3.678459000
H	-5.514430000	-4.893498000	-1.000047000
C	-3.868876000	-3.497912000	-1.088725000
C	-4.712418000	-4.611462000	-1.685640000
C	-3.227210000	-2.422665000	-3.713348000
C	-4.300879000	-1.357458000	-3.561225000
C	1.305110000	-3.907063000	2.662344000
C	0.741179000	-3.223476000	3.894673000
H	-3.417295000	-3.800256000	-0.139458000
H	-4.473142000	-2.616181000	-0.856578000

Co	-1.314620000	-1.208131000	-1.001695000
Co	0.940892000	0.235694000	-1.695882000
H	2.019732000	2.583502000	-3.928454000
C	2.853677000	1.878403000	-3.894669000
H	3.264684000	1.812065000	-4.906837000
Co	0.996406000	-1.261771000	0.638966000
H	-5.176784000	-4.307561000	-2.625987000
H	-4.629431000	-0.998814000	-4.538633000
H	-5.178289000	-1.741403000	-3.037284000
H	-3.919206000	-0.506687000	-2.994592000
H	0.053781000	-2.424792000	3.612645000
H	0.198623000	-3.943039000	4.511188000
H	1.528566000	-2.785115000	4.511257000
S	-1.073490000	0.322670000	-2.628107000
S	-2.879119000	0.179843000	-0.126615000
S	0.768648000	-1.956869000	-1.453107000
S	-1.038603000	-2.100187000	1.051016000
S	0.694779000	2.390467000	-1.237964000
S	2.481077000	0.186610000	-0.098408000
C	3.904741000	2.343399000	-2.903884000
H	4.213039000	3.367476000	-3.123005000
H	4.796597000	1.714584000	-2.937387000
H	3.513077000	2.313760000	-1.887146000
S	0.739880000	0.028504000	2.416311000
Co	-1.322289000	1.615050000	-0.851575000
Co	-1.324809000	0.087727000	1.516781000
Co	0.916096000	1.506755000	0.773566000
P	-2.532467000	3.128298000	-1.733439000
S	-1.102343000	2.302830000	1.240777000
P	-2.557877000	0.115162000	3.479491000
P	2.085083000	3.055792000	1.674038000
H	-3.447348000	1.799537000	-3.464357000
C	-1.647872000	4.259680000	-2.860966000
H	-2.344919000	5.053816000	-3.146335000
C	-3.310708000	4.282070000	-0.553079000
H	-2.493628000	4.703198000	0.038132000
H	-3.750500000	5.102146000	-1.129003000
H	-4.465979000	1.796921000	-2.050250000
C	-3.910061000	2.455324000	-2.722737000
H	-0.857743000	4.721215000	-2.263092000
H	-3.510828000	2.263994000	3.216271000
H	-4.527389000	1.023598000	2.536539000
C	-3.954382000	1.287664000	3.430330000
C	-3.293922000	-1.508340000	3.880631000
H	-3.739785000	-1.460760000	4.879160000
H	-2.453799000	-2.206856000	3.935050000

C	-1.616988000	0.533855000	4.987387000
H	-0.808466000	-0.200418000	5.044389000
H	-2.258211000	0.380681000	5.860843000
H	3.010222000	3.919559000	-0.320552000
C	1.179738000	4.585370000	2.099533000
H	0.379180000	4.281858000	2.778683000
H	1.864166000	5.221874000	2.669019000
C	3.467297000	3.615839000	0.624133000
H	4.052229000	2.720361000	0.399538000
H	2.040504000	2.258799000	3.907286000
C	2.854772000	2.610030000	3.268769000
H	3.252814000	3.523431000	3.721042000
C	-4.818176000	3.480467000	-3.379885000
H	-1.834861000	3.150152000	-4.721071000
C	-1.060167000	3.587072000	-4.087854000
H	-0.507750000	4.311194000	-4.690001000
H	-0.376176000	2.787646000	-3.798417000
C	-4.341713000	3.629082000	0.349861000
H	-4.689964000	4.336006000	1.105361000
H	-3.915928000	2.764176000	0.859777000
H	-5.213338000	3.290580000	-0.213664000
H	-5.603012000	2.977613000	-3.948619000
H	-5.308835000	4.122887000	-2.646111000
H	-4.272782000	4.121457000	-4.075342000
C	-4.840013000	1.337394000	4.663266000
H	-5.643868000	2.064094000	4.526862000
H	-4.279734000	1.633406000	5.552507000
H	-5.305489000	0.371130000	4.868096000
H	-5.176017000	-1.324509000	2.807933000
H	-3.856471000	-2.002372000	1.850399000
C	-4.303087000	-1.979345000	2.846427000
H	-4.654468000	-2.984821000	3.085876000
C	-1.044915000	1.941243000	4.961853000
H	-1.832222000	2.697700000	4.947426000
H	-0.428504000	2.120274000	5.845035000
H	-0.427499000	2.086713000	4.073693000
C	4.337180000	4.719672000	1.201320000
C	0.611597000	5.331872000	0.905837000
H	0.020769000	6.187484000	1.238907000
H	1.401172000	5.707250000	0.251724000
H	-0.030881000	4.679192000	0.312390000
H	4.797729000	4.425278000	2.146325000
H	3.769366000	5.635352000	1.376407000
H	5.143770000	4.964370000	0.507193000
C	3.927694000	1.544274000	3.140621000
H	4.264108000	1.216601000	4.126145000

H	4.799901000	1.912210000	2.596952000
H	3.542009000	0.676981000	2.604189000

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C	-1.523229000	-4.302779000	-2.423142000
C	-0.929703000	-5.058595000	-1.247556000
H	-0.361049000	-5.921077000	-1.600868000
C	1.352296000	-0.251336000	-5.091535000
C	0.796505000	-1.663348000	-5.098369000
C	3.638837000	-0.904273000	-3.426413000
C	4.547594000	-0.964794000	-4.642355000
H	5.374210000	-1.654520000	-4.459982000
C	3.131608000	-4.183353000	0.451705000
C	4.141030000	-3.538502000	-0.483244000
H	4.472943000	-4.249171000	-1.242655000
C	4.664124000	-3.315434000	3.270424000
H	-2.214103000	-4.936633000	-2.988066000
H	-0.736075000	-3.988949000	-3.113569000
H	-0.259745000	-4.416883000	-0.673252000
H	-1.704081000	-5.426004000	-0.571153000
H	-4.128457000	-5.347232000	-1.688334000
H	-2.393556000	-1.997705000	-4.208301000
H	-3.643463000	-3.218420000	-3.989476000
H	1.587699000	-2.412253000	-5.023679000
H	0.115353000	-1.811056000	-4.258654000
H	4.184797000	-0.594091000	-2.531490000
H	3.218755000	-1.885766000	-3.192799000
H	4.017553000	-1.318927000	-5.528563000
H	4.982245000	0.008603000	-4.878576000
H	2.299810000	-4.604217000	-0.121294000
H	3.579504000	-5.004458000	1.019558000
H	3.701739000	-2.677116000	-0.989390000
H	5.025866000	-3.195245000	0.056631000
H	4.112101000	-3.936815000	3.978456000
H	5.150381000	-3.979201000	2.552681000
H	2.114923000	-4.870164000	3.101039000
H	0.671452000	-4.539452000	2.149782000
P	-2.427252000	-2.781284000	-1.970230000
H	0.546179000	0.476707000	-5.215291000
H	0.248447000	-1.850111000	-6.024027000
H	2.054398000	-0.101015000	-5.917587000
P	2.210983000	0.223325000	-3.552029000
P	2.374834000	-2.988077000	1.608049000
C	3.760705000	-2.306361000	2.583376000
H	3.304347000	-1.624400000	3.306380000
H	4.323362000	-1.669331000	1.894618000

H	5.451782000	-2.805086000	3.829029000
H	-5.478540000	-4.684165000	-0.776010000
C	-3.797419000	-3.343894000	-0.904763000
C	-4.686227000	-4.431470000	-1.483496000
C	-3.209031000	-2.313805000	-3.552635000
C	-4.246656000	-1.212932000	-3.426887000
C	1.452246000	-4.070315000	2.755962000
C	0.827489000	-3.331101000	3.927651000
H	-3.329551000	-3.662703000	0.029884000
H	-4.369539000	-2.446189000	-0.657245000
Co	-1.244137000	-1.251889000	-1.065595000
Co	1.001119000	0.221976000	-1.797471000
H	2.063555000	2.534154000	-4.047959000
C	2.914061000	1.849905000	-3.987756000
H	3.343407000	1.775925000	-4.991813000
Co	1.034374000	-1.338540000	0.584306000
H	-5.166273000	-4.115622000	-2.411730000
H	-4.620271000	-0.928078000	-4.412401000
H	-5.101825000	-1.531662000	-2.827497000
H	-3.816716000	-0.328446000	-2.955597000
H	0.163215000	-2.539183000	3.576952000
H	0.246028000	-4.018933000	4.545026000
H	1.584749000	-2.872527000	4.567122000
S	-1.022324000	0.218282000	-2.711025000
S	-2.875091000	0.023714000	-0.230004000
S	0.797823000	-1.970392000	-1.551314000
S	-1.041361000	-2.178191000	0.945138000
S	0.683781000	2.359578000	-1.347262000
S	2.506804000	0.184425000	-0.179065000
C	3.938050000	2.353751000	-2.987914000
H	4.231764000	3.378626000	-3.222369000
H	4.841246000	1.740479000	-2.993126000
H	3.528397000	2.337491000	-1.977792000
S	0.698900000	0.004401000	2.364403000
Co	-1.388251000	1.562491000	-0.962710000
Co	-1.389170000	-0.011573000	1.484690000
Co	0.868967000	1.447253000	0.668514000
P	-2.659343000	3.342324000	-1.817138000
S	-1.163723000	2.215300000	1.186516000
P	-2.640050000	0.025354000	3.482595000
P	2.016097000	3.014324000	1.588557000
H	-3.575320000	2.127323000	-3.635153000
C	-1.727275000	4.511000000	-2.866760000
H	-2.363433000	5.366080000	-3.114627000
C	-3.430123000	4.409715000	-0.551933000
H	-2.606928000	4.762446000	0.076307000

H	-3.869691000	5.289314000	-1.031839000
H	-4.607916000	2.055684000	-2.235111000
C	-4.037084000	2.747652000	-2.861426000
H	-0.913243000	4.884564000	-2.238613000
H	-3.617409000	2.157544000	3.169576000
H	-4.640911000	0.890852000	2.556462000
C	-4.048880000	1.186102000	3.428156000
C	-3.353954000	-1.596249000	3.933054000
H	-3.792344000	-1.541431000	4.934363000
H	-2.503619000	-2.282803000	3.990498000
C	-1.686884000	0.484342000	4.972875000
H	-0.860776000	-0.230972000	5.025161000
H	-2.307700000	0.327448000	5.860233000
H	2.944276000	3.900283000	-0.396695000
C	1.088156000	4.529519000	2.016059000
H	0.289690000	4.213464000	2.691916000
H	1.763166000	5.171901000	2.590111000
C	3.397812000	3.599861000	0.550695000
H	3.998989000	2.714799000	0.328155000
H	1.967698000	2.223873000	3.823990000
C	2.782821000	2.573764000	3.185804000
H	3.175473000	3.491823000	3.633587000
C	-4.931633000	3.814181000	-3.469407000
H	-1.956275000	3.545131000	-4.801754000
C	-1.163875000	3.860507000	-4.119927000
H	-0.524049000	4.561047000	-4.660258000
H	-0.570484000	2.979565000	-3.865874000
C	-4.453921000	3.669267000	0.293300000
H	-4.803373000	4.299610000	1.113447000
H	-4.021616000	2.762258000	0.719978000
H	-5.327207000	3.379024000	-0.294469000
H	-5.718646000	3.356181000	-4.072604000
H	-5.418787000	4.419392000	-2.702264000
H	-4.372251000	4.488605000	-4.121118000
C	-4.907742000	1.275577000	4.677495000
H	-5.723003000	1.988000000	4.533122000
H	-4.330055000	1.610941000	5.541316000
H	-5.357006000	0.312973000	4.930648000
H	-5.251676000	-1.461450000	2.881265000
H	-3.927177000	-2.111082000	1.912028000
C	-4.363645000	-2.096137000	2.912494000
H	-4.690176000	-3.108738000	3.157356000
C	-1.145509000	1.903698000	4.923079000
H	-1.949027000	2.643164000	4.915535000
H	-0.517818000	2.105631000	5.793414000
H	-0.547062000	2.054473000	4.022773000

C	4.246146000	4.715136000	1.137781000
C	0.514206000	5.272670000	0.823143000
H	-0.078732000	6.126488000	1.157208000
H	1.300249000	5.650549000	0.166091000
H	-0.128076000	4.616226000	0.234415000
H	4.706974000	4.423782000	2.083549000
H	3.662440000	5.620562000	1.313782000
H	5.051960000	4.976183000	0.448690000
C	3.861474000	1.512171000	3.069222000
H	4.210800000	1.211823000	4.058991000
H	4.725330000	1.873872000	2.508091000
H	3.476580000	0.628370000	2.559754000

6Fe_1_2_M2

Fe	6.154615000	6.271025000	6.559110000
Fe	8.353796000	7.753250000	5.947561000
Fe	8.360464000	6.230832000	8.228497000
Fe	6.064074000	9.025388000	6.786949000
Fe	6.150302000	7.516450000	8.997158000
Fe	8.381224000	8.998264000	8.305243000
S	6.366008000	7.796591000	4.898626000
S	4.499673000	7.513572000	7.471780000
S	8.239385000	5.515452000	6.081605000
S	6.303159000	5.318797000	8.590074000
S	8.108664000	9.938274000	6.292108000
S	9.984085000	7.661789000	7.471639000
S	8.170187000	7.547952000	10.041398000
S	6.337907000	9.779498000	8.901753000
P	5.068509000	4.669511000	5.476414000
P	9.698906000	4.634510000	9.143075000
P	4.775071000	10.644728000	5.820421000
P	4.921176000	7.555104000	10.905853000
P	9.705361000	10.597498000	9.035323000
C	6.020806000	3.153810000	5.107577000
C	6.499751000	2.408657000	6.341620000
C	10.441719000	3.514854000	7.910233000
C	11.476793000	4.171815000	7.013607000
C	11.997564000	4.263273000	10.750133000
C	11.083751000	5.301428000	10.120120000
C	3.620352000	4.091326000	6.431279000
C	2.802865000	2.977750000	5.798764000
C	4.398920000	5.126517000	3.838862000
C	3.299941000	6.173013000	3.911304000
C	8.799254000	3.503618000	10.256452000
C	8.193796000	4.180946000	11.472686000
C	5.680501000	11.808667000	4.747221000

C	3.977276000	11.743840000	7.039503000
C	3.425904000	9.969551000	4.797772000
C	3.521248000	8.720025000	10.832413000
C	4.172461000	5.936083000	11.307853000
C	5.813606000	7.965283000	12.445875000
C	8.856406000	12.157557000	9.474992000
C	11.019740000	11.071760000	7.861750000
C	10.563431000	10.216474000	10.603202000
C	2.515811000	11.000271000	4.150640000
C	6.268884000	11.189725000	3.492047000
C	2.936684000	11.047244000	7.897150000
C	2.639054000	8.782388000	12.067866000
C	3.116827000	5.473552000	10.318914000
C	6.360157000	9.380757000	12.500056000
C	11.988755000	12.139447000	8.339510000
C	8.159243000	12.861538000	8.324306000
C	11.543540000	9.062601000	10.510440000
H	7.120515000	1.557327000	6.055454000
H	11.831946000	3.458053000	6.268465000
H	5.396928000	2.510450000	4.479774000
H	6.869963000	3.472871000	4.497678000
H	7.088414000	3.064449000	6.985194000
H	5.664024000	2.026603000	6.931547000
H	3.394117000	2.071324000	5.655302000
H	5.248431000	5.501179000	3.261578000
H	4.046761000	4.217390000	3.342259000
H	9.607767000	3.128058000	7.319109000
H	10.872130000	2.669849000	8.457505000
H	11.056061000	5.029337000	6.486472000
H	12.343359000	4.514634000	7.582010000
H	11.459453000	3.615571000	11.444793000
H	12.475576000	3.630435000	10.000178000
H	9.489789000	2.706928000	10.551022000
H	8.017232000	3.047730000	9.643623000
H	10.631835000	5.946946000	10.877352000
H	11.633624000	5.965450000	9.448441000
H	12.791428000	4.757261000	11.313828000
H	1.957747000	2.717449000	6.439538000
H	4.008993000	3.794283000	7.408992000
H	3.013654000	4.982693000	6.612735000
H	2.398124000	3.269205000	4.827528000
H	3.030619000	6.516127000	2.910540000
H	2.396855000	5.776914000	4.379462000
H	3.627870000	7.036657000	4.491402000
H	7.508511000	4.974290000	11.170227000
H	7.638619000	3.455931000	12.070827000

H	8.958290000	4.624629000	12.113476000
H	3.910833000	9.341014000	4.046811000
H	4.988846000	12.620184000	4.498475000
H	4.786266000	12.140273000	7.658466000
H	3.542048000	12.585869000	6.492258000
H	2.867647000	9.287547000	5.444517000
H	6.469225000	12.235593000	5.372366000
H	3.956874000	9.695743000	10.603508000
H	2.947195000	8.431991000	9.947450000
H	3.760640000	6.001170000	12.319984000
H	5.001406000	5.224075000	11.342079000
H	6.627357000	7.239279000	12.523507000
H	5.131181000	7.776096000	13.280378000
H	10.504151000	11.379652000	6.948294000
H	8.133669000	11.889158000	10.250750000
H	9.597144000	12.814226000	9.942183000
H	11.539502000	10.144578000	7.606204000
H	9.773177000	9.989178000	11.324670000
H	11.058739000	11.129892000	10.946904000
H	5.495311000	10.769934000	2.846136000
H	6.803920000	11.948254000	2.917969000
H	6.971154000	10.392549000	3.737502000
H	2.571751000	11.720500000	8.675050000
H	3.358979000	10.164706000	8.378320000
H	2.076259000	10.727214000	7.306470000
H	1.746982000	10.500816000	3.557724000
H	2.005718000	11.619000000	4.891477000
H	3.064878000	11.662861000	3.478999000
H	1.824081000	9.492646000	11.913389000
H	3.194853000	9.110853000	12.948121000
H	2.187988000	7.814993000	12.297384000
H	2.253213000	6.141396000	10.308384000
H	3.520308000	5.432061000	9.306270000
H	2.760289000	4.476767000	10.585318000
H	5.563122000	10.125571000	12.453438000
H	6.906478000	9.537956000	13.432112000
H	7.040827000	9.567235000	11.668151000
H	7.659799000	13.764727000	8.680966000
H	8.863003000	13.158031000	7.543903000
H	7.410163000	12.211227000	7.870143000
H	12.533649000	11.827573000	9.232643000
H	11.482129000	13.079474000	8.567162000
H	12.728252000	12.348784000	7.564027000
H	11.982315000	8.853545000	11.488210000
H	12.360396000	9.279244000	9.818918000
H	11.040491000	8.161875000	10.159525000

6Fe_1_4_M2

Fe	6.123774000	6.253399000	6.631226000
Fe	8.319189000	7.732740000	6.000678000
Fe	8.368164000	6.218133000	8.280607000
Fe	6.065589000	9.097107000	6.780962000
Fe	6.082165000	7.577043000	9.135160000
Fe	8.360200000	9.054986000	8.361194000
S	6.346776000	7.765660000	4.956085000
S	4.504525000	7.625437000	7.451688000
S	8.194834000	5.510827000	6.142950000
S	6.336427000	5.338939000	8.685156000
S	8.107713000	9.936104000	6.306780000
S	9.947704000	7.668685000	7.526089000
S	8.179017000	7.562591000	10.069273000
S	6.309924000	9.851511000	8.887250000
P	5.072197000	4.610893000	5.591503000
P	9.720643000	4.612298000	8.968935000
P	4.925961000	10.702930000	5.778477000
P	4.709427000	7.524032000	11.047672000
P	9.696070000	10.667074000	9.047596000
C	6.030656000	3.096460000	5.242588000
C	6.545074000	2.390846000	6.485057000
C	10.512664000	3.575914000	7.692219000
C	11.491766000	4.325589000	6.805239000
C	12.045735000	4.219373000	10.550999000
C	11.096428000	5.259499000	9.979904000
C	3.643645000	4.052993000	6.583380000
C	2.822840000	2.920861000	5.988519000
C	4.386887000	5.043176000	3.955465000
C	3.286160000	6.088756000	4.013293000
C	8.891671000	3.384177000	10.038258000
C	8.354645000	3.961399000	11.337369000
C	5.836962000	11.811646000	4.651102000
C	4.140355000	11.867618000	6.945950000
C	3.551521000	10.033727000	4.777698000
C	3.324077000	8.706527000	10.934382000
C	3.951761000	5.901596000	11.404181000
C	5.584877000	7.928406000	12.599593000
C	8.850265000	12.232351000	9.463965000
C	11.009907000	11.106533000	7.862318000
C	10.548369000	10.281807000	10.616813000
C	2.659116000	11.059877000	4.100442000
C	6.402917000	11.121657000	3.422115000
C	3.082154000	11.227590000	7.828127000
C	2.370481000	8.742825000	12.115992000

C	2.974289000	5.452651000	10.330473000
C	6.144302000	9.340820000	12.634637000
C	12.011247000	12.146459000	8.335648000
C	8.163733000	12.918012000	8.295794000
C	11.515017000	9.114737000	10.535386000
H	7.171436000	1.540559000	6.208604000
H	11.887938000	3.660810000	6.035541000
H	5.396411000	2.432150000	4.647852000
H	6.861661000	3.406376000	4.603757000
H	7.138434000	3.071646000	7.097513000
H	5.727555000	2.014068000	7.103101000
H	3.414447000	2.011599000	5.866603000
H	5.231776000	5.407032000	3.364493000
H	4.032819000	4.122959000	3.480793000
H	9.699257000	3.154962000	7.095427000
H	11.004638000	2.739915000	8.199136000
H	11.010478000	5.168742000	6.307500000
H	12.338754000	4.711579000	7.375823000
H	11.530204000	3.512540000	11.203918000
H	12.544511000	3.648932000	9.765332000
H	9.600382000	2.572980000	10.230320000
H	8.077424000	2.966922000	9.439890000
H	10.630161000	5.850074000	10.773054000
H	11.625216000	5.975794000	9.345955000
H	12.822983000	4.704428000	11.144943000
H	1.983885000	2.678328000	6.643908000
H	4.049087000	3.781049000	7.561457000
H	3.034244000	4.945010000	6.752261000
H	2.409905000	3.184452000	5.012846000
H	2.991767000	6.387008000	3.005442000
H	2.396321000	5.710102000	4.519668000
H	3.623176000	6.979042000	4.546648000
H	7.680861000	4.797476000	11.141537000
H	7.803330000	3.199877000	11.891927000
H	9.158724000	4.323004000	11.981300000
H	4.014469000	9.366970000	4.045714000
H	5.158455000	12.622318000	4.367526000
H	4.951122000	12.276755000	7.554651000
H	3.722940000	12.695522000	6.364955000
H	2.980677000	9.386553000	5.449067000
H	6.639056000	12.257319000	5.245388000
H	3.786037000	9.682951000	10.762680000
H	2.799932000	8.462263000	10.005698000
H	3.473556000	5.936986000	12.387837000
H	4.785535000	5.196703000	11.476312000
H	6.395685000	7.198323000	12.680175000

H	4.906111000	7.749604000	13.439211000
H	10.494101000	11.430949000	6.954749000
H	8.120262000	11.972811000	10.236054000
H	9.587497000	12.894548000	9.928780000
H	11.501741000	10.165851000	7.600662000
H	9.754888000	10.070946000	11.339909000
H	11.055537000	11.191508000	10.953261000
H	5.613968000	10.698962000	2.796981000
H	6.960783000	11.835192000	2.813000000
H	7.079792000	10.312437000	3.698993000
H	2.727657000	11.939182000	8.576081000
H	3.485110000	10.357713000	8.348888000
H	2.217800000	10.901070000	7.246688000
H	1.873891000	10.558525000	3.530921000
H	2.169226000	11.716098000	4.822430000
H	3.217017000	11.686623000	3.402084000
H	1.582670000	9.479973000	11.947266000
H	2.881423000	9.016466000	13.041340000
H	1.885358000	7.777729000	12.275512000
H	2.100061000	6.105073000	10.283565000
H	3.447935000	5.457997000	9.347238000
H	2.620580000	4.440001000	10.533388000
H	5.351134000	10.090387000	12.601075000
H	6.711565000	9.500989000	13.553439000
H	6.808502000	9.517750000	11.786830000
H	7.648746000	13.818678000	8.635734000
H	8.876408000	13.214378000	7.523609000
H	7.427930000	12.255572000	7.836984000
H	12.561448000	11.811683000	9.217045000
H	11.530679000	13.095753000	8.580792000
H	12.743749000	12.345976000	7.551073000
H	11.960154000	8.921233000	11.513266000
H	12.328205000	9.309479000	9.833104000
H	11.001448000	8.210104000	10.208869000

6Fe_1_6_M1

Fe	6.235414000	6.375442000	6.565360000
Fe	8.479261000	7.820127000	5.894150000
Fe	8.481935000	6.269173000	8.127811000
Fe	6.194521000	9.105789000	6.707091000
Fe	6.297706000	7.621344000	9.010359000
Fe	8.448700000	9.006920000	8.285404000
S	6.441710000	7.836856000	4.879373000
S	4.629642000	7.682311000	7.462228000
S	8.261051000	5.563700000	5.999635000
S	6.454142000	5.411956000	8.589067000

S	8.216363000	10.040601000	6.288341000
S	10.103799000	7.710444000	7.471415000
S	8.347098000	7.542152000	9.978237000
S	6.425193000	9.862913000	8.831837000
P	9.755972000	7.825604000	3.998355000
P	9.657446000	4.621264000	8.983926000
P	4.911169000	10.572169000	5.719252000
P	4.977340000	7.553904000	10.857722000
P	9.630510000	10.693767000	9.212793000
C	8.857770000	7.454186000	2.454599000
C	8.314383000	6.040077000	2.359837000
C	11.133121000	6.636592000	4.071282000
C	12.039692000	6.604609000	2.852058000
C	10.351295000	3.450568000	7.765180000
C	11.432546000	4.062297000	6.891574000
C	11.969095000	4.142029000	10.568157000
C	11.099692000	5.215920000	9.936033000
C	8.769879000	3.515265000	10.135138000
C	8.257291000	4.200464000	11.389201000
C	10.518921000	9.446168000	3.648797000
C	11.552420000	9.866552000	4.677171000
C	5.741917000	11.675141000	4.521218000
C	4.133782000	11.787984000	6.840459000
C	3.526395000	9.816480000	4.798628000
C	3.601471000	8.744117000	10.792656000
C	4.218075000	5.926608000	11.174599000
C	5.875359000	7.908022000	12.406318000
C	8.698593000	12.199487000	9.660004000
C	11.002705000	11.272882000	8.161459000
C	10.407862000	10.230097000	10.801367000
C	2.588806000	10.781149000	4.092955000
C	6.384295000	10.980117000	3.334676000
C	3.130223000	11.180889000	7.803837000
C	2.666034000	8.731461000	11.989862000
C	3.199058000	5.496179000	10.134306000
C	6.458988000	9.307445000	12.479059000
C	11.854032000	12.394051000	8.733072000
C	8.112572000	12.951018000	8.477695000
C	11.497036000	9.178995000	10.673817000
H	12.835313000	5.870950000	2.996586000
H	11.706652000	3.378575000	6.085917000
H	9.112553000	5.295962000	2.392120000
H	7.622629000	5.827243000	3.175585000
H	11.689795000	6.881254000	4.979773000
H	10.673218000	5.662383000	4.253199000
H	11.496676000	6.322382000	1.948192000

H	12.516099000	7.570102000	2.670667000
H	9.505703000	3.117938000	7.157876000
H	10.727127000	2.575761000	8.304205000
H	11.086399000	4.994936000	6.445093000
H	12.336931000	4.278632000	7.463478000
H	11.416255000	3.547787000	11.298201000
H	12.380688000	3.457427000	9.823923000
H	9.444696000	2.692179000	10.389168000
H	7.941063000	3.087293000	9.565456000
H	8.045626000	8.183290000	2.395259000
H	7.778494000	5.909493000	1.418123000
H	9.545565000	7.666944000	1.629581000
H	10.698629000	5.897920000	10.690326000
H	11.672610000	5.841509000	9.246355000
H	12.811826000	4.598018000	11.091962000
H	9.694952000	10.163436000	3.616645000
H	10.952086000	9.400860000	2.644571000
H	7.590188000	5.024995000	11.133421000
H	7.705653000	3.491774000	12.010083000
H	9.072866000	4.605259000	11.991985000
H	11.906115000	10.878238000	4.469845000
H	12.420146000	9.204185000	4.672384000
H	11.125140000	9.852021000	5.679953000
H	3.982928000	9.116645000	4.093852000
H	4.999425000	12.406931000	4.188185000
H	4.956497000	12.256067000	7.388106000
H	3.671645000	12.566796000	6.226301000
H	2.992154000	9.195152000	5.522235000
H	6.495210000	12.223176000	5.094095000
H	4.062858000	9.724670000	10.652147000
H	3.067010000	8.527594000	9.864113000
H	3.770063000	5.970062000	12.172864000
H	5.045280000	5.213826000	11.220747000
H	6.668551000	7.158446000	12.468485000
H	5.185956000	7.723609000	13.236403000
H	10.545276000	11.561717000	7.211978000
H	7.905287000	11.871510000	10.336768000
H	9.372279000	12.840170000	10.237479000
H	11.603802000	10.385331000	7.946067000
H	9.595489000	9.862879000	11.434186000
H	10.793150000	11.142368000	11.267168000
H	5.655057000	10.417956000	2.747918000
H	6.848116000	11.714645000	2.672856000
H	7.153406000	10.281846000	3.666306000
H	2.787524000	11.928233000	8.522032000
H	3.579131000	10.354904000	8.356314000

H	2.252253000	10.796981000	7.280772000
H	1.794266000	10.229346000	3.586837000
H	2.111935000	11.472817000	4.790368000
H	3.107192000	11.372634000	3.335862000
H	1.879469000	9.476938000	11.857388000
H	3.187898000	8.969451000	12.918825000
H	2.178616000	7.762987000	12.116261000
H	2.350274000	6.181218000	10.090484000
H	3.646609000	5.450057000	9.140581000
H	2.812815000	4.505003000	10.377805000
H	5.680455000	10.072455000	12.461102000
H	7.026846000	9.432158000	13.402863000
H	7.128033000	9.489253000	11.636271000
H	7.526840000	13.804182000	8.825344000
H	8.891710000	13.331517000	7.814173000
H	7.460663000	12.302675000	7.890505000
H	12.317099000	12.112038000	9.680644000
H	11.270369000	13.300877000	8.901925000
H	12.657911000	12.648250000	8.039282000
H	11.856746000	8.884196000	11.661419000
H	12.353124000	9.551303000	10.107884000
H	11.122983000	8.287792000	10.167909000

6Fe_1_6_M2

Fe	6.166351000	6.269031000	6.467215000
Fe	8.513419000	7.733385000	5.663721000
Fe	8.429655000	6.173806000	8.074891000
Fe	6.168615000	9.021117000	6.659364000
Fe	6.190188000	7.521981000	8.938152000
Fe	8.416082000	8.982437000	8.258494000
S	6.411056000	7.762356000	4.754111000
S	4.565543000	7.591387000	7.363955000
S	8.245673000	5.487939000	5.912168000
S	6.388672000	5.319543000	8.485727000
S	8.240870000	9.957285000	6.203011000
S	10.026982000	7.626899000	7.370083000
S	8.240740000	7.469838000	9.894001000
S	6.373200000	9.763196000	8.803243000
P	5.027804000	4.584358000	5.583649000
P	9.616055000	4.588586000	9.042224000
P	4.830662000	10.708592000	5.748586000
P	5.037424000	7.579099000	10.827057000
P	9.589061000	10.627792000	9.121037000
C	5.968159000	3.073494000	5.174416000
C	6.561137000	2.365874000	6.380409000
C	10.381072000	3.411525000	7.872900000

C	11.426995000	4.035769000	6.964616000
C	11.902880000	4.210227000	10.690534000
C	11.007640000	5.243017000	10.027683000
C	3.648484000	4.016946000	6.636971000
C	2.799208000	2.887094000	6.080560000
C	4.260263000	5.011466000	3.980508000
C	3.191503000	6.086634000	4.083672000
C	8.711296000	3.484622000	10.181713000
C	8.137538000	4.187695000	11.399010000
C	5.733429000	11.873160000	4.670500000
C	4.053969000	11.809086000	6.982217000
C	3.462490000	10.054924000	4.734197000
C	3.631497000	8.742289000	10.787648000
C	4.296124000	5.967857000	11.269309000
C	5.970273000	8.011168000	12.336631000
C	8.675642000	12.146614000	9.563530000
C	10.945946000	11.178856000	8.032575000
C	10.393488000	10.184288000	10.700949000
C	2.556965000	11.094621000	4.095558000
C	6.301309000	11.245650000	3.409279000
C	3.004327000	11.118775000	7.835544000
C	2.785410000	8.811210000	12.047638000
C	3.226537000	5.499390000	10.298520000
C	6.544769000	9.416429000	12.335523000
C	11.833407000	12.280979000	8.586152000
C	8.047228000	12.868681000	8.384314000
C	11.461600000	9.112939000	10.567475000
H	7.165870000	1.514297000	6.062658000
H	11.783972000	3.303083000	6.238862000
H	5.303944000	2.407653000	4.615086000
H	6.758847000	3.390069000	4.489149000
H	7.195610000	3.044503000	6.952147000
H	5.785303000	1.990624000	7.051063000
H	3.384969000	1.979195000	5.924802000
H	5.081334000	5.348262000	3.341478000
H	3.858053000	4.097165000	3.533811000
H	9.559362000	2.997711000	7.282112000
H	10.804994000	2.587434000	8.455019000
H	11.014974000	4.882903000	6.413760000
H	12.291753000	4.388908000	7.529690000
H	11.350574000	3.583413000	11.393508000
H	12.379739000	3.554320000	9.959783000
H	9.389926000	2.679297000	10.478945000
H	7.911478000	3.030683000	9.590819000
H	10.560899000	5.913695000	10.766200000
H	11.575435000	5.884644000	9.348273000

H	12.698387000	4.704864000	11.251686000
H	1.994020000	2.640481000	6.775675000
H	4.101553000	3.742427000	7.593169000
H	3.045160000	4.906470000	6.839196000
H	2.338244000	3.155246000	5.127904000
H	2.839630000	6.371567000	3.090362000
H	2.326793000	5.741936000	4.654446000
H	3.582461000	6.979091000	4.574713000
H	7.475093000	5.001327000	11.099513000
H	7.565385000	3.486397000	12.009715000
H	8.922057000	4.612347000	12.028533000
H	3.930983000	9.418453000	3.978433000
H	5.056007000	12.698558000	4.429810000
H	4.872184000	12.178368000	7.606529000
H	3.632971000	12.671874000	6.457113000
H	2.900952000	9.378695000	5.384781000
H	6.537453000	12.284198000	5.287570000
H	4.056486000	9.718283000	10.540941000
H	3.032759000	8.449677000	9.920670000
H	3.899444000	6.044192000	12.286462000
H	5.123440000	5.254076000	11.298416000
H	6.771529000	7.272455000	12.418897000
H	5.302786000	7.861313000	13.190686000
H	10.473489000	11.478202000	7.093986000
H	7.908170000	11.839594000	10.278997000
H	9.370190000	12.801591000	10.098675000
H	11.520655000	10.279362000	7.795917000
H	9.591713000	9.845087000	11.362080000
H	10.805449000	11.099630000	11.136947000
H	5.514942000	10.844540000	2.766961000
H	6.850709000	11.992183000	2.833064000
H	6.986591000	10.431757000	3.648739000
H	2.652272000	11.787875000	8.623085000
H	3.411223000	10.222727000	8.305544000
H	2.136770000	10.820516000	7.243912000
H	1.773278000	10.606588000	3.512550000
H	2.065526000	11.721562000	4.842254000
H	3.106910000	11.749763000	3.417278000
H	1.963843000	9.517451000	11.911076000
H	3.365477000	9.149544000	12.908286000
H	2.344781000	7.844479000	12.298785000
H	2.358791000	6.161964000	10.302505000
H	3.615872000	5.461348000	9.280265000
H	2.880086000	4.499716000	10.567157000
H	5.761600000	10.175510000	12.281869000
H	7.115931000	9.593075000	13.249110000

H	7.209640000	9.559801000	11.482221000
H	7.482235000	13.737017000	8.728983000
H	8.800942000	13.221515000	7.677798000
H	7.367528000	12.207966000	7.844666000
H	12.317113000	11.987857000	9.519921000
H	11.272962000	13.199223000	8.772089000
H	12.622645000	12.520783000	7.871059000
H	11.840009000	8.828555000	11.551117000
H	12.309755000	9.460337000	9.974570000
H	11.059898000	8.220412000	10.086462000

6Fe_1_6_M3

Fe	6.224625000	6.267986000	6.526189000
Fe	8.382092000	7.774439000	5.720886000
Fe	8.374827000	6.335292000	8.035356000
Fe	6.083573000	9.001708000	6.582946000
Fe	6.102828000	7.568351000	8.927416000
Fe	8.307388000	9.015623000	8.181620000
S	6.344071000	7.686682000	4.760251000
S	4.514661000	7.524167000	7.329087000
S	8.286692000	5.507146000	5.960345000
S	6.452768000	5.320727000	8.565865000
S	8.094235000	9.944993000	6.142468000
S	9.969715000	7.736348000	7.321491000
S	8.127461000	7.541387000	9.897952000
S	6.242137000	9.775034000	8.695167000
P	4.954304000	4.636351000	5.585125000
P	9.710094000	7.821828000	3.982492000
P	4.897251000	10.674948000	5.709942000
P	4.942461000	7.595610000	10.785282000
P	9.604538000	10.493887000	9.222649000
C	5.896937000	3.139453000	5.140399000
C	6.492888000	2.389353000	6.318352000
C	8.899887000	7.369986000	2.407044000
C	8.373803000	5.947058000	2.346677000
C	11.128367000	6.683298000	4.135458000
C	12.072625000	6.629586000	2.946525000
C	3.608174000	4.075664000	6.674849000
C	2.739123000	2.959321000	6.119592000
C	4.169404000	5.111915000	4.009723000
C	3.099869000	6.180470000	4.147968000
C	10.434709000	9.447875000	3.579933000
C	11.416844000	9.950874000	4.621247000
C	5.782936000	11.774160000	4.549339000
C	4.170300000	11.855191000	6.900831000
C	3.474078000	10.049364000	4.746956000

C	3.499773000	8.711916000	10.704846000
C	4.256006000	5.969699000	11.258905000
C	5.836563000	8.087840000	12.299637000
C	8.702058000	12.000758000	9.730715000
C	10.980526000	11.101571000	8.191431000
C	10.377787000	9.943820000	10.781323000
C	2.597458000	11.098207000	4.083771000
C	6.314504000	11.065972000	3.315314000
C	3.086343000	11.237932000	7.768204000
C	2.633549000	8.774546000	11.951652000
C	3.212997000	5.440286000	10.291310000
C	6.381004000	9.504682000	12.277226000
C	11.876612000	12.151352000	8.827047000
C	8.165095000	12.825019000	8.573323000
C	11.401342000	8.835619000	10.602968000
H	7.050078000	1.520708000	5.963449000
H	12.884077000	5.925955000	3.142839000
H	5.217788000	2.498368000	4.568669000
H	6.681591000	3.471516000	4.455501000
H	7.177053000	3.022868000	6.883847000
H	5.721161000	2.030970000	7.002302000
H	3.314037000	2.050470000	5.933434000
H	4.981465000	5.460001000	3.366048000
H	3.764368000	4.200171000	3.559257000
H	9.178030000	5.213335000	2.430853000
H	7.664555000	5.760635000	3.154619000
H	11.651312000	6.977084000	5.049271000
H	10.698163000	5.701192000	4.348948000
H	11.566286000	6.297346000	2.038133000
H	12.526969000	7.600891000	2.740649000
H	8.082200000	8.085009000	2.279004000
H	7.864337000	5.772245000	1.396951000
H	9.616936000	7.554906000	1.601226000
H	1.954003000	2.707770000	6.835252000
H	4.089603000	3.782098000	7.610852000
H	3.019051000	4.966578000	6.906607000
H	9.591282000	10.136725000	3.482296000
H	10.906400000	9.372293000	2.595373000
H	2.250908000	3.247232000	5.186603000
H	2.729129000	6.472144000	3.163641000
H	2.247996000	5.826438000	4.731599000
H	3.498365000	7.067938000	4.639749000
H	11.752855000	10.960186000	4.376086000
H	12.300362000	9.312687000	4.683861000
H	10.951852000	9.975979000	5.606629000
H	3.894808000	9.361518000	4.008321000

H	5.108306000	12.589502000	4.271641000
H	5.001231000	12.205341000	7.519166000
H	3.790962000	12.720434000	6.349288000
H	2.898607000	9.425856000	5.436921000
H	6.605637000	12.216637000	5.117521000
H	3.899371000	9.696869000	10.451062000
H	2.922137000	8.390831000	9.833547000
H	3.847014000	6.055607000	12.270344000
H	5.111459000	5.291061000	11.313380000
H	6.650251000	7.366906000	12.413189000
H	5.157621000	7.941868000	13.145242000
H	10.516144000	11.477116000	7.275960000
H	7.883315000	11.659876000	10.369561000
H	9.373516000	12.596140000	10.357103000
H	11.549695000	10.216274000	7.896810000
H	9.559902000	9.611513000	11.425570000
H	10.826213000	10.821887000	11.256552000
H	5.507661000	10.650916000	2.707790000
H	6.876118000	11.761910000	2.688898000
H	6.977973000	10.245417000	3.594100000
H	2.789859000	11.926853000	8.561522000
H	3.438807000	10.315681000	8.232338000
H	2.193417000	11.000959000	7.186681000
H	1.769438000	10.622115000	3.554282000
H	2.165341000	11.788592000	4.810880000
H	3.153510000	11.688958000	3.353281000
H	1.795345000	9.456328000	11.793717000
H	3.191876000	9.140194000	12.815440000
H	2.215676000	7.799804000	12.210817000
H	2.315216000	6.061718000	10.286644000
H	3.606147000	5.414109000	9.274581000
H	2.913405000	4.427928000	10.568882000
H	5.582824000	10.246496000	12.205484000
H	6.942978000	9.709429000	13.190652000
H	7.046565000	9.647140000	11.424716000
H	7.575479000	13.664227000	8.947365000
H	8.971150000	13.234309000	7.961099000
H	7.527083000	12.221250000	7.925530000
H	12.360836000	11.779271000	9.731772000
H	11.322885000	13.054649000	9.089955000
H	12.665626000	12.443408000	8.131134000
H	11.783425000	8.514685000	11.573652000
H	12.252754000	9.166652000	10.005115000
H	10.961745000	7.967570000	10.109645000

6Fe_1_6_M4

Fe	6.288069000	6.209092000	6.557679000
Fe	8.427417000	7.746451000	5.807727000
Fe	8.537924000	6.229080000	8.104211000
Fe	6.226054000	8.931802000	6.717075000
Fe	6.277216000	7.486482000	8.962438000
Fe	8.407429000	8.976390000	8.268248000
S	6.410775000	7.722855000	4.842046000
S	4.640466000	7.486745000	7.391326000
S	8.352866000	5.493417000	5.975732000
S	6.525829000	5.296094000	8.567033000
S	8.136985000	9.980227000	6.222324000
S	10.096994000	7.728111000	7.351796000
S	8.312870000	7.477098000	9.958422000
S	6.373592000	9.741421000	8.793378000
P	5.029895000	4.670458000	5.654893000
P	9.681268000	7.808391000	3.912114000
P	9.721528000	4.566069000	9.021176000
P	4.900658000	7.600345000	10.721945000
P	9.653527000	10.634888000	9.245949000
C	5.931629000	3.156481000	5.165204000
C	6.559039000	2.397558000	6.321301000
C	8.788868000	7.348286000	2.390714000
C	8.267849000	5.922682000	2.372585000
C	11.107627000	6.678389000	4.018220000
C	11.994948000	6.631807000	2.785400000
C	10.481168000	3.413858000	7.820039000
C	11.560430000	4.058118000	6.966391000
C	12.005568000	4.126757000	10.667105000
C	11.124575000	5.181565000	10.019698000
C	3.681819000	4.082798000	6.732917000
C	2.795221000	2.991002000	6.158553000
C	4.216363000	5.145690000	4.089722000
C	3.181464000	6.248118000	4.231901000
C	8.828614000	3.429809000	10.140152000
C	8.273175000	4.100210000	11.384564000
C	10.365386000	9.450348000	3.515849000
C	11.388967000	9.944046000	4.522148000
C	3.486048000	8.729686000	10.497645000
C	4.180150000	5.992614000	11.201582000
C	5.708695000	8.109853000	12.280436000
C	8.703482000	12.111457000	9.739213000
C	10.987386000	11.241000000	8.162487000
C	10.467852000	10.117766000	10.794654000
C	2.515576000	8.818277000	11.663261000
C	3.191880000	5.437650000	10.193706000
C	6.360112000	9.480632000	12.265365000

C	11.855709000	12.345795000	8.741352000
C	8.115503000	12.895571000	8.579216000
C	11.535933000	9.056022000	10.598396000
H	7.137763000	1.549160000	5.950690000
H	12.823434000	5.939706000	2.949036000
H	11.885636000	3.375608000	6.178652000
H	5.235902000	2.519507000	4.610367000
H	6.700882000	3.481790000	4.459566000
H	7.226277000	3.044688000	6.892651000
H	5.803658000	2.008837000	7.007367000
H	3.359408000	2.083702000	5.934694000
H	5.019843000	5.459122000	3.417575000
H	3.771926000	4.242532000	3.659956000
H	9.077467000	5.191943000	2.423246000
H	7.601329000	5.746256000	3.217673000
H	11.666991000	6.985087000	4.905804000
H	10.691442000	5.695184000	4.251119000
H	11.450538000	6.286402000	1.904680000
H	12.426323000	7.607560000	2.553712000
H	9.661573000	3.055553000	7.191263000
H	10.871878000	2.548325000	8.363270000
H	11.190341000	4.970630000	6.496275000
H	12.438980000	4.319506000	7.559367000
H	11.445820000	3.505009000	11.368543000
H	12.462498000	3.466083000	9.927610000
H	9.504727000	2.611570000	10.405681000
H	8.017893000	2.997480000	9.547307000
H	7.963919000	8.059704000	2.302076000
H	7.711597000	5.739336000	1.451483000
H	9.467345000	7.532271000	1.551475000
H	10.686285000	5.845545000	10.769733000
H	11.702321000	5.829122000	9.353913000
H	12.815940000	4.598845000	11.226726000
H	2.017738000	2.722486000	6.876602000
H	4.164967000	3.758547000	7.657975000
H	3.101804000	4.971644000	6.993534000
H	9.508236000	10.127465000	3.473130000
H	10.790261000	9.400112000	2.508187000
H	2.296084000	3.311590000	5.242289000
H	2.768868000	6.507585000	3.255246000
H	2.351258000	5.941339000	4.871159000
H	3.620508000	7.148715000	4.663503000
H	7.607374000	4.923201000	11.118787000
H	7.707775000	3.383206000	11.983223000
H	9.067671000	4.504686000	12.014989000
H	11.693915000	10.964212000	4.282152000

H	12.285932000	9.321624000	4.525279000
H	10.971501000	9.939505000	5.528988000
H	3.916994000	9.706282000	10.262276000
H	2.986903000	8.400220000	9.582765000
H	3.718700000	6.112463000	12.186873000
H	5.028143000	5.312770000	11.322337000
H	6.454484000	7.337232000	12.488971000
H	4.952806000	8.044644000	13.069308000
H	10.495122000	11.558316000	7.239770000
H	7.912708000	11.751051000	10.402339000
H	9.370702000	12.737847000	10.340220000
H	11.580465000	10.361909000	7.896875000
H	9.669784000	9.744262000	11.441612000
H	10.880389000	11.012501000	11.271383000
H	1.706020000	9.509897000	11.421998000
H	2.997961000	9.186352000	12.570704000
H	2.061112000	7.852373000	11.892378000
H	2.303204000	6.066315000	10.112002000
H	3.647530000	5.375416000	9.206163000
H	2.866710000	4.437661000	10.486887000
H	5.644492000	10.270474000	12.028972000
H	6.793690000	9.702775000	13.242659000
H	7.154335000	9.516427000	11.519278000
H	7.528129000	13.735086000	8.955054000
H	8.893764000	13.301310000	7.929941000
H	7.460520000	12.270527000	7.970598000
H	12.358934000	12.031078000	9.657620000
H	11.275467000	13.242314000	8.966887000
H	12.628929000	12.629403000	8.024579000
H	11.921562000	8.723854000	11.564025000
H	12.379463000	9.433898000	10.017480000
H	11.130596000	8.187740000	10.077405000

6Fe_1_6_M5

Fe	6.311158000	6.334512000	6.397712000
Fe	8.456409000	7.746373000	5.779162000
Fe	8.479147000	6.221014000	8.083983000
Fe	6.192477000	9.053215000	6.618934000
Fe	6.215899000	7.529674000	8.877361000
Fe	8.450270000	8.970298000	8.128933000
S	6.475376000	7.858271000	4.725563000
S	4.629449000	7.579344000	7.275859000
S	8.357840000	5.501380000	5.937457000
S	6.445268000	5.340411000	8.440658000
S	8.205919000	9.955716000	6.110349000
S	10.098210000	7.627005000	7.338680000

S	8.231500000	7.536354000	9.882706000
S	6.419074000	9.763523000	8.737659000
P	5.070779000	4.683185000	5.434775000
P	9.790138000	7.712656000	3.936825000
P	9.637917000	4.647766000	9.068093000
P	4.813536000	10.600289000	5.902491000
P	9.648114000	10.633467000	9.121636000
C	5.991584000	3.159797000	5.032026000
C	6.545990000	2.420366000	6.236637000
C	8.937399000	7.259061000	2.386987000
C	8.337083000	5.864665000	2.382046000
C	11.190084000	6.552597000	4.082683000
C	12.114021000	6.472195000	2.879634000
C	10.392970000	3.428323000	7.933138000
C	11.490491000	4.005220000	7.056562000
C	11.903189000	4.253927000	10.742424000
C	11.037240000	5.292174000	10.049226000
C	3.685067000	4.168166000	6.500950000
C	2.804291000	3.067431000	5.933599000
C	4.330562000	5.145766000	3.832452000
C	3.275613000	6.231724000	3.943799000
C	8.715002000	3.573635000	10.221397000
C	8.128853000	4.291945000	11.423791000
C	10.533083000	9.325398000	3.514796000
C	11.538982000	9.810867000	4.542395000
C	5.600143000	11.894818000	4.877021000
C	3.987742000	11.588474000	7.197472000
C	3.459081000	9.952322000	4.864243000
C	8.713227000	12.145011000	9.530202000
C	11.029472000	11.178289000	8.063449000
C	10.391418000	10.164859000	10.718722000
C	2.488331000	10.984638000	4.315633000
C	6.146885000	11.397560000	3.549923000
C	3.055596000	10.791874000	8.092945000
C	11.896292000	12.288047000	8.634692000
C	8.125015000	12.867448000	8.331447000
C	11.460785000	9.093761000	10.598450000
H	7.129317000	1.556587000	5.912167000
H	12.920704000	5.761977000	3.072666000
H	11.809048000	3.274881000	6.310250000
H	5.319205000	2.519032000	4.452455000
H	6.800340000	3.467900000	4.364118000
H	7.192124000	3.071339000	6.826707000
H	5.749731000	2.058225000	6.889723000
H	3.359480000	2.140792000	5.776705000
H	5.159784000	5.481458000	3.204197000

H	3.923255000	4.238453000	3.375334000
H	9.103892000	5.092094000	2.469100000
H	7.643615000	5.743472000	3.215348000
H	11.730379000	6.850251000	4.985326000
H	10.744450000	5.580650000	4.309057000
H	11.588320000	6.132926000	1.985089000
H	12.575512000	7.435254000	2.652517000
H	9.574671000	3.041777000	7.320049000
H	10.766703000	2.593805000	8.534208000
H	11.140755000	4.897201000	6.535233000
H	12.368449000	4.282758000	7.642929000
H	11.335687000	3.672627000	11.471567000
H	12.352249000	3.555027000	10.033983000
H	9.394915000	2.776221000	10.537487000
H	7.923224000	3.104445000	9.631530000
H	8.154450000	8.010153000	2.251024000
H	7.793761000	5.690080000	1.451239000
H	9.650351000	7.384210000	1.566141000
H	10.599343000	5.986402000	10.770584000
H	11.624050000	5.907353000	9.361687000
H	12.718907000	4.741542000	11.280242000
H	1.991503000	2.847152000	6.628326000
H	4.134306000	3.878754000	7.454026000
H	3.115247000	5.077327000	6.707998000
H	9.697059000	10.025766000	3.436210000
H	10.985062000	9.246128000	2.521218000
H	2.352443000	3.354640000	4.982191000
H	2.943302000	6.542143000	2.951540000
H	2.398777000	5.888649000	4.495908000
H	3.676281000	7.105380000	4.458153000
H	7.434803000	5.076102000	11.118000000
H	7.584019000	3.587150000	12.054731000
H	8.905615000	4.752513000	12.037668000
H	11.875370000	10.821192000	4.302130000
H	12.420241000	9.167504000	4.579139000
H	11.093396000	9.824640000	5.537248000
H	3.944264000	9.396342000	4.057658000
H	4.865431000	12.691295000	4.724082000
H	4.789484000	12.042618000	7.785952000
H	3.451934000	12.403677000	6.701125000
H	2.942802000	9.207003000	5.474400000
H	6.404327000	12.312475000	5.488734000
H	10.574197000	11.471889000	7.114521000
H	7.922885000	11.832118000	10.217041000
H	9.390025000	12.797917000	10.090679000
H	11.614262000	10.279378000	7.852077000

H	9.563632000	9.814425000	11.340545000
H	10.786629000	11.073579000	11.183637000
H	5.353197000	11.023680000	2.900051000
H	6.653666000	12.206998000	3.021032000
H	6.862431000	10.587650000	3.702415000
H	2.628230000	11.437509000	8.862338000
H	3.585833000	9.978669000	8.591088000
H	2.227766000	10.357818000	7.528643000
H	1.726994000	10.497976000	3.702618000
H	1.970467000	11.519591000	5.113786000
H	2.989766000	11.722908000	3.686974000
H	7.555381000	13.738792000	8.659812000
H	8.900546000	13.215755000	7.646408000
H	7.456559000	12.208272000	7.776356000
H	12.350151000	12.003218000	9.585728000
H	11.327999000	13.206077000	8.794178000
H	12.707181000	12.522247000	7.942000000
H	11.794184000	8.777932000	11.588590000
H	12.335045000	9.454151000	10.052984000
H	11.073621000	8.220088000	10.073442000

6Fe_1_6_M6

Fe	6.151316000	6.247716000	6.613139000
Fe	8.365245000	7.650863000	5.815941000
Fe	8.432683000	6.156002000	8.126510000
Fe	6.135279000	9.004930000	6.668400000
Fe	6.245386000	7.578228000	9.005082000
Fe	8.394296000	8.880905000	8.202104000
S	6.306498000	7.688392000	4.884940000
S	4.555185000	7.619600000	7.493605000
S	8.174118000	5.419863000	6.036832000
S	6.403846000	5.339575000	8.672257000
S	8.158922000	9.871883000	6.213528000
S	10.013422000	7.572381000	7.371933000
S	8.301004000	7.509155000	9.966335000
S	6.453923000	9.826339000	8.788896000
P	4.997156000	4.644247000	5.575732000
P	9.693216000	7.820773000	4.046715000
P	9.761264000	4.635912000	8.970094000
P	4.985027000	10.604906000	5.705485000
P	4.929434000	7.566858000	10.861127000
C	5.912071000	3.120774000	5.146534000
C	6.442796000	2.364244000	6.352687000
C	8.820079000	7.531850000	2.466633000
C	8.275220000	6.123087000	2.305051000
C	11.056470000	6.609859000	4.054676000

C	11.993330000	6.651877000	2.859809000
C	10.460277000	3.441072000	7.779483000
C	11.455824000	4.053482000	6.811932000
C	12.123875000	4.318028000	10.511510000
C	11.196713000	5.329769000	9.859131000
C	3.608955000	4.063515000	6.614207000
C	2.745652000	2.958756000	6.028434000
C	4.225875000	5.108736000	3.985836000
C	3.143974000	6.164965000	4.135452000
C	8.951240000	3.524929000	10.176860000
C	8.417299000	4.212720000	11.420582000
C	10.491662000	9.438571000	3.775658000
C	11.480693000	9.831201000	4.859411000
C	5.887700000	11.665803000	4.525640000
C	4.292684000	11.830007000	6.871547000
C	3.548656000	9.978307000	4.768923000
C	3.570299000	8.773663000	10.770271000
C	4.154933000	5.957894000	11.228241000
C	5.843258000	7.948229000	12.392976000
C	2.674164000	11.029025000	4.105671000
C	6.429754000	10.935475000	3.310391000
C	3.239958000	11.257188000	7.803738000
C	2.662748000	8.827501000	11.988230000
C	3.117238000	5.520505000	10.210690000
C	6.407380000	9.356080000	12.457612000
H	7.057301000	1.520078000	6.033776000
H	12.760642000	5.881016000	2.955941000
H	11.755204000	3.323582000	6.057348000
H	5.252585000	2.487578000	4.545549000
H	6.736328000	3.432968000	4.499789000
H	7.053906000	3.014934000	6.980772000
H	5.632553000	1.969588000	6.969125000
H	3.320710000	2.049462000	5.843867000
H	5.037731000	5.482564000	3.355822000
H	3.835710000	4.205433000	3.507801000
H	9.075084000	5.380450000	2.284656000
H	7.602519000	5.868075000	3.125870000
H	11.596993000	6.777724000	4.989641000
H	10.580226000	5.631222000	4.155352000
H	11.466708000	6.472175000	1.920496000
H	12.505439000	7.612411000	2.778704000
H	9.605893000	3.024907000	7.239078000
H	10.912911000	2.623676000	8.348692000
H	11.018117000	4.910905000	6.300873000
H	12.359456000	4.391308000	7.322902000
H	11.611375000	3.729539000	11.274853000

H	12.549649000	3.624257000	9.783754000
H	9.674341000	2.747782000	10.442817000
H	8.138901000	3.033560000	9.633908000
H	8.006715000	8.261159000	2.432180000
H	7.719546000	6.036933000	1.369405000
H	9.509978000	7.779428000	1.653951000
H	10.785614000	6.026521000	10.594688000
H	11.727238000	5.951668000	9.133574000
H	12.955690000	4.830039000	10.999122000
H	1.939391000	2.700570000	6.718240000
H	4.060484000	3.756248000	7.561483000
H	3.015554000	4.952894000	6.843756000
H	9.681591000	10.169579000	3.712760000
H	10.974449000	9.406844000	2.793828000
H	2.285371000	3.259446000	5.085250000
H	2.805220000	6.510214000	3.156731000
H	2.273841000	5.778350000	4.669404000
H	3.519776000	7.026685000	4.688784000
H	7.689924000	4.981366000	11.155534000
H	7.927495000	3.487146000	12.073166000
H	9.214418000	4.689430000	11.994676000
H	11.894120000	10.819847000	4.652287000
H	12.315063000	9.129591000	4.919425000
H	11.000446000	9.864710000	5.838372000
H	3.954554000	9.278418000	4.034106000
H	5.212211000	12.472885000	4.225948000
H	5.145167000	12.211044000	7.440184000
H	3.892496000	12.665349000	6.289136000
H	2.975791000	9.369656000	5.473902000
H	6.702174000	12.123042000	5.093128000
H	4.043981000	9.739972000	10.580573000
H	3.011818000	8.527478000	9.863544000
H	3.722431000	6.027758000	12.231542000
H	4.974650000	5.236383000	11.276395000
H	6.644886000	7.207580000	12.456082000
H	5.159768000	7.758514000	13.227143000
H	5.629949000	10.498778000	2.708817000
H	6.987499000	11.623532000	2.671991000
H	7.099053000	10.128220000	3.611277000
H	2.955544000	11.993317000	8.557966000
H	3.618469000	10.371437000	8.315124000
H	2.335605000	10.971200000	7.263091000
H	1.841006000	10.552528000	3.585026000
H	2.249189000	11.725396000	4.831169000
H	3.227546000	11.612371000	3.367292000
H	1.878805000	9.572108000	11.836774000

H	3.208281000	9.107552000	12.891261000
H	2.171482000	7.870515000	12.174394000
H	2.266242000	6.203579000	10.180895000
H	3.549187000	5.478761000	9.210688000
H	2.738070000	4.528218000	10.461675000
H	5.618454000	10.109968000	12.425825000
H	6.959577000	9.494132000	13.388649000
H	7.088949000	9.545734000	11.627631000

6Fe_1_8_M1

Fe	6.209840000	6.375275000	6.663770000
Fe	8.481929000	7.717943000	5.894601000
Fe	8.437134000	6.217391000	8.222965000
Fe	6.216210000	9.077176000	6.719155000
Fe	6.246290000	7.614152000	9.060359000
Fe	8.440379000	8.976107000	8.352193000
S	6.430821000	7.783646000	4.903454000
S	4.558806000	7.717621000	7.459870000
S	8.186033000	5.476161000	6.085333000
S	6.379010000	5.364931000	8.688847000
S	8.246071000	9.923904000	6.319196000
S	10.047745000	7.645386000	7.500444000
S	8.256560000	7.491268000	10.055828000
S	6.404681000	9.835975000	8.853488000
P	9.628990000	7.829109000	4.014112000
P	9.798914000	4.631479000	8.978183000
P	4.996290000	10.576971000	5.697009000
P	4.866455000	7.550887000	10.920281000
P	9.608880000	10.647807000	9.230145000
C	8.730366000	7.454397000	2.469050000
C	8.208055000	6.030900000	2.382409000
C	11.024205000	6.652375000	4.032199000
C	11.894586000	6.630227000	2.786626000
C	10.554301000	3.531443000	7.731624000
C	11.564760000	4.233388000	6.842763000
C	12.136327000	4.237438000	10.549952000
C	11.201992000	5.277226000	9.954711000
C	8.974401000	3.439401000	10.094513000
C	8.444172000	4.051499000	11.379899000
C	10.397448000	9.447208000	3.655230000
C	11.474424000	9.836049000	4.652426000
C	5.883760000	11.653383000	4.517278000
C	4.226519000	11.812453000	6.802340000
C	3.610819000	9.859493000	4.748817000
C	3.535086000	8.789945000	10.810034000
C	4.046098000	5.951973000	11.223437000

C	5.740687000	7.885719000	12.486171000
C	8.693271000	12.177418000	9.629953000
C	10.998861000	11.186566000	8.180241000
C	10.364018000	10.219843000	10.839343000
C	2.715516000	10.851558000	4.026010000
C	6.504038000	10.933376000	3.334660000
C	3.197157000	11.232510000	7.755216000
C	2.559030000	8.814840000	11.973760000
C	3.058441000	5.548114000	10.142237000
C	6.354163000	9.273234000	12.560029000
C	11.861352000	12.306256000	8.737412000
C	8.112454000	12.893040000	8.423243000
C	11.438903000	9.150435000	10.748170000
H	12.705868000	5.909626000	2.908751000
H	11.897640000	3.571176000	6.041099000
H	9.019893000	5.301111000	2.394668000
H	7.540920000	5.803033000	3.214789000
H	11.608980000	6.899785000	4.922071000
H	10.584091000	5.670986000	4.225562000
H	11.329407000	6.336870000	1.900234000
H	12.349906000	7.602436000	2.587828000
H	9.724067000	3.141685000	7.136627000
H	11.007541000	2.680861000	8.249310000
H	11.128815000	5.124294000	6.390673000
H	12.448439000	4.543788000	7.403908000
H	11.613685000	3.567621000	11.235330000
H	12.608228000	3.624989000	9.779173000
H	9.681593000	2.632302000	10.308157000
H	8.156572000	3.004180000	9.513401000
H	7.906252000	8.169659000	2.408182000
H	7.651103000	5.889717000	1.454505000
H	9.407671000	7.674259000	1.637947000
H	10.756260000	5.900181000	10.735182000
H	11.738095000	5.965458000	9.295767000
H	12.935102000	4.722871000	11.114565000
H	9.587204000	10.180185000	3.662540000
H	10.794750000	9.414631000	2.636243000
H	7.745737000	4.861560000	11.164092000
H	7.922409000	3.297595000	11.972424000
H	9.248242000	4.459333000	11.996029000
H	11.808991000	10.860143000	4.476048000
H	12.347946000	9.185692000	4.576527000
H	11.097302000	9.770439000	5.673325000
H	4.059848000	9.146365000	4.052886000
H	5.176600000	12.417682000	4.180302000
H	5.048882000	12.271495000	7.357866000

H	3.787790000	12.594190000	6.174752000
H	3.044390000	9.254344000	5.461543000
H	6.655268000	12.164808000	5.099237000
H	4.036325000	9.753028000	10.684515000
H	3.025136000	8.592332000	9.863290000
H	3.561953000	6.006998000	12.203804000
H	4.850232000	5.214820000	11.301307000
H	6.518511000	7.120901000	12.562805000
H	5.039585000	7.717539000	13.309736000
H	10.554997000	11.463224000	7.220857000
H	7.899026000	11.881117000	10.320142000
H	9.374073000	12.831401000	10.183565000
H	11.588523000	10.286244000	7.987572000
H	9.540450000	9.879630000	11.473075000
H	10.757693000	11.137746000	11.286495000
H	5.752409000	10.426068000	2.726711000
H	7.028614000	11.642607000	2.691059000
H	7.220605000	10.183901000	3.672609000
H	2.849970000	11.996029000	8.453859000
H	3.625366000	10.411076000	8.330451000
H	2.324953000	10.850505000	7.221342000
H	1.917116000	10.322668000	3.501927000
H	2.243083000	11.554606000	4.714883000
H	3.265534000	11.430070000	3.281201000
H	1.808374000	9.592098000	11.816867000
H	3.058406000	9.028943000	12.920760000
H	2.029057000	7.866543000	12.080214000
H	2.224424000	6.249209000	10.073463000
H	3.541580000	5.502836000	9.165107000
H	2.645199000	4.561995000	10.360535000
H	5.591257000	10.053869000	12.539629000
H	6.921537000	9.387981000	13.485423000
H	7.030294000	9.441219000	11.719908000
H	7.532374000	13.761908000	8.740100000
H	8.894482000	13.243829000	7.746946000
H	7.456983000	12.228573000	7.858231000
H	12.306684000	12.039217000	9.697758000
H	11.291401000	13.226724000	8.876737000
H	12.678778000	12.530133000	8.049110000
H	11.778884000	8.866063000	11.745699000
H	12.309082000	9.499979000	10.189228000
H	11.059481000	8.256811000	10.250964000

6Fe_1_8_M2

Fe	6.213963000	6.333958000	6.629766000
Fe	8.395866000	7.822344000	5.962791000

Fe	8.478935000	6.262608000	8.168542000
Fe	6.158628000	9.081299000	6.693880000
Fe	6.217703000	7.576598000	9.017381000
Fe	8.318794000	8.991844000	8.381874000
S	6.417303000	7.793523000	4.880121000
S	4.584086000	7.656382000	7.429256000
S	8.258625000	5.586429000	6.013451000
S	6.448798000	5.377204000	8.629647000
S	8.164192000	10.055187000	6.325841000
S	10.049980000	7.766281000	7.508913000
S	8.222160000	7.490390000	10.036727000
S	6.308801000	9.820771000	8.841308000
P	5.037771000	4.735969000	5.699125000
P	9.729130000	4.571237000	8.883199000
P	4.933542000	10.605177000	5.699953000
P	4.864604000	7.619848000	10.837987000
P	9.635094000	10.640495000	9.310202000
C	5.964251000	3.218599000	5.273569000
C	6.575918000	2.492609000	6.458144000
C	10.544531000	3.565671000	7.593881000
C	11.542627000	4.340180000	6.750291000
C	12.022577000	4.100639000	10.501123000
C	11.092472000	5.165896000	9.945270000
C	3.660517000	4.160763000	6.749286000
C	2.815375000	3.030677000	6.186515000
C	4.269505000	5.159183000	4.097493000
C	3.178136000	6.208294000	4.208204000
C	8.869545000	3.315350000	9.895815000
C	8.345020000	3.849549000	11.218264000
C	5.811581000	11.688763000	4.520607000
C	4.177424000	11.823594000	6.834042000
C	3.533912000	9.918685000	4.750891000
C	3.443507000	8.752133000	10.686656000
C	4.152414000	5.994766000	11.265165000
C	5.709696000	8.090357000	12.387685000
C	8.719545000	12.150989000	9.774740000
C	10.984546000	11.187035000	8.215544000
C	10.422232000	10.150842000	10.882690000
C	2.635685000	10.929455000	4.058295000
C	6.421098000	10.979453000	3.324785000
C	3.115482000	11.233648000	7.744222000
C	2.502045000	8.802111000	11.877876000
C	3.140184000	5.495522000	10.250701000
C	6.318501000	9.481184000	12.385067000
C	11.881139000	12.279157000	8.774647000
C	8.130409000	12.922293000	8.606814000

C	11.465069000	9.056417000	10.739212000
H	7.144112000	1.623953000	6.119699000
H	11.947214000	3.702676000	5.962133000
H	5.279893000	2.563624000	4.725759000
H	6.742248000	3.528571000	4.571015000
H	7.250591000	3.151627000	7.005774000
H	5.813791000	2.140146000	7.156319000
H	3.401631000	2.122142000	6.037255000
H	5.084657000	5.516793000	3.462807000
H	3.889622000	4.237301000	3.647100000
H	9.741577000	3.169250000	6.966389000
H	11.022854000	2.709298000	8.079137000
H	11.074250000	5.204572000	6.276515000
H	12.383097000	4.698817000	7.348098000
H	11.490234000	3.379116000	11.124076000
H	12.527602000	3.548269000	9.706594000
H	9.552734000	2.475568000	10.053899000
H	8.044697000	2.946677000	9.280320000
H	10.617839000	5.737140000	10.747889000
H	11.640111000	5.896980000	9.344162000
H	12.795656000	4.558622000	11.121712000
H	2.005336000	2.785911000	6.876632000
H	4.115684000	3.879742000	7.702110000
H	3.055480000	5.047630000	6.955863000
H	2.360855000	3.297097000	5.230382000
H	2.841302000	6.518596000	3.217288000
H	2.309157000	5.831402000	4.751123000
H	3.543596000	7.089013000	4.736466000
H	7.711993000	4.725083000	11.061038000
H	7.752805000	3.088240000	11.729600000
H	9.157679000	4.139710000	11.887090000
H	3.975758000	9.226627000	4.030009000
H	5.096836000	12.452172000	4.197433000
H	5.001628000	12.238482000	7.420623000
H	3.770988000	12.639514000	6.228798000
H	2.970514000	9.299539000	5.453918000
H	6.585770000	12.200595000	5.098369000
H	3.870319000	9.736047000	10.476171000
H	2.920501000	8.451551000	9.774761000
H	3.713249000	6.066140000	12.265126000
H	5.000023000	5.307063000	11.331341000
H	6.486882000	7.335944000	12.538569000
H	4.989944000	7.977106000	13.204385000
H	10.504287000	11.495231000	7.283356000
H	7.930526000	11.822529000	10.456675000
H	9.405307000	12.778728000	10.352987000

H	11.552726000	10.286553000	7.968132000
H	9.607812000	9.821474000	11.533776000
H	10.852991000	11.050834000	11.333003000
H	5.665096000	10.461326000	2.731266000
H	6.915448000	11.701682000	2.672290000
H	7.163399000	10.244034000	3.636700000
H	2.797020000	11.965969000	8.488545000
H	3.499022000	10.357211000	8.267672000
H	2.231058000	10.926531000	7.182904000
H	1.826332000	10.415624000	3.535634000
H	2.177915000	11.624137000	4.765214000
H	3.180509000	11.516127000	3.316471000
H	1.685867000	9.500264000	11.680859000
H	3.008109000	9.140699000	12.783884000
H	2.054410000	7.828755000	12.087651000
H	2.245618000	6.120938000	10.231940000
H	3.568685000	5.494701000	9.248563000
H	2.828048000	4.477395000	10.490457000
H	5.558531000	10.257370000	12.273343000
H	6.844159000	9.664863000	13.324260000
H	7.029925000	9.587451000	11.565249000
H	7.562696000	13.780238000	8.971936000
H	8.906935000	13.298226000	7.938040000
H	7.460910000	12.291578000	8.020423000
H	12.371723000	11.971120000	9.700030000
H	11.327198000	13.197796000	8.977184000
H	12.665006000	12.523132000	8.055117000
H	11.843356000	8.764265000	11.720550000
H	12.316168000	9.386188000	10.140456000
H	11.040264000	8.172978000	10.261444000

6Fe_1_8_M3

Fe	6.186231000	6.125402000	6.511674000
Fe	8.443320000	7.651357000	5.800885000
Fe	8.430198000	6.146159000	8.101780000
Fe	6.157705000	8.928066000	6.664560000
Fe	6.163549000	7.452926000	9.000643000
Fe	8.408237000	8.890211000	8.273181000
S	6.408283000	7.619882000	4.847465000
S	4.590890000	7.459145000	7.388726000
S	8.269687000	5.381046000	5.991730000
S	6.431019000	5.220818000	8.570576000
S	8.197468000	9.820012000	6.250824000
S	10.055773000	7.568596000	7.427069000
S	8.222162000	7.386045000	9.975741000
S	6.361445000	9.667420000	8.781016000

P	4.950028000	4.616166000	5.553370000
P	9.667299000	7.835237000	3.975473000
P	5.032158000	10.631803000	5.777100000
P	4.946692000	7.588670000	10.837509000
P	9.525458000	10.571011000	9.200850000
C	5.832358000	3.089950000	5.072250000
C	6.392202000	2.290392000	6.235874000
C	8.798122000	7.443492000	2.416473000
C	8.290407000	6.015336000	2.322545000
C	11.081707000	6.680752000	4.033506000
C	11.974203000	6.663457000	2.803724000
C	3.578385000	4.052170000	6.617384000
C	2.679377000	2.976661000	6.030703000
C	4.165357000	5.122567000	3.984219000
C	3.124028000	6.215361000	4.147103000
C	10.404738000	9.467915000	3.623849000
C	11.448121000	9.883531000	4.645645000
C	5.956080000	11.737911000	4.654311000
C	4.269886000	11.799412000	6.957115000
C	3.639733000	10.011264000	4.768919000
C	3.534967000	8.738260000	10.724610000
C	4.222550000	5.977660000	11.305958000
C	5.838286000	8.065064000	12.358420000
C	8.576521000	12.076776000	9.612003000
C	10.911023000	11.158730000	8.169887000
C	10.282950000	10.125109000	10.803148000
C	2.775585000	11.067212000	4.100690000
C	6.504430000	11.040611000	3.421791000
C	3.168024000	11.168306000	7.790892000
C	2.652087000	8.832782000	11.957532000
C	3.191762000	5.455225000	10.321180000
C	6.427616000	9.463940000	12.333768000
C	11.749924000	12.282390000	8.755082000
C	8.016083000	12.795809000	8.397632000
C	11.374352000	9.072333000	10.702870000
H	6.935135000	1.418375000	5.867063000
H	12.795200000	5.957979000	2.945968000
H	5.136902000	2.485130000	4.481596000
H	6.634332000	3.403490000	4.398301000
H	7.081547000	2.888229000	6.833694000
H	5.600018000	1.930735000	6.895607000
H	3.230069000	2.058784000	5.817327000
H	4.979354000	5.460995000	3.337351000
H	3.733544000	4.231343000	3.518952000
H	9.107988000	5.292355000	2.344256000
H	7.618070000	5.784947000	3.150745000

H	11.644032000	6.943800000	4.933270000
H	10.656482000	5.694065000	4.235001000
H	11.430505000	6.353880000	1.909138000
H	12.416617000	7.641790000	2.604954000
H	7.967193000	8.150568000	2.345782000
H	7.743763000	5.869340000	1.388922000
H	9.483117000	7.668416000	1.593169000
H	1.885387000	2.723844000	6.736198000
H	4.047675000	3.716847000	7.545974000
H	3.011463000	4.949651000	6.878202000
H	9.576356000	10.180699000	3.608409000
H	10.826889000	9.442167000	2.614718000
H	2.202104000	3.304618000	5.105271000
H	2.764708000	6.550301000	3.172162000
H	2.260216000	5.866650000	4.716416000
H	3.543323000	7.075408000	4.670125000
H	11.754275000	10.918760000	4.483698000
H	12.342402000	9.260747000	4.583813000
H	11.052237000	9.798928000	5.658030000
H	4.083584000	9.337082000	4.031749000
H	5.296588000	12.564955000	4.374699000
H	5.080480000	12.153175000	7.598910000
H	3.899372000	12.664002000	6.398454000
H	3.050612000	9.374679000	5.434632000
H	6.770938000	12.161228000	5.247396000
H	3.962510000	9.710916000	10.468510000
H	2.962896000	8.421941000	9.847933000
H	3.794992000	6.076107000	12.308647000
H	5.067190000	5.287231000	11.381406000
H	6.627235000	7.319110000	12.485306000
H	5.146449000	7.946040000	13.197909000
H	10.466551000	11.448833000	7.214699000
H	7.768515000	11.754392000	10.273449000
H	9.228415000	12.735180000	10.193876000
H	11.520084000	10.275282000	7.960399000
H	9.465455000	9.768535000	11.435213000
H	10.663391000	11.044279000	11.259505000
H	5.704911000	10.659356000	2.783630000
H	7.102281000	11.733261000	2.826045000
H	7.136246000	10.196195000	3.702331000
H	2.847215000	11.848154000	8.582482000
H	3.514558000	10.243719000	8.254180000
H	2.291745000	10.930304000	7.185135000
H	1.967759000	10.593605000	3.538949000
H	2.315855000	11.740022000	4.827240000
H	3.346850000	11.675850000	3.397011000

H	1.834027000	9.534559000	11.782573000
H	3.206738000	9.189410000	12.827479000
H	2.205766000	7.870592000	12.215755000
H	2.312560000	6.101221000	10.276795000
H	3.610743000	5.391533000	9.315978000
H	2.856394000	4.458750000	10.614276000
H	5.653320000	10.229661000	12.250968000
H	6.986250000	9.655650000	13.252004000
H	7.105900000	9.581953000	11.487681000
H	7.384925000	13.631874000	8.705022000
H	8.810106000	13.194977000	7.763334000
H	7.416277000	12.115578000	7.791082000
H	12.206597000	11.997628000	9.704729000
H	11.159214000	13.184725000	8.924144000
H	12.558211000	12.545562000	8.069830000
H	11.736645000	8.809001000	11.698047000
H	12.228481000	9.431157000	10.125304000
H	11.004625000	8.162378000	10.227739000

6Fe_1_8_M4

Fe	6.264794000	6.174514000	6.522067000
Fe	8.510760000	7.644465000	5.833025000
Fe	8.471035000	6.215952000	8.162500000
Fe	6.216673000	8.851522000	6.731139000
Fe	6.228578000	7.386430000	8.998626000
Fe	8.409111000	8.951389000	8.274560000
S	6.488582000	7.682703000	4.827767000
S	4.610021000	7.418746000	7.438053000
S	8.348183000	5.419610000	6.034054000
S	6.483188000	5.196576000	8.539128000
S	8.175580000	9.865724000	6.236020000
S	10.088523000	7.696083000	7.438036000
S	8.262017000	7.479088000	9.995915000
S	6.342977000	9.662014000	8.836584000
P	4.922797000	4.758381000	5.446238000
P	9.718135000	7.678314000	4.013360000
P	9.827052000	4.588117000	9.106394000
P	5.000538000	7.535470000	10.858491000
P	9.537170000	10.604310000	9.161566000
C	5.781419000	3.240817000	4.892582000
C	6.320496000	2.384274000	6.025661000
C	8.858261000	7.206163000	2.472609000
C	8.319196000	5.787172000	2.458772000
C	11.165022000	6.568282000	4.105526000
C	12.069946000	6.545331000	2.885236000
C	10.591670000	3.430617000	7.921566000

C	11.628996000	4.085514000	7.026271000
C	12.130593000	4.303262000	10.737206000
C	11.207255000	5.303329000	10.062290000
C	3.537668000	4.159612000	6.475272000
C	2.612578000	3.141361000	5.830954000
C	4.152322000	5.361182000	3.905742000
C	3.154026000	6.487106000	4.115560000
C	8.956916000	3.474138000	10.260604000
C	8.349681000	4.173488000	11.464100000
C	10.404482000	9.314821000	3.581585000
C	11.434591000	9.824698000	4.572827000
C	3.589473000	8.679184000	10.696738000
C	4.274176000	5.925956000	11.331163000
C	5.869485000	8.031162000	12.385946000
C	8.578249000	12.098342000	9.588442000
C	10.889966000	11.202568000	8.092962000
C	10.342493000	10.200276000	10.752411000
C	2.673384000	8.774587000	11.905214000
C	3.268378000	5.380813000	10.332964000
C	6.439051000	9.438315000	12.366674000
C	11.716467000	12.353263000	8.641278000
C	7.944408000	12.803284000	8.401996000
C	11.444029000	9.161184000	10.638560000
H	6.876298000	1.533172000	5.627361000
H	12.906780000	5.863329000	3.049654000
H	11.960484000	3.389288000	6.253690000
H	5.091292000	2.669336000	4.264338000
H	6.597542000	3.576873000	4.246861000
H	6.991124000	2.958858000	6.667167000
H	5.516449000	1.989651000	6.650202000
H	3.142460000	2.228189000	5.553077000
H	4.975408000	5.693377000	3.267152000
H	3.683663000	4.506964000	3.407403000
H	9.118550000	5.046916000	2.534072000
H	7.634554000	5.627077000	3.293091000
H	11.713110000	6.868722000	5.002827000
H	10.764040000	5.574220000	4.318954000
H	11.541147000	6.202544000	1.993940000
H	12.490108000	7.529257000	2.667841000
H	9.768244000	3.028628000	7.324652000
H	11.020728000	2.596656000	8.485366000
H	11.216870000	4.968141000	6.535771000
H	12.509658000	4.396056000	7.591499000
H	11.597627000	3.685281000	11.462206000
H	12.609607000	3.637461000	10.016778000
H	9.662125000	2.696709000	10.570902000

H	8.176433000	2.985081000	9.671340000
H	8.043840000	7.925525000	2.353310000
H	7.777574000	5.596320000	1.530190000
H	9.554330000	7.369350000	1.644274000
H	10.746452000	5.973991000	10.792135000
H	11.750247000	5.948889000	9.366617000
H	12.923361000	4.827033000	11.275243000
H	1.818607000	2.859173000	6.525394000
H	3.997484000	3.759565000	7.383432000
H	2.991034000	5.052641000	6.789806000
H	9.548218000	9.992734000	3.532034000
H	10.825302000	9.251333000	2.573396000
H	2.134629000	3.537553000	4.933012000
H	2.776351000	6.841774000	3.154934000
H	2.296784000	6.159202000	4.706953000
H	3.613281000	7.332844000	4.629635000
H	7.643902000	4.943054000	11.148425000
H	7.817115000	3.454588000	12.089810000
H	9.111242000	4.651921000	12.083218000
H	11.724436000	10.848913000	4.330832000
H	12.339515000	9.213832000	4.564400000
H	11.034375000	9.814315000	5.586976000
H	4.019243000	9.651574000	10.443913000
H	3.045306000	8.358792000	9.804203000
H	3.821460000	6.041949000	12.321078000
H	5.118390000	5.239580000	11.440583000
H	6.667653000	7.296984000	12.524837000
H	5.166964000	7.904615000	13.215641000
H	10.420934000	11.468239000	7.142640000
H	7.811968000	11.775153000	10.297980000
H	9.252771000	12.769943000	10.128858000
H	11.512580000	10.328351000	7.885023000
H	9.545741000	9.843136000	11.410117000
H	10.721322000	11.131485000	11.184405000
H	1.862923000	9.478221000	11.705488000
H	3.203204000	9.131551000	12.790534000
H	2.216933000	7.813800000	12.151279000
H	2.396450000	6.031638000	10.243399000
H	3.715608000	5.281492000	9.342933000
H	2.916603000	4.396717000	10.647864000
H	5.655643000	10.192313000	12.267929000
H	6.977885000	9.639199000	13.294770000
H	7.131185000	9.564403000	11.532969000
H	7.380981000	13.675262000	8.738987000
H	8.695162000	13.149415000	7.688834000
H	7.258311000	12.141701000	7.871826000

H	12.193597000	12.098944000	9.589805000
H	11.111740000	13.248210000	8.798359000
H	12.508753000	12.615299000	7.937147000
H	11.818429000	8.891705000	11.628122000
H	12.289296000	9.531715000	10.055354000
H	11.076033000	8.256397000	10.153937000

6Fe_1_8_M5

Fe	6.242776000	6.241859000	6.474958000
Fe	8.477647000	7.690547000	5.841416000
Fe	8.392233000	6.232416000	8.129658000
Fe	6.236338000	8.998580000	6.682268000
Fe	6.228318000	7.508721000	8.878047000
Fe	8.482391000	8.921647000	8.269620000
S	6.465157000	7.748325000	4.825377000
S	4.619170000	7.582402000	7.329307000
S	8.276156000	5.436550000	6.014277000
S	6.346481000	5.297334000	8.521269000
S	8.290678000	9.873495000	6.259786000
S	10.086557000	7.572476000	7.440203000
S	8.176967000	7.464748000	9.999041000
S	6.443092000	9.733872000	8.807387000
P	5.045573000	4.694607000	5.510273000
P	9.648906000	7.776169000	3.982619000
P	9.731227000	4.639550000	9.043945000
P	4.935947000	10.552515000	5.851770000
P	9.590325000	10.597477000	9.155968000
C	5.929669000	3.143404000	5.114554000
C	6.446117000	2.382000000	6.322579000
C	8.759301000	7.366489000	2.440691000
C	8.225222000	5.946013000	2.395043000
C	11.059714000	6.616657000	4.020496000
C	11.927685000	6.579261000	2.773848000
C	10.501324000	3.506175000	7.840354000
C	11.548225000	4.156731000	6.954937000
C	12.008133000	4.297934000	10.686592000
C	11.095812000	5.324944000	10.036741000
C	3.617459000	4.181240000	6.525831000
C	2.731555000	3.098940000	5.931869000
C	4.333164000	5.146180000	3.888964000
C	3.272050000	6.228346000	3.975087000
C	8.831178000	3.499460000	10.148243000
C	8.234771000	4.140629000	11.387878000
C	10.393736000	9.397863000	3.596373000
C	11.471969000	9.812500000	4.581820000
C	5.798379000	11.766774000	4.790687000

C	4.119374000	11.627087000	7.081647000
C	3.582578000	9.911475000	4.808679000
C	8.660758000	12.131340000	9.501051000
C	11.014545000	11.128063000	8.145060000
C	10.292855000	10.208462000	10.797890000
C	2.660582000	10.953585000	4.198848000
C	6.384004000	11.177541000	3.519437000
C	3.131156000	10.907935000	7.983125000
C	11.848477000	12.267592000	8.705426000
C	8.090211000	12.819429000	8.274338000
C	11.378942000	9.147949000	10.762033000
H	7.002676000	1.498152000	6.004538000
H	12.750907000	5.874722000	2.909428000
H	11.897917000	3.448958000	6.201101000
H	5.250510000	2.520314000	4.524567000
H	6.756395000	3.426535000	4.457279000
H	7.108465000	3.007428000	6.923183000
H	5.630739000	2.046535000	6.966505000
H	3.274960000	2.163869000	5.783079000
H	5.171617000	5.483946000	3.274350000
H	3.936460000	4.238519000	3.424405000
H	9.030335000	5.208888000	2.416704000
H	7.572282000	5.752653000	3.247792000
H	11.642236000	6.888255000	4.905031000
H	10.631617000	5.634213000	4.235362000
H	11.364663000	6.256711000	1.896096000
H	12.366803000	7.553574000	2.550579000
H	9.680281000	3.106954000	7.239259000
H	10.924700000	2.670924000	8.407073000
H	11.137657000	5.026890000	6.442647000
H	12.416238000	4.483971000	7.530190000
H	11.465401000	3.651676000	11.378812000
H	12.501941000	3.662878000	9.948666000
H	9.531567000	2.701920000	10.417291000
H	8.047878000	3.048370000	9.533261000
H	7.939617000	8.085093000	2.360815000
H	7.651720000	5.784236000	1.480316000
H	9.439511000	7.556923000	1.605081000
H	10.624981000	5.967378000	10.784872000
H	11.649104000	5.992320000	9.371193000
H	12.789873000	4.802616000	11.257672000
H	1.896553000	2.887020000	6.602572000
H	4.029497000	3.875580000	7.490959000
H	3.053808000	5.096279000	6.726263000
H	9.572034000	10.118484000	3.600674000
H	10.785087000	9.358908000	2.575321000

H	2.309724000	3.397553000	4.970172000
H	2.966793000	6.547236000	2.976665000
H	2.380427000	5.879605000	4.499191000
H	3.654254000	7.098992000	4.508092000
H	7.506659000	4.907884000	11.124143000
H	7.726941000	3.384543000	11.989277000
H	8.999932000	4.603188000	12.014305000
H	11.783729000	10.842520000	4.398865000
H	12.357790000	9.179807000	4.499288000
H	11.106261000	9.744143000	5.606844000
H	4.065564000	9.310023000	4.034380000
H	5.094728000	12.572877000	4.562001000
H	4.922078000	12.073630000	7.674350000
H	3.631951000	12.441383000	6.536481000
H	3.027135000	9.207708000	5.433754000
H	6.589933000	12.196090000	5.410340000
H	10.603379000	11.382152000	7.165119000
H	7.861121000	11.851249000	10.191361000
H	9.335614000	12.799402000	10.044992000
H	11.618216000	10.229321000	7.991823000
H	9.450012000	9.874897000	11.409216000
H	10.663874000	11.138405000	11.239257000
H	5.607462000	10.787382000	2.858559000
H	6.938607000	11.938505000	2.966955000
H	7.065204000	10.357672000	3.752415000
H	2.704422000	11.605149000	8.706483000
H	3.615632000	10.102291000	8.536625000
H	2.305622000	10.475638000	7.414228000
H	1.895416000	10.467909000	3.589783000
H	2.145219000	11.538935000	4.962527000
H	3.200252000	11.646882000	3.550796000
H	7.533965000	13.712647000	8.565288000
H	8.874431000	13.126845000	7.579547000
H	7.413834000	12.152332000	7.738945000
H	12.259841000	12.029278000	9.688267000
H	11.267346000	13.186710000	8.799544000
H	12.689390000	12.480616000	8.042283000
H	11.683626000	8.878294000	11.774948000
H	12.266718000	9.497128000	10.231103000
H	11.022945000	8.246995000	10.261155000

6Fe_1_8_M6

Fe	6.226871000	6.247992000	6.571580000
Fe	8.436847000	7.682708000	5.794996000
Fe	8.468417000	6.282448000	8.121553000
Fe	6.189877000	8.959850000	6.705318000

Fe	6.242154000	7.499573000	8.999984000
Fe	8.413432000	8.921862000	8.220430000
S	6.388761000	7.717301000	4.860718000
S	4.605367000	7.544426000	7.478525000
S	8.275945000	5.466313000	6.008300000
S	6.499912000	5.292894000	8.593593000
S	8.183663000	9.905574000	6.233970000
S	10.110354000	7.701945000	7.325784000
S	8.319277000	7.535540000	9.997698000
S	6.412051000	9.743122000	8.840204000
P	4.939988000	4.752812000	5.559431000
P	9.685140000	7.751801000	3.999969000
P	9.814558000	4.646029000	9.055572000
P	5.014842000	10.576456000	5.769765000
P	4.958906000	7.524321000	10.795039000
C	5.837907000	3.240361000	5.053253000
C	6.391509000	2.419439000	6.205276000
C	8.808119000	7.351243000	2.447401000
C	8.250671000	5.940232000	2.391136000
C	11.095824000	6.596068000	4.055265000
C	12.001126000	6.588745000	2.835271000
C	10.529589000	3.463685000	7.862917000
C	11.550753000	4.085538000	6.927414000
C	12.151574000	4.354355000	10.626690000
C	11.225231000	5.360571000	9.964157000
C	3.574049000	4.144361000	6.606791000
C	2.682422000	3.077305000	5.994273000
C	4.143373000	5.265602000	3.998941000
C	3.076079000	6.326909000	4.198343000
C	8.963292000	3.547613000	10.238801000
C	8.394053000	4.248021000	11.459560000
C	10.419854000	9.380724000	3.621226000
C	11.433579000	9.864891000	4.643231000
C	5.907721000	11.656599000	4.597821000
C	4.324318000	11.785328000	6.953651000
C	3.577009000	9.969253000	4.825300000
C	3.544893000	8.668784000	10.674660000
C	4.226724000	5.902327000	11.212374000
C	5.796784000	7.962872000	12.358150000
C	2.714539000	11.034218000	4.168240000
C	6.439875000	10.952360000	3.363036000
C	3.233842000	11.209451000	7.839288000
C	2.621628000	8.714405000	11.880446000
C	3.230774000	5.390806000	10.188826000
C	6.323658000	9.384659000	12.427350000
H	6.965648000	1.572172000	5.825033000

H	12.811032000	5.869369000	2.972631000
H	11.855477000	3.366613000	6.164620000
H	5.159494000	2.639833000	4.439547000
H	6.647436000	3.576400000	4.399352000
H	7.047822000	3.020217000	6.837113000
H	5.594111000	2.021118000	6.835964000
H	3.241131000	2.171625000	5.750998000
H	4.946134000	5.644790000	3.361108000
H	3.734417000	4.376161000	3.510739000
H	9.042353000	5.189368000	2.432831000
H	7.572329000	5.759574000	3.226783000
H	11.652474000	6.851499000	4.960781000
H	10.664697000	5.608202000	4.236187000
H	11.462660000	6.303814000	1.929376000
H	12.459012000	7.564246000	2.661350000
H	9.682195000	3.065959000	7.297377000
H	10.961694000	2.631536000	8.427207000
H	11.134789000	4.959402000	6.425377000
H	12.448154000	4.400644000	7.462861000
H	11.632075000	3.759178000	11.379989000
H	12.595253000	3.667380000	9.903343000
H	9.674533000	2.768180000	10.530166000
H	8.165877000	3.058837000	9.672252000
H	8.000721000	8.083132000	2.360502000
H	7.697325000	5.786945000	1.462595000
H	9.498163000	7.533890000	1.617983000
H	10.794583000	6.050435000	10.694567000
H	11.757017000	5.989336000	9.244998000
H	12.970124000	4.873581000	11.128906000
H	1.893597000	2.795637000	6.694760000
H	4.047375000	3.785621000	7.524693000
H	2.999212000	5.028293000	6.895720000
H	9.582846000	10.080567000	3.551056000
H	10.867260000	9.317409000	2.624205000
H	2.198300000	3.426503000	5.080279000
H	2.725336000	6.706897000	3.236877000
H	2.210656000	5.933520000	4.734898000
H	3.470053000	7.164534000	4.773820000
H	7.679039000	5.017755000	11.166703000
H	7.880683000	3.528540000	12.100515000
H	9.174484000	4.725221000	12.055395000
H	11.801789000	10.855325000	4.369881000
H	12.295405000	9.197393000	4.704923000
H	10.990314000	9.932230000	5.637778000
H	3.978897000	9.274475000	4.083953000
H	5.223819000	12.463937000	4.318761000

H	5.170327000	12.128245000	7.554785000
H	3.958761000	12.646879000	6.386816000
H	2.995882000	9.360289000	5.522771000
H	6.724833000	12.111038000	5.163360000
H	3.976997000	9.651448000	10.469783000
H	3.003293000	8.382872000	9.769203000
H	3.766000000	5.989270000	12.201282000
H	5.067857000	5.210605000	11.309816000
H	6.614802000	7.245514000	12.469262000
H	5.089110000	7.768151000	13.170237000
H	5.635932000	10.519448000	2.764261000
H	6.982530000	11.657389000	2.730112000
H	7.120251000	10.145464000	3.638368000
H	2.964060000	11.918174000	8.624409000
H	3.567375000	10.285995000	8.313391000
H	2.329444000	10.986311000	7.270065000
H	1.870948000	10.570218000	3.653058000
H	2.304905000	11.737283000	4.896002000
H	3.271911000	11.608711000	3.426088000
H	1.810242000	9.423763000	11.705027000
H	3.145358000	9.035568000	12.782651000
H	2.166091000	7.743283000	12.083880000
H	2.353477000	6.037303000	10.121778000
H	3.684579000	5.342318000	9.199003000
H	2.885899000	4.390173000	10.456525000
H	5.519935000	10.119253000	12.345570000
H	6.827272000	9.552052000	13.381194000
H	7.040045000	9.580928000	11.628729000

6Fe_1_10_M2

Fe	6.226585000	6.269759000	6.360358000
Fe	8.453835000	7.727351000	5.706393000
Fe	8.465723000	6.182970000	8.015498000
Fe	6.193372000	9.083161000	6.553271000
Fe	6.186473000	7.513303000	8.844696000
Fe	8.453831000	8.973015000	8.169972000
S	6.440506000	7.795974000	4.698630000
S	4.621782000	7.602752000	7.222936000
S	8.307415000	5.493324000	5.833919000
S	6.425395000	5.321023000	8.393946000
S	8.274794000	9.936154000	6.112587000
S	10.066776000	7.635009000	7.289167000
S	8.243478000	7.474306000	9.818923000
S	6.409365000	9.750726000	8.672729000
P	5.050081000	4.581759000	5.557054000
P	9.626088000	4.611634000	9.042944000

P	4.930321000	10.747060000	5.835307000
P	5.059624000	7.563513000	10.756624000
P	9.536628000	10.605577000	9.197138000
C	5.980407000	3.062608000	5.157798000
C	6.603322000	2.371016000	6.357380000
C	10.398435000	3.416252000	7.897192000
C	11.461275000	4.020403000	6.995304000
C	11.896679000	4.245122000	10.713511000
C	11.008403000	5.273956000	10.035010000
C	3.671456000	4.043310000	6.622648000
C	2.809238000	2.917533000	6.077522000
C	4.287803000	5.000391000	3.949488000
C	3.226378000	6.084152000	4.029416000
C	8.701905000	3.525671000	10.183418000
C	8.118010000	4.242707000	11.387431000
C	5.812080000	11.976876000	4.812004000
C	4.103974000	11.779168000	7.093688000
C	3.582749000	10.124241000	4.770854000
C	3.650104000	8.721998000	10.735746000
C	4.319398000	5.948405000	11.190423000
C	5.987189000	7.992179000	12.271531000
C	8.592178000	12.111373000	9.617694000
C	10.918581000	11.190020000	8.155154000
C	10.305257000	10.146694000	10.789390000
C	2.664609000	11.180743000	4.179284000
C	6.346489000	11.431109000	3.498750000
C	3.057612000	11.022649000	7.891677000
C	2.810054000	8.780674000	12.000256000
C	3.244662000	5.494176000	10.218217000
C	6.539381000	9.406430000	12.273269000
C	11.771586000	12.299526000	8.747355000
C	8.047042000	12.851018000	8.408050000
C	11.393440000	9.095888000	10.650768000
H	7.176961000	1.499367000	6.036523000
H	11.821310000	3.275386000	6.283843000
H	5.297730000	2.390743000	4.628283000
H	6.751811000	3.364179000	4.444516000
H	7.274098000	3.048879000	6.886909000
H	5.846649000	2.029051000	7.066456000
H	3.383575000	2.000518000	5.933423000
H	5.113200000	5.317880000	3.306344000
H	3.879233000	4.080809000	3.519071000
H	9.582808000	2.996998000	7.302103000
H	10.809384000	2.599293000	8.498585000
H	11.064124000	4.863875000	6.428411000
H	12.321558000	4.372906000	7.567418000

H	11.337918000	3.623910000	11.416352000
H	12.380254000	3.583752000	9.992265000
H	9.374761000	2.721184000	10.495854000
H	7.907290000	3.068983000	9.587959000
H	10.554803000	5.949237000	10.764808000
H	11.582698000	5.910514000	9.356491000
H	12.686966000	4.744192000	11.277978000
H	2.001495000	2.689872000	6.775956000
H	4.124225000	3.772080000	7.579454000
H	3.079799000	4.942306000	6.815940000
H	2.351035000	3.180197000	5.122113000
H	2.873509000	6.343099000	3.029511000
H	2.361507000	5.759297000	4.611451000
H	3.623750000	6.987868000	4.494243000
H	7.461207000	5.055061000	11.073111000
H	7.537791000	3.548984000	11.999117000
H	8.897311000	4.671345000	12.020655000
H	4.070870000	9.537924000	3.987762000
H	5.128380000	12.814058000	4.640283000
H	4.895520000	12.149790000	7.750003000
H	3.667600000	12.647712000	6.591531000
H	3.027552000	9.404620000	5.378372000
H	6.629769000	12.352825000	5.432830000
H	4.071681000	9.700697000	10.494246000
H	3.046326000	8.435124000	9.870462000
H	3.927496000	6.013068000	12.210086000
H	5.144499000	5.231883000	11.206879000
H	6.800774000	7.266303000	12.346236000
H	5.326227000	7.827195000	13.127635000
H	10.468400000	11.493090000	7.206719000
H	7.776173000	11.786184000	10.268128000
H	9.243496000	12.758353000	10.212967000
H	11.514621000	10.303444000	7.923343000
H	9.495972000	9.776755000	11.423790000
H	10.690882000	11.057634000	11.257054000
H	5.539422000	11.120017000	2.832753000
H	6.925313000	12.197092000	2.979904000
H	6.996694000	10.570556000	3.662704000
H	2.685392000	11.634116000	8.715971000
H	3.476481000	10.106253000	8.307764000
H	2.201855000	10.745633000	7.273106000
H	1.897047000	10.709811000	3.561769000
H	2.152554000	11.756208000	4.952884000
H	3.207586000	11.882641000	3.543549000
H	1.985414000	9.484993000	11.872381000
H	3.393116000	9.115365000	12.860262000

H	2.373935000	7.810902000	12.247713000
H	2.369692000	6.146388000	10.250098000
H	3.623011000	5.491173000	9.195289000
H	2.911760000	4.483390000	10.461631000
H	5.743498000	10.153225000	12.240164000
H	7.125695000	9.586131000	13.176622000
H	7.182684000	9.568156000	11.407189000
H	7.423800000	13.690269000	8.722771000
H	8.849215000	13.248827000	7.783523000
H	7.441592000	12.186164000	7.789718000
H	12.234662000	12.001182000	9.689907000
H	11.190386000	13.205120000	8.931577000
H	12.575399000	12.563143000	8.057229000
H	11.743590000	8.776227000	11.634045000
H	12.255259000	9.476556000	10.099796000
H	11.018865000	8.219037000	10.121107000

6Fe_1_4

Fe	6.205167000	6.253336000	6.535580000
Fe	8.429712000	7.657376000	5.775742000
Fe	8.441659000	6.141317000	8.066536000
Fe	6.150674000	8.995421000	6.643047000
Fe	6.196040000	7.507247000	8.950383000
Fe	8.400908000	8.904258000	8.212919000
S	6.378916000	7.726209000	4.806949000
S	4.544053000	7.573647000	7.386496000
S	8.215823000	5.424864000	5.919018000
S	6.396397000	5.286228000	8.558097000
S	8.183344000	9.857168000	6.186475000
S	10.029941000	7.570206000	7.357526000
S	8.215067000	7.414490000	9.903953000
S	6.378878000	9.724221000	8.750937000
P	4.947507000	4.616180000	5.549063000
P	9.747329000	7.788215000	4.016797000
P	9.773778000	4.647679000	9.002385000
P	4.929975000	10.606052000	5.810092000
P	4.971500000	7.590837000	10.775469000
P	9.510804000	10.550963000	9.170730000
C	5.851813000	3.087309000	5.131739000
C	6.433611000	2.357953000	6.330130000
C	8.884252000	7.501090000	2.428978000
C	8.320260000	6.100548000	2.263651000
C	11.110808000	6.575139000	4.028152000
C	12.035981000	6.589687000	2.823764000
C	10.538695000	3.459658000	7.842884000
C	11.544377000	4.093879000	6.899496000

C	12.092756000	4.345830000	10.621662000
C	11.164299000	5.346840000	9.956287000
C	3.565349000	4.095821000	6.617737000
C	2.669348000	3.006958000	6.052000000
C	4.200213000	5.097206000	3.956039000
C	3.151104000	6.187350000	4.087426000
C	8.931388000	3.516841000	10.168924000
C	8.331067000	4.189131000	11.390580000
C	10.556715000	9.397948000	3.719718000
C	11.605458000	9.745032000	4.761093000
C	5.814637000	11.739461000	4.679439000
C	4.177834000	11.769518000	7.001920000
C	3.525170000	9.984094000	4.820818000
C	3.578689000	8.767047000	10.710496000
C	4.212076000	5.992562000	11.236342000
C	5.878413000	8.024664000	12.302413000
C	8.577485000	12.070770000	9.573524000
C	10.910103000	11.131525000	8.152590000
C	10.263003000	10.126581000	10.782902000
C	2.646507000	11.037605000	4.167977000
C	6.363556000	11.077843000	3.428080000
C	3.095990000	11.135088000	7.857186000
C	2.712308000	8.850280000	11.955533000
C	3.153585000	5.514656000	10.258731000
C	6.466709000	9.423814000	12.306687000
C	11.741084000	12.262438000	8.734337000
C	8.022888000	12.796908000	8.360810000
C	11.373525000	9.096039000	10.679429000
H	7.003514000	1.486996000	6.000997000
H	12.815568000	5.833138000	2.935776000
H	11.880880000	3.371668000	6.153110000
H	5.166371000	2.443290000	4.571634000
H	6.646816000	3.388308000	4.444280000
H	7.099876000	3.012471000	6.893776000
H	5.653066000	2.007806000	7.008475000
H	3.216622000	2.077910000	5.882283000
H	5.029747000	5.439649000	3.331223000
H	3.787584000	4.199168000	3.485819000
H	9.109118000	5.345641000	2.259921000
H	7.631892000	5.859823000	3.075457000
H	11.660333000	6.759430000	4.955212000
H	10.635155000	5.598812000	4.152896000
H	11.501679000	6.372188000	1.896845000
H	12.533206000	7.554189000	2.703407000
H	9.710245000	3.021285000	7.279117000
H	10.994186000	2.653796000	8.426269000

H	11.100926000	4.942617000	6.378174000
H	12.426084000	4.453030000	7.433987000
H	11.563706000	3.717966000	11.341148000
H	12.573997000	3.688980000	9.894367000
H	9.650415000	2.745835000	10.462607000
H	8.149307000	3.019405000	9.588149000
H	8.080646000	8.241541000	2.387098000
H	7.778544000	6.018242000	1.319230000
H	9.582367000	7.737569000	1.620100000
H	10.707479000	6.012275000	10.693414000
H	11.705364000	5.996754000	9.263439000
H	12.884408000	4.866875000	11.164237000
H	1.860453000	2.786397000	6.751463000
H	4.023936000	3.791539000	7.562018000
H	3.002682000	5.006413000	6.839789000
H	9.754770000	10.140781000	3.722761000
H	10.985474000	9.386675000	2.713089000
H	2.212446000	3.305431000	5.106516000
H	2.818313000	6.516181000	3.101193000
H	2.273337000	5.839334000	4.635241000
H	3.556262000	7.050538000	4.616478000
H	7.599555000	4.943555000	11.098153000
H	7.830002000	3.451675000	12.021163000
H	9.092403000	4.682486000	11.998378000
H	11.959156000	10.769092000	4.625794000
H	12.472263000	9.084335000	4.696056000
H	11.194724000	9.654191000	5.766373000
H	3.962805000	9.316425000	4.074152000
H	5.129167000	12.552379000	4.421500000
H	4.998109000	12.131521000	7.626552000
H	3.790669000	12.628773000	6.446379000
H	2.948887000	9.341703000	5.491974000
H	6.627181000	12.176694000	5.265679000
H	4.020648000	9.736955000	10.470606000
H	2.991058000	8.479816000	9.834329000
H	3.802750000	6.086296000	12.246933000
H	5.036890000	5.276596000	11.286927000
H	6.671297000	7.278641000	12.401544000
H	5.195284000	7.883909000	13.145621000
H	10.478250000	11.408191000	7.187857000
H	7.767281000	11.762510000	10.238989000
H	9.240390000	12.721974000	10.151275000
H	11.521806000	10.245872000	7.962006000
H	9.448987000	9.746803000	11.405077000
H	10.621169000	11.050396000	11.247055000
H	5.568077000	10.657411000	2.809418000

H	6.906510000	11.805121000	2.821073000
H	7.049029000	10.269258000	3.686578000
H	2.783972000	11.815127000	8.652342000
H	3.456910000	10.214765000	8.316502000
H	2.210932000	10.888323000	7.267614000
H	1.832303000	10.562816000	3.616394000
H	2.194649000	11.706935000	4.902797000
H	3.205426000	11.650352000	3.458049000
H	1.901604000	9.566028000	11.803512000
H	3.281893000	9.183790000	12.825026000
H	2.255988000	7.889561000	12.201961000
H	2.287878000	6.180033000	10.245303000
H	3.556180000	5.470244000	9.246414000
H	2.801249000	4.518166000	10.532295000
H	5.690993000	10.190531000	12.250432000
H	7.036291000	9.594316000	13.222568000
H	7.133896000	9.561365000	11.454968000
H	7.410590000	13.646085000	8.670945000
H	8.820204000	13.178390000	7.719697000
H	7.406154000	12.127311000	7.759811000
H	12.175623000	11.995500000	9.699798000
H	11.151078000	13.170248000	8.873209000
H	12.565419000	12.509356000	8.062088000
H	11.700373000	8.783321000	11.673054000
H	12.244452000	9.491416000	10.153328000
H	11.030435000	8.213367000	10.139517000

6Fe_1_6

Fe	6.220109000	6.265749000	6.590504000
Fe	8.435248000	7.678036000	5.895062000
Fe	8.436877000	6.180664000	8.205223000
Fe	6.165081000	9.028684000	6.715195000
Fe	6.209537000	7.524132000	8.993542000
Fe	8.407793000	8.946996000	8.309307000
S	6.397755000	7.728693000	4.907699000
S	4.565063000	7.609758000	7.427550000
S	8.237379000	5.443823000	6.086236000
S	6.372831000	5.307366000	8.622743000
S	8.202491000	9.880893000	6.286932000
S	10.029823000	7.617889000	7.495668000
S	8.207196000	7.489701000	10.031520000
S	6.366301000	9.785062000	8.834218000
P	5.043684000	4.706153000	5.593247000
P	9.593423000	7.804748000	4.021757000
P	9.778520000	4.612278000	8.990653000
P	5.013453000	10.612223000	5.748992000

P	4.893330000	7.532060000	10.858240000
P	9.571692000	10.605464000	9.180140000
C	5.950661000	3.175920000	5.169532000
C	6.470704000	2.402027000	6.368499000
C	8.695530000	7.390690000	2.484119000
C	8.175698000	5.964668000	2.441068000
C	11.010127000	6.651834000	4.045198000
C	11.872353000	6.622854000	2.794619000
C	10.550082000	3.496766000	7.766674000
C	11.571492000	4.188484000	6.881864000
C	12.098272000	4.229221000	10.596400000
C	11.171328000	5.262440000	9.979577000
C	3.638799000	4.137619000	6.613688000
C	2.772392000	3.043512000	6.012981000
C	4.295822000	5.167665000	3.991053000
C	3.221383000	6.233496000	4.114573000
C	8.942143000	3.426955000	10.107488000
C	8.376684000	4.055856000	11.369328000
C	10.333760000	9.427494000	3.626930000
C	11.409904000	9.844333000	4.613700000
C	5.931559000	11.710254000	4.611947000
C	4.246117000	11.813257000	6.894801000
C	3.621344000	9.982168000	4.747302000
C	3.509485000	8.710105000	10.738278000
C	4.141836000	5.916021000	11.246839000
C	5.773097000	7.956208000	12.400211000
C	8.657990000	12.138812000	9.574362000
C	10.963531000	11.147069000	8.132923000
C	10.327477000	10.194865000	10.794090000
C	2.756743000	11.026936000	4.062909000
C	6.496921000	11.007000000	3.391293000
C	3.166798000	11.206122000	7.773668000
C	2.602317000	8.790002000	11.954471000
C	3.102920000	5.468480000	10.234364000
C	6.331742000	9.367082000	12.437476000
C	11.821644000	12.271962000	8.685768000
C	8.074276000	12.846636000	8.364669000
C	11.401799000	9.124430000	10.713961000
H	7.055534000	1.540744000	6.039452000
H	12.696912000	5.918323000	2.922479000
H	11.913064000	3.517754000	6.090835000
H	5.283134000	2.554695000	4.564497000
H	6.778012000	3.483494000	4.524825000
H	7.108453000	3.031137000	6.991601000
H	5.655620000	2.030146000	6.992751000
H	3.340194000	2.128749000	5.832873000

H	5.117803000	5.526251000	3.366231000
H	3.903483000	4.260989000	3.520932000
H	8.989182000	5.236539000	2.447680000
H	7.540996000	5.760369000	3.304734000
H	11.595634000	6.921759000	4.928171000
H	10.587038000	5.667124000	4.258823000
H	11.305812000	6.304876000	1.917351000
H	12.309475000	7.598966000	2.574987000
H	9.727876000	3.102141000	7.163537000
H	10.995610000	2.651368000	8.299345000
H	11.141571000	5.075486000	6.416039000
H	12.448964000	4.503187000	7.450271000
H	11.567571000	3.567675000	11.283867000
H	12.577947000	3.607326000	9.837944000
H	9.649386000	2.628238000	10.350485000
H	8.139476000	2.977723000	9.515654000
H	7.867062000	8.100100000	2.414448000
H	7.589288000	5.799767000	1.534975000
H	9.364536000	7.590396000	1.641646000
H	10.716098000	5.893424000	10.747988000
H	11.714588000	5.944982000	9.320495000
H	12.891394000	4.720320000	11.164212000
H	1.956110000	2.791656000	6.693272000
H	4.076695000	3.822707000	7.564296000
H	3.053577000	5.033382000	6.838108000
H	9.512367000	10.147964000	3.630944000
H	10.725156000	9.387679000	2.605931000
H	2.324904000	3.351048000	5.065857000
H	2.893246000	6.564927000	3.127446000
H	2.344368000	5.863083000	4.648713000
H	3.600737000	7.100455000	4.656380000
H	7.679948000	4.858303000	11.121621000
H	7.844900000	3.309244000	11.962582000
H	9.163119000	4.479783000	11.997267000
H	11.716129000	10.877127000	4.436397000
H	12.299104000	9.216652000	4.528923000
H	11.043652000	9.766734000	5.637638000
H	4.066408000	9.298895000	4.019653000
H	5.262016000	12.524235000	4.317889000
H	5.060887000	12.208558000	7.506873000
H	3.853075000	12.646027000	6.303918000
H	3.030572000	9.355151000	5.420509000
H	6.737259000	12.152384000	5.203618000
H	3.965684000	9.677556000	10.513809000
H	2.954531000	8.425452000	9.840359000
H	3.715577000	5.976924000	12.253262000

H	4.971476000	5.205076000	11.285307000
H	6.579657000	7.224143000	12.492290000
H	5.079299000	7.784071000	13.229283000
H	10.519445000	11.418758000	7.172231000
H	7.863837000	11.845290000	10.265739000
H	9.338147000	12.796866000	10.123867000
H	11.556375000	10.248077000	7.943978000
H	9.504134000	9.860026000	11.430855000
H	10.720796000	11.117149000	11.232407000
H	5.707685000	10.593810000	2.759991000
H	7.077520000	11.704234000	2.783683000
H	7.149292000	10.184463000	3.687523000
H	2.838141000	11.922254000	8.529399000
H	3.540157000	10.316943000	8.282991000
H	2.290741000	10.914959000	7.190876000
H	1.953384000	10.544234000	3.502368000
H	2.290756000	11.706101000	4.779554000
H	3.329134000	11.629952000	3.355223000
H	1.799303000	9.508442000	11.777475000
H	3.143139000	9.118058000	12.844230000
H	2.135738000	7.829099000	12.180602000
H	2.230753000	6.125071000	10.233906000
H	3.521203000	5.464690000	9.227513000
H	2.758130000	4.458914000	10.465361000
H	5.541330000	10.118661000	12.388452000
H	6.886296000	9.527442000	13.364028000
H	7.007140000	9.535445000	11.597718000
H	7.485660000	13.711831000	8.676291000
H	8.855142000	13.201365000	7.688872000
H	7.427087000	12.173586000	7.800561000
H	12.268882000	12.009688000	9.646567000
H	11.247785000	13.190379000	8.823187000
H	12.637688000	12.497726000	7.996247000
H	11.742278000	8.849278000	11.714067000
H	12.271904000	9.467887000	10.150910000
H	11.020663000	8.227332000	10.224736000

6Fe_1_8

Fe	6.217765000	6.335578000	6.475706000
Fe	8.408047000	7.793719000	5.739021000
Fe	8.434563000	6.308743000	8.049585000
Fe	6.212546000	9.044732000	6.635613000
Fe	6.180678000	7.596465000	8.945386000
Fe	8.406125000	9.032840000	8.205749000
S	6.366042000	7.799133000	4.764308000
S	4.574472000	7.641873000	7.355710000

S	8.251781000	5.569228000	5.924073000
S	6.423989000	5.399098000	8.498105000
S	8.186187000	10.011234000	6.183582000
S	10.025970000	7.751857000	7.308237000
S	8.227039000	7.563342000	9.891383000
S	6.359689000	9.824613000	8.767327000
P	5.066873000	4.704198000	5.578621000
P	9.679971000	7.751604000	3.956146000
P	9.614878000	4.720862000	8.996883000
P	4.904485000	10.669085000	5.717628000
P	5.016607000	7.510239000	10.788933000
P	9.603164000	10.563351000	9.232198000
C	5.998958000	3.190797000	5.152698000
C	6.595760000	2.472168000	6.349752000
C	8.827663000	7.315143000	2.398101000
C	8.247518000	5.912649000	2.368110000
C	11.083721000	6.591869000	4.067882000
C	11.995147000	6.522021000	2.854805000
C	10.374347000	3.532611000	7.832355000
C	11.467893000	4.142403000	6.973586000
C	11.886217000	4.289388000	10.656218000
C	11.014616000	5.341712000	9.992213000
C	3.697537000	4.120107000	6.635779000
C	2.854176000	2.986317000	6.078366000
C	4.274064000	5.120716000	3.984215000
C	3.180909000	6.167989000	4.105676000
C	8.713692000	3.606436000	10.132237000
C	8.149544000	4.290305000	11.364213000
C	10.434007000	9.360598000	3.523642000
C	11.448434000	9.855327000	4.538601000
C	5.771012000	11.787338000	4.566018000
C	4.172899000	11.819637000	6.929416000
C	3.503039000	9.985523000	4.771941000
C	3.601030000	8.665621000	10.769040000
C	4.272954000	5.887520000	11.183027000
C	5.912767000	7.910529000	12.331523000
C	8.699172000	12.080918000	9.708571000
C	10.985654000	11.161306000	8.198562000
C	10.380099000	10.067785000	10.808802000
C	2.586069000	11.012106000	4.128548000
C	6.341858000	11.104775000	3.336255000
C	3.138149000	11.174558000	7.834040000
C	2.729150000	8.683517000	12.012965000
C	3.206886000	5.456568000	10.191649000
C	6.451298000	9.329152000	12.382156000
C	11.862319000	12.240628000	8.810997000

C	8.164224000	12.885314000	8.536622000
C	11.450732000	9.005246000	10.636099000
H	7.205936000	1.627773000	6.022979000
H	12.803796000	5.809565000	3.031083000
H	11.789309000	3.438676000	6.203227000
H	5.326867000	2.532195000	4.594188000
H	6.787500000	3.506791000	4.464876000
H	7.224973000	3.148731000	6.929499000
H	5.821641000	2.084941000	7.015488000
H	3.445156000	2.082841000	5.916649000
H	5.077436000	5.481425000	3.336405000
H	3.890222000	4.197867000	3.539146000
H	9.026161000	5.150216000	2.438584000
H	7.558734000	5.762997000	3.200804000
H	11.636312000	6.882644000	4.965472000
H	10.644006000	5.616397000	4.290280000
H	11.459632000	6.192344000	1.962374000
H	12.454875000	7.486996000	2.632161000
H	9.559022000	3.161066000	7.206739000
H	10.752049000	2.683378000	8.409726000
H	11.112563000	5.048574000	6.482318000
H	12.345264000	4.406256000	7.567211000
H	11.321668000	3.681785000	11.366196000
H	12.341791000	3.615155000	9.928342000
H	9.395972000	2.798602000	10.413666000
H	7.909479000	3.159101000	9.542696000
H	8.032911000	8.056695000	2.278300000
H	7.703241000	5.746222000	1.436269000
H	9.534452000	7.464956000	1.576166000
H	10.574902000	6.014034000	10.732911000
H	11.598146000	5.977849000	9.321367000
H	12.697534000	4.766045000	11.210493000
H	2.054393000	2.731678000	6.776887000
H	4.158623000	3.843699000	7.587123000
H	3.088669000	5.003508000	6.846401000
H	9.602051000	10.065296000	3.439870000
H	10.882466000	9.271704000	2.529279000
H	2.385970000	3.253993000	5.129064000
H	2.822672000	6.465042000	3.117991000
H	2.324386000	5.793634000	4.669750000
H	3.553490000	7.056594000	4.616105000
H	7.480307000	5.104080000	11.082073000
H	7.587060000	3.577877000	11.971317000
H	8.938334000	4.710930000	11.991177000
H	11.798335000	10.855452000	4.275445000
H	12.321005000	9.200786000	4.587422000

H	11.009026000	9.897752000	5.535732000
H	3.944785000	9.321235000	4.025138000
H	5.065011000	12.575963000	4.286893000
H	5.010704000	12.203504000	7.517567000
H	3.748728000	12.664445000	6.377902000
H	2.961267000	9.338019000	5.466132000
H	6.568345000	12.257295000	5.147569000
H	4.026022000	9.652410000	10.568315000
H	3.021678000	8.404655000	9.879027000
H	3.872117000	5.931518000	12.200247000
H	5.097290000	5.170027000	11.191520000
H	6.732292000	7.190494000	12.401172000
H	5.239725000	7.716245000	13.172027000
H	10.527527000	11.502193000	7.266361000
H	7.879516000	11.753009000	10.353305000
H	9.370354000	12.687913000	10.323856000
H	11.567321000	10.273961000	7.935419000
H	9.569883000	9.694605000	11.440409000
H	10.781665000	10.963449000	11.291973000
H	5.560259000	10.651254000	2.723637000
H	6.872150000	11.829863000	2.715840000
H	7.041879000	10.318461000	3.621171000
H	2.820867000	11.875788000	8.608093000
H	3.548230000	10.290012000	8.322475000
H	2.249548000	10.870800000	7.277567000
H	1.776496000	10.508629000	3.596272000
H	2.129147000	11.673606000	4.867074000
H	3.116269000	11.632504000	3.403681000
H	1.908153000	9.392921000	11.889052000
H	3.290820000	8.987487000	12.898377000
H	2.286677000	7.706439000	12.216963000
H	2.325234000	6.098607000	10.242472000
H	3.590292000	5.495578000	9.171717000
H	2.883175000	4.434002000	10.395509000
H	5.648059000	10.068578000	12.363530000
H	7.026630000	9.486723000	13.296661000
H	7.102943000	9.523241000	11.528646000
H	7.573272000	13.730866000	8.894513000
H	8.971860000	13.283488000	7.918998000
H	7.529728000	12.268646000	7.897953000
H	12.331187000	11.907094000	9.738765000
H	11.296572000	13.148140000	9.030275000
H	12.662823000	12.514232000	8.120526000
H	11.789240000	8.637694000	11.606788000
H	12.322405000	9.392630000	10.105311000
H	11.063284000	8.160131000	10.066918000

6Fe_1_10

Fe	6.225538000	6.282635000	6.521376000
Fe	8.414802000	7.733721000	5.774379000
Fe	8.494048000	6.245290000	8.072571000
Fe	6.154460000	9.060702000	6.599320000
Fe	6.248787000	7.566583000	8.943858000
Fe	8.452365000	9.037959000	8.174916000
S	6.387238000	7.644773000	4.700296000
S	4.539953000	7.516547000	7.411970000
S	8.256354000	5.482394000	5.952537000
S	6.483336000	5.363280000	8.538127000
S	8.305141000	10.003034000	6.153006000
S	10.057295000	7.685945000	7.330205000
S	8.303700000	7.550057000	9.867056000
S	6.397091000	9.807962000	8.851695000
P	5.008729000	4.662113000	5.684246000
P	9.795967000	7.753572000	3.879233000
P	9.648183000	4.629340000	9.004989000
P	4.776770000	10.853536000	5.622866000
P	5.013768000	7.431447000	10.760629000
P	9.578810000	10.623862000	9.235236000
C	5.927719000	3.152886000	5.214178000
C	6.563344000	2.421154000	6.383021000
C	8.946401000	7.328658000	2.319216000
C	8.426511000	5.902573000	2.263474000
C	11.178404000	6.573313000	4.019756000
C	12.121958000	6.504580000	2.831072000
C	10.393442000	3.435702000	7.838292000
C	11.463511000	4.046641000	6.950659000
C	11.936866000	4.224444000	10.645797000
C	11.058236000	5.267693000	9.976636000
C	3.679201000	4.066715000	6.781104000
C	2.815413000	2.942305000	6.236340000
C	4.168468000	5.090089000	4.119039000
C	3.119763000	6.179642000	4.256301000
C	8.752180000	3.536482000	10.162018000
C	8.205913000	4.246439000	11.387675000
C	10.562336000	9.368553000	3.508312000
C	11.584914000	9.805776000	4.543012000
C	5.696844000	11.950488000	4.489944000
C	4.080351000	11.995380000	6.865714000
C	3.359751000	10.211043000	4.667856000
C	3.604116000	8.590596000	10.728055000
C	4.278442000	5.807619000	11.161296000
C	5.909461000	7.818747000	12.308875000

C	8.658626000	12.140140000	9.675219000
C	10.981927000	11.213252000	8.222038000
C	10.331280000	10.145799000	10.831343000
C	2.457530000	11.254927000	4.032181000
C	6.259225000	11.223790000	3.278945000
C	3.086508000	11.318833000	7.795480000
C	2.732546000	8.616018000	11.972246000
C	3.199891000	5.374333000	10.186542000
C	6.430889000	9.240094000	12.413450000
C	11.837533000	12.310505000	8.832244000
C	8.103668000	12.893610000	8.478844000
C	11.419742000	9.095284000	10.691816000
H	7.161391000	1.579942000	6.026828000
H	12.914799000	5.777409000	3.018945000
H	11.779948000	3.334654000	6.185972000
H	5.236176000	2.499889000	4.672908000
H	6.691846000	3.473990000	4.501677000
H	7.213586000	3.090141000	6.948856000
H	5.812042000	2.026782000	7.070315000
H	3.399052000	2.043651000	6.027732000
H	4.960603000	5.405432000	3.434809000
H	3.732195000	4.172433000	3.712668000
H	9.237142000	5.172566000	2.310823000
H	7.744984000	5.708779000	3.093038000
H	11.708916000	6.844675000	4.936546000
H	10.715972000	5.603006000	4.219190000
H	11.605778000	6.196738000	1.919636000
H	12.601014000	7.466032000	2.635387000
H	9.568125000	3.050349000	7.234321000
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H	11.087025000	4.940039000	6.451265000
H	12.347884000	4.330363000	7.524334000
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H	12.385912000	3.541241000	9.922218000
H	9.431880000	2.728621000	10.449658000
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H	8.117790000	8.036735000	2.231367000
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H	11.633933000	5.893818000	9.289710000
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H	2.049744000	2.671020000	6.966141000
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H	3.080909000	4.948198000	7.024177000
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H	2.301588000	3.230363000	5.317242000
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H	2.289692000	5.862582000	4.891003000
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H	5.232431000	7.591317000	13.138240000
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