

Electronic Supplementary Information

Understanding the unique reactivity patterns of nickel/JoSPOphos manifold in the Nickel-catalyzed enantioselective C–H cyclization of imidazoles

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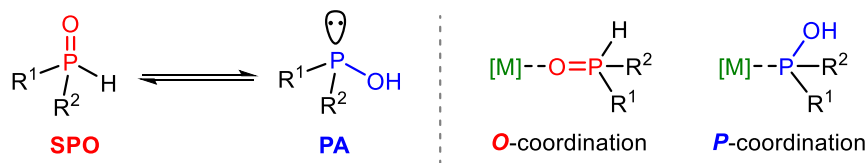
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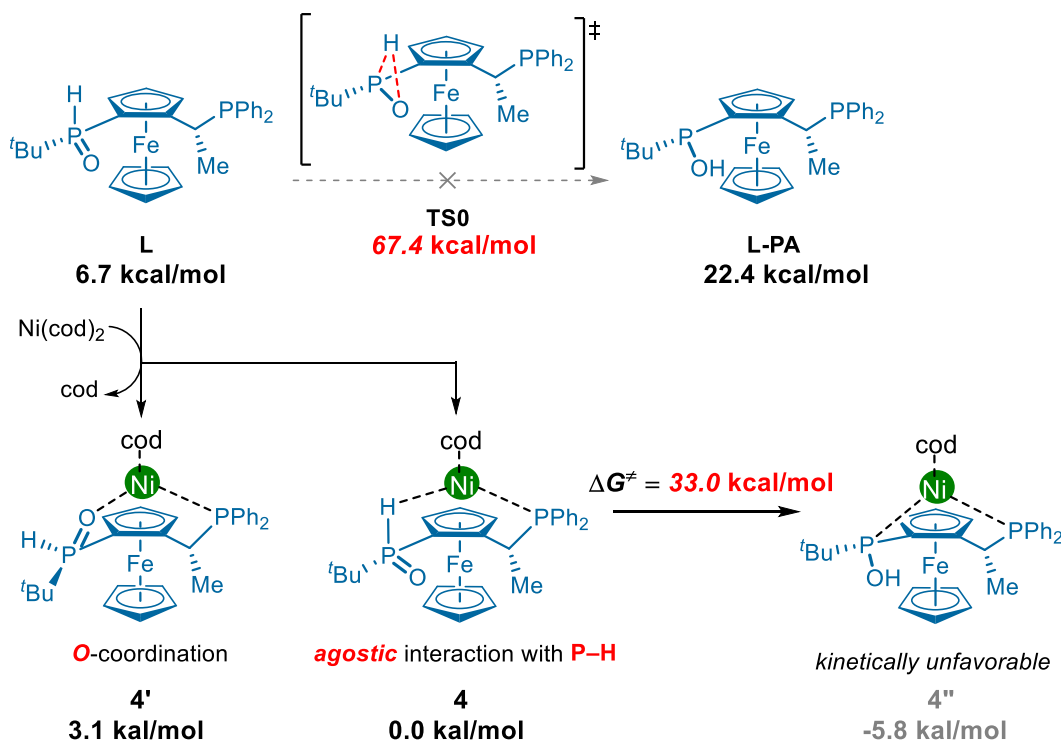
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1. The coordination mode of JoSPOphos with nickel.

(a) General SPO-PA tautomeric equilibrium and possible coordination modes



(b) SPO-PA tautomeric equilibrium in JoSPOphos ligand (L)



Scheme S1 SPO-PA tautomeric equilibrium and two different coordination modes of **L** with nickel(0). All energies are presented with respect to complex **4**.

For the JoSPOphos ligand, the secondary phosphine oxide (SPO) and phosphine groups are separately introduced to the chiral ferrocenyl backbone. For SPOs, there generally exists a tautomeric equilibrium between the pentavalent phosphine oxide and the trivalent phosphinous acid (PA), which will lead to different coordination modes with a transition metal (Scheme S1a). We first investigated the tautomeric behavior of JoSPOphos to determine the dominate species. As shown in Scheme S1b, due to the severe strain in the transition state **TS0**, the tautomeric conversion is kinetically unfavorable, with a significantly high energy barrier of 60.7 kcal/mol with respect to **L**. In addition, the possibility of intermolecular hydrogen transfer process is excluded due to the steric hindrance caused by the ^tBu

group. Ligand exchange of the precatalyst $\text{Ni}(\text{cod})_2$ with **L** forms the *O*-coordinated complex **4'**, which is exergonic by 3.6 kcal/mol. Interestingly, we located another more stable isomeric form **4**, which is 3.1 kcal/mol lower in energy than **4'**. This result is further verified by additional calculations employing B3LYP-D3(BJ) and M06^[1] density functionals in combination with def2-TZVP basis set (see Table S1).

Table S1. The energy differences between complexes **4** and **4'** calculated by using different methods.

Methods	$\Delta\Delta G_{\text{sol}} = \Delta G_{\text{sol}}(\mathbf{4}') - \Delta G_{\text{sol}}(\mathbf{4})$
B3LYP-D3(BJ)/def2-QZVP// B3LYP-D3(BJ)/def2-TZVP	2.8 kcal/mol
M06/def2-QZVP//M06/def2-TZVP	3.7 kcal/mol

We also considered the coordination of the **L-PA** ligand with nickel. As shown in Scheme S1, although the corresponding complex **4''** is 5.8 kcal/mol more stable than complex **4**, the transformation requires a relatively high barrier of 33.0 kcal/mol. The free energy profile for the conversion from complex **4** to **4''** is given in Fig. S1.

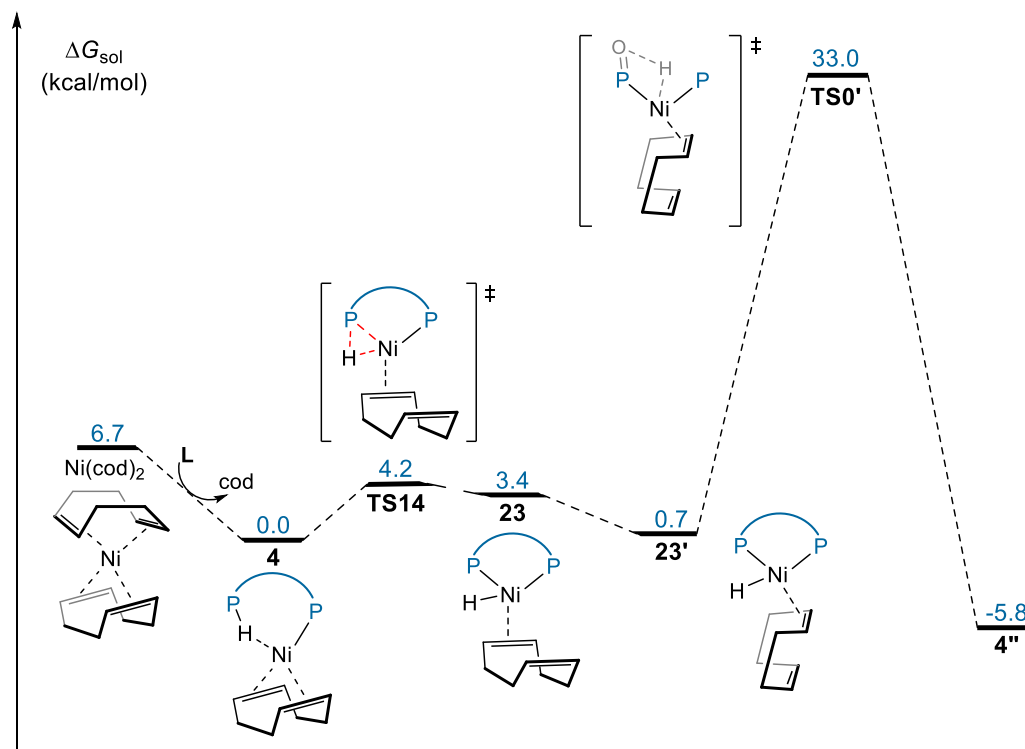


Fig. S1 Free energy profile for the formation of complex **4''**.

2. Mechanism of the formation of π -allyl nickel(II) complex **3**.

The calculated energy profile for the formation of **3** is given in Fig. S2. The optimized structures of the representative transition states are shown in Fig. S3. All energies are presented with respect to complex **4**, which is formed by ligand exchange of the precatalyst Ni(cod)₂ with **L**. This ligand substitution is exergonic by 6.7 kcal/mol. Complex **4** then undergoes facile oxidative addition of P–H bond through **TS14** with a low activation free energy of 4.2 kcal/mol, forming the square planar nickel hydride complex **23**. The subsequent migratory insertion of the C=C into Ni–H bond only requires a barrier of 0.7 kcal/mol from **23**. We also considered the possibility of direct transformation from complex **4** to **24** via LLHT, in which the oxidative addition of P–H bond and migratory insertion occur concurrently. However, we failed to locate the corresponding LLHT transition state.

Upon formation of **24**, the traditional chain walking involving consecutive β -hydride elimination/migratory insertion occurs to yield the π -allyl nickel(II) complex **3**. Rotation of the Ni–C1 bond in **24** occurs first to result in intermediate **25**. Then a facile β -hydride elimination takes place via **TS16** to generate another new nickel hydride **26**, in which the two C=C bonds becomes one carbon closer. The subsequent migratory insertion of the newly formed C1=C8 into Ni–H bond occurs through **TS17**, which gives another agostic intermediate **28**. In analogous to the **25** \rightarrow **26** \rightarrow **27** \rightarrow **28** transformation, **29** \rightarrow **30** \rightarrow **21** \rightarrow **20** proceeds to form the agostic intermediate **20**. The σ -allyl nickel(II) complex **20** ultimately isomerizes to the π -allyl nickel(II) complex **3**, which is exergonic by 14.0 kcal/mol. As compared to the precatalyst Ni(cod)₂, the complex **3** is 25.2 kcal/mol more stable, explaining why it can be isolated in experiment.

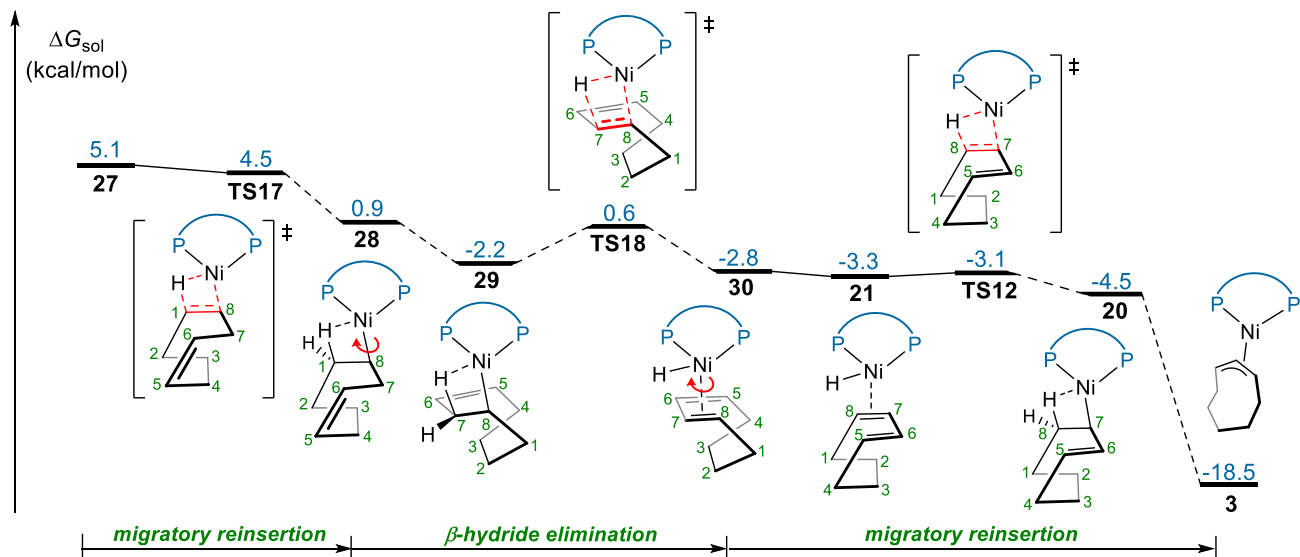
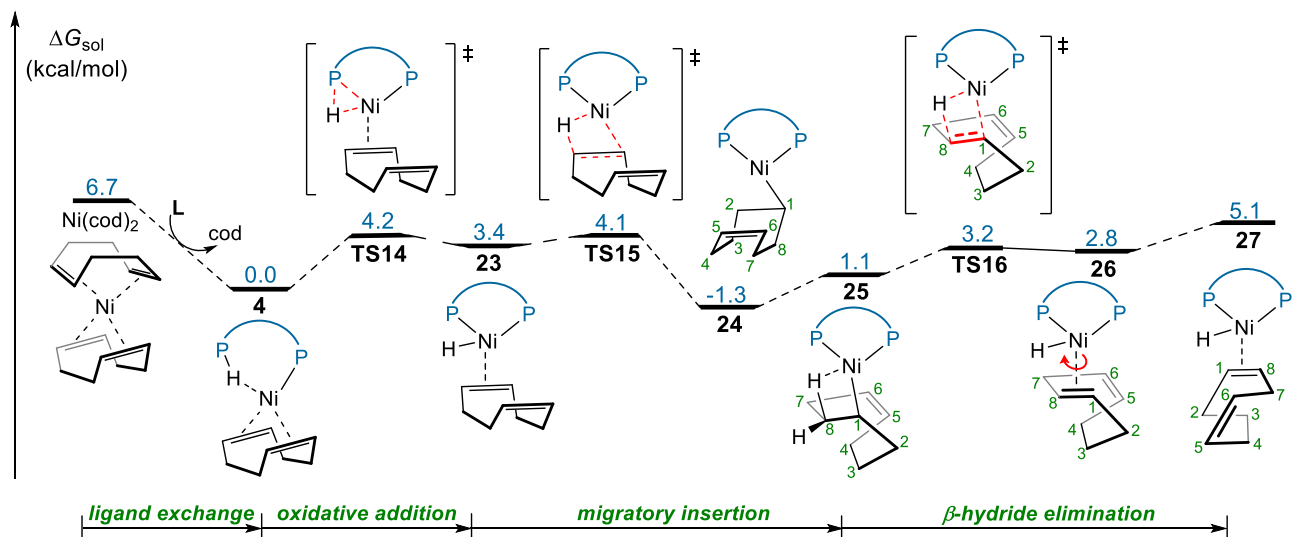


Fig. S2 Free energy profile for the formation of complex 3 *via* chain walking mechanism.

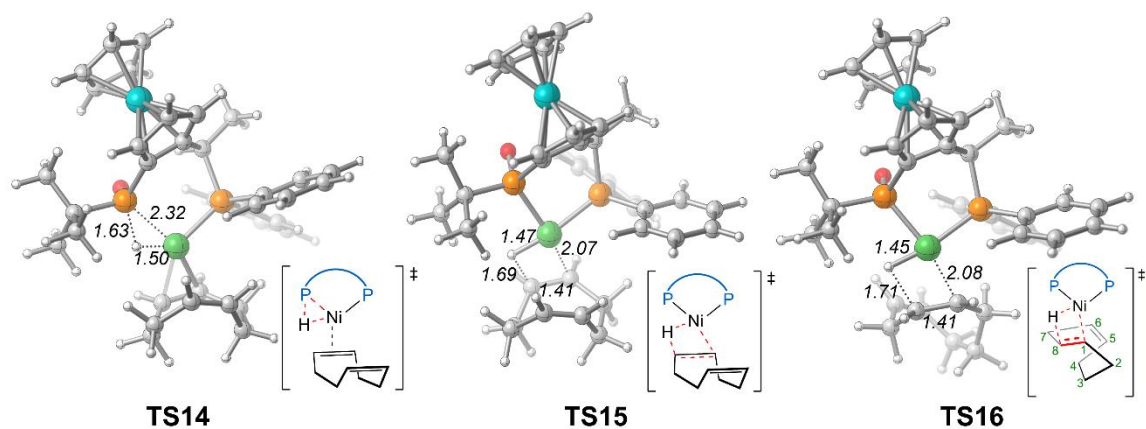


Fig. S3 Optimized structures of transition states TS14, TS15 and TS16 with selected bond distances in Å.

3. The complete free energy profile for nickel(II)-promoted hydroarylation *via* σ -CAM.

The complete energy profile for the nickel(II)-promoted hydroarylation *via* the σ -CAM mechanism is given in Fig. S4, which includes the possible coordination of the cyclooctene (coe) with the intermediate and the proton abstraction from an additional substrate **1a**. In addition, we also located a reverse LLHT transition state from intermediate **7** (Fig. S5). Although the reverse LLHT process is very facile, this reaction pathway is disfavored due to the higher barrier of the preceding migratory insertion.

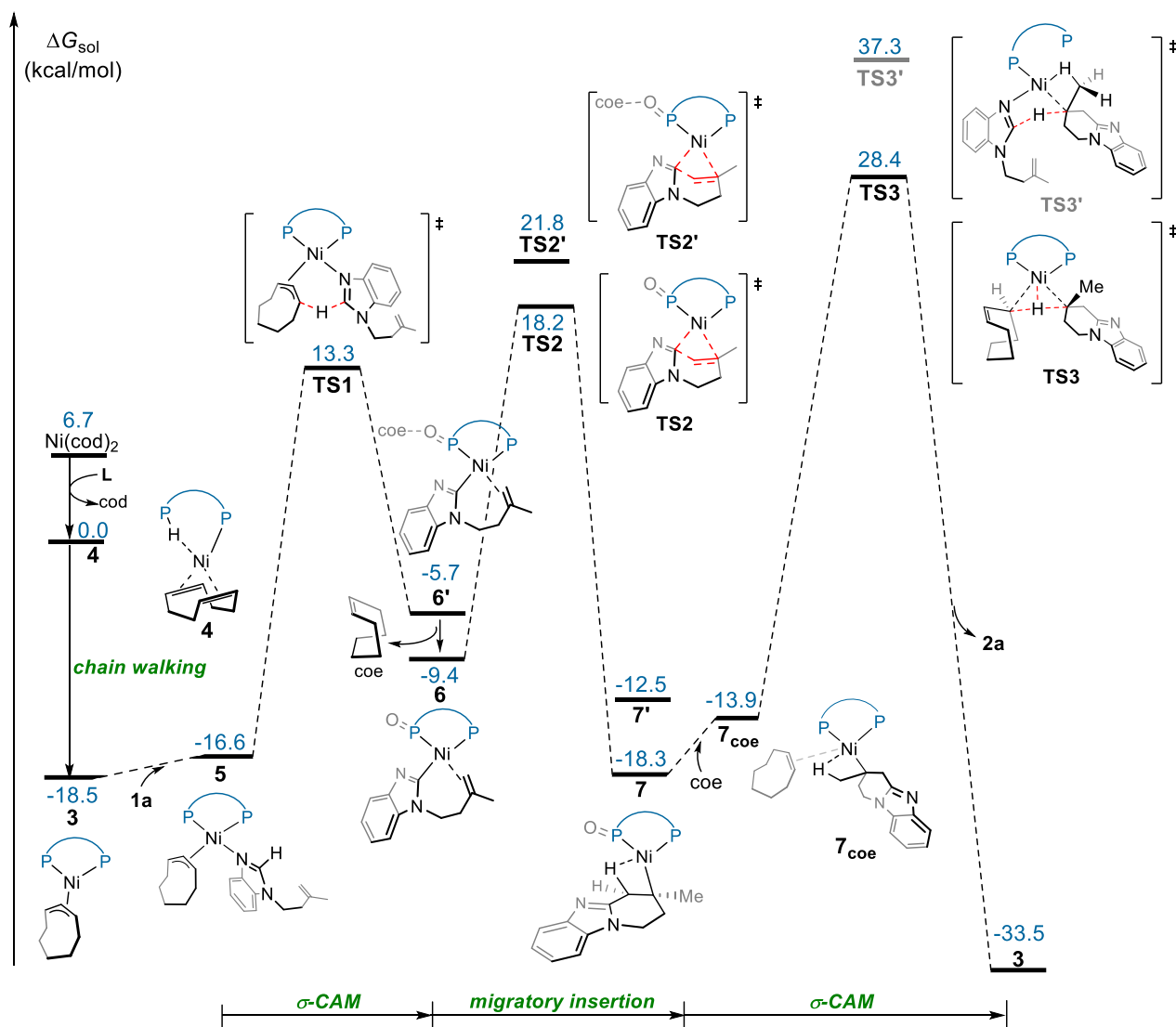


Fig. S4 The complete free energy profile for the nickel(II)-promoted hydroarylation *via* the σ -CAM mechanism.

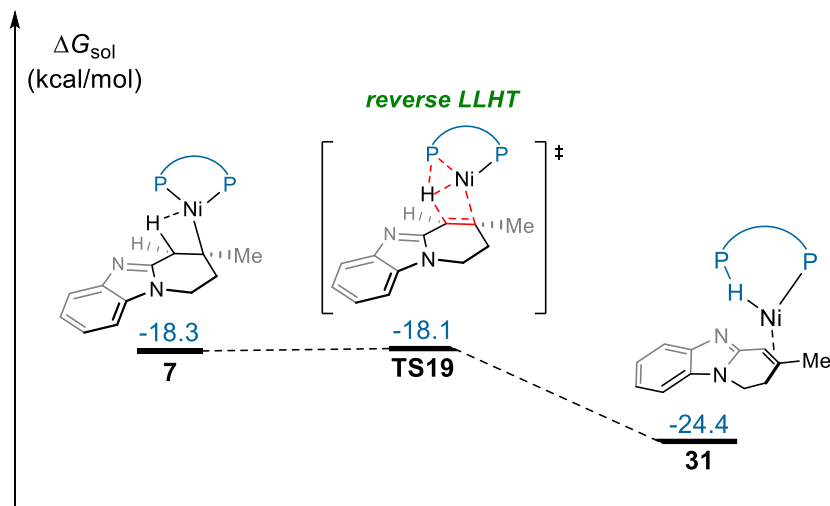


Fig. S5 Free energy profile for the reverse LLHT from 7.

From complex 3, we also considered the σ -complex-assisted metathesis step. As shown in Fig. S6, during this process, the hydrogen transfers from $\text{C}(\text{sp}^2)\text{-H}$ to the P(V) atom of JoSPOphos. However, this process requires a significantly higher barrier (TS20, $\Delta G^\ddagger = 43.7$ kcal/mol relative to 3).

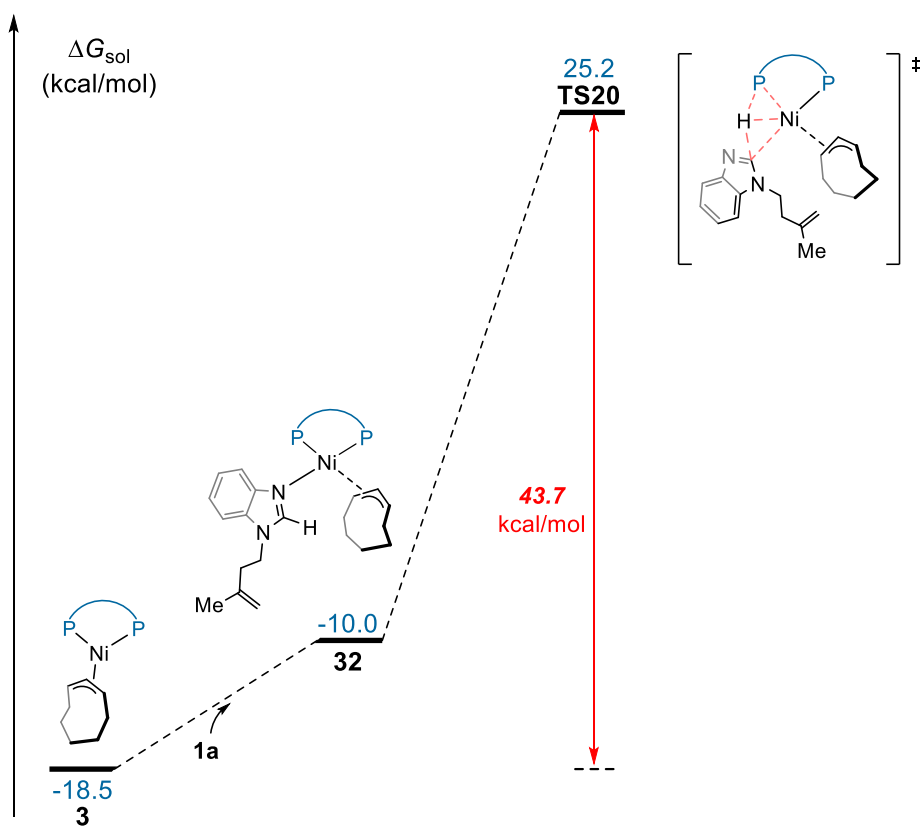


Fig. S6 Free energy profile for the σ -complex-assisted metathesis from complex 3.

4. On the energy difference between various substrate-coordinated complexes.

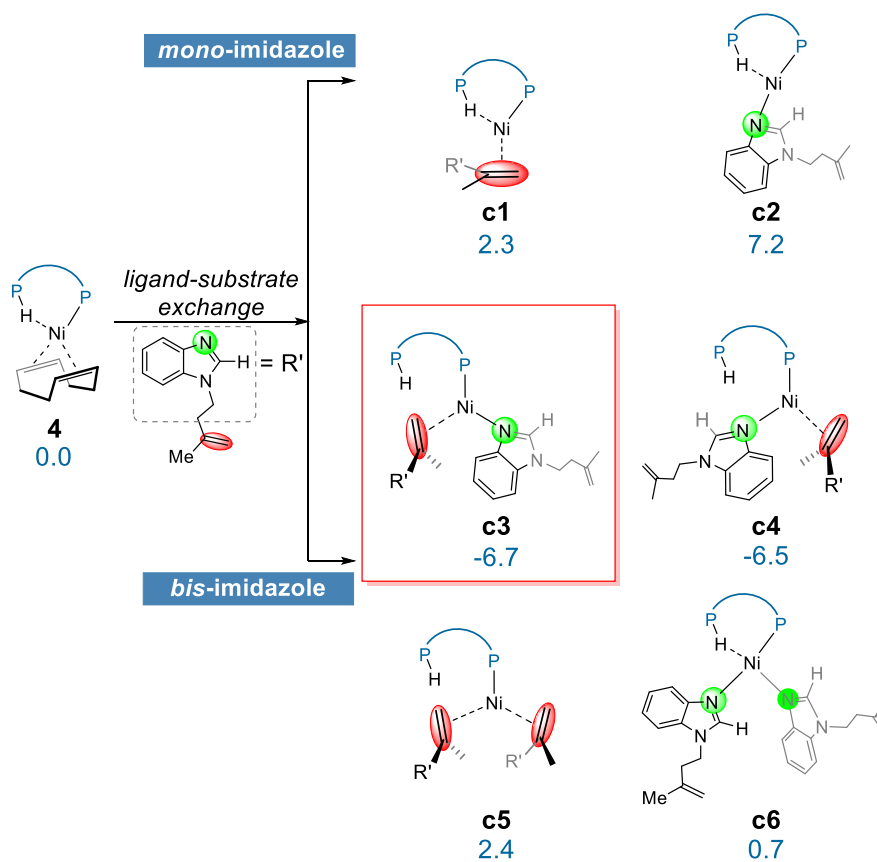
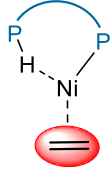
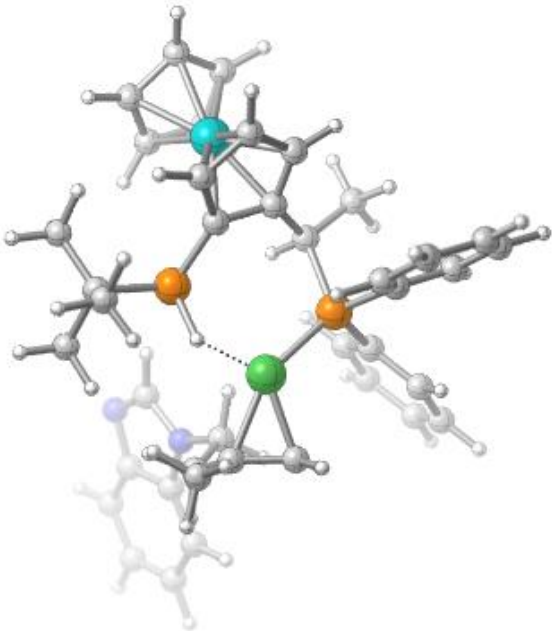
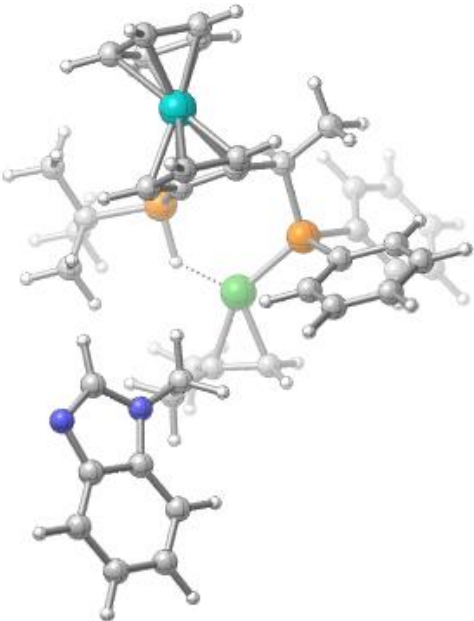
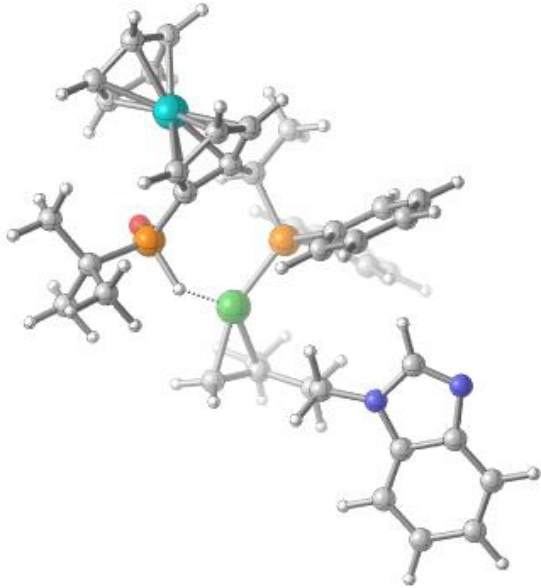
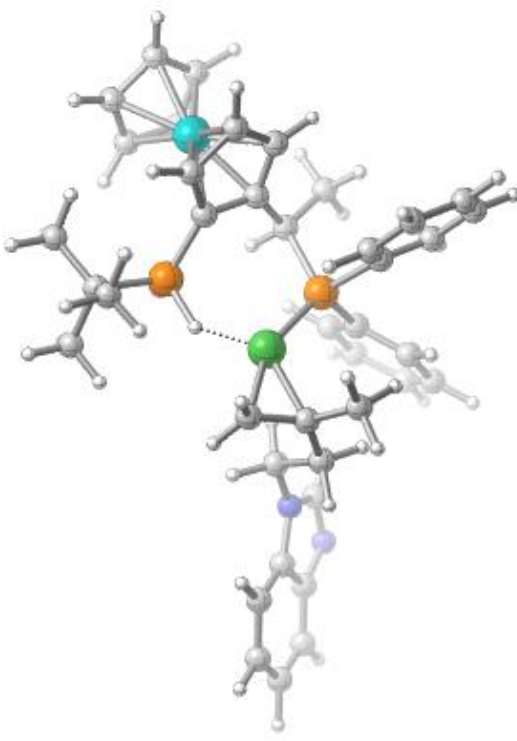
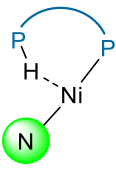
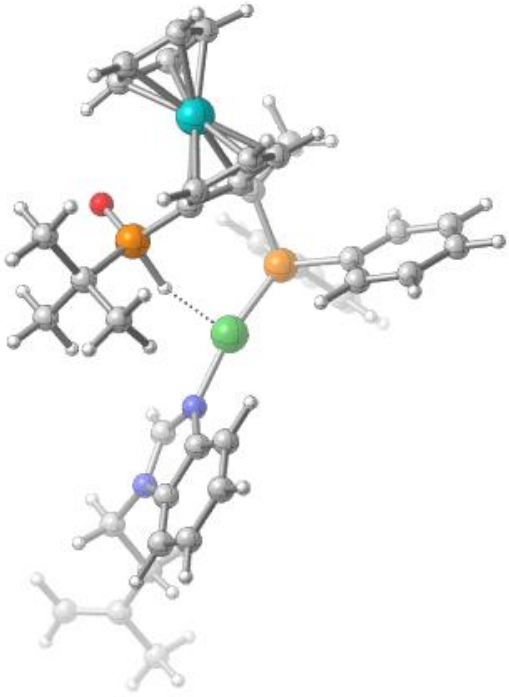
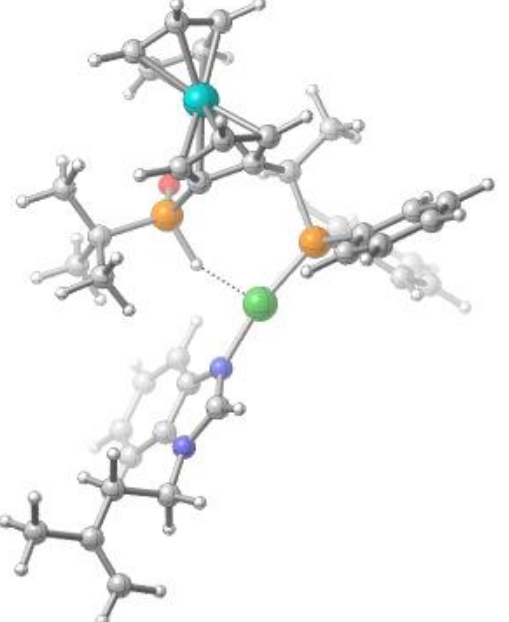
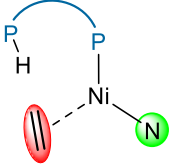


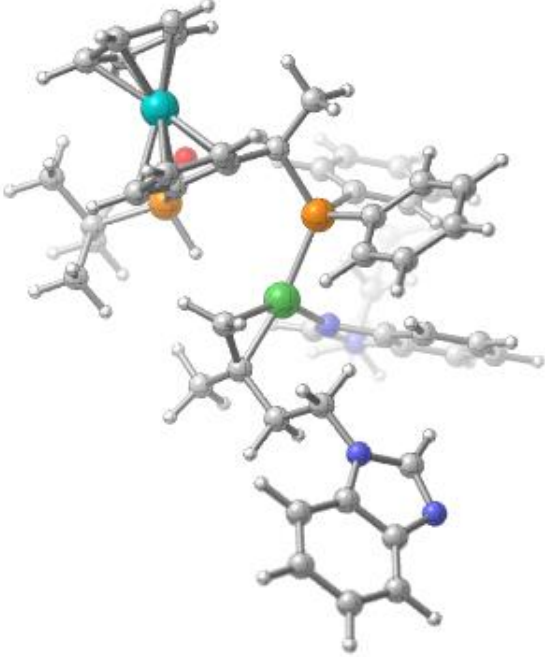
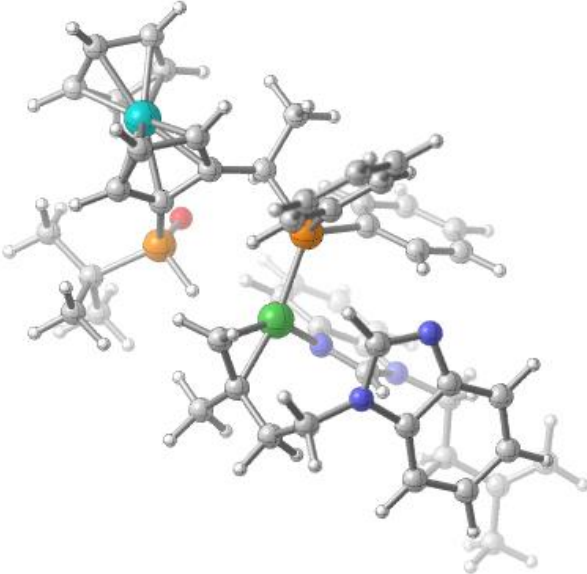
Fig. S7 The possible ligand-substrate exchanges and corresponding substrate-coordinated complexes with energies in kcal/mol.

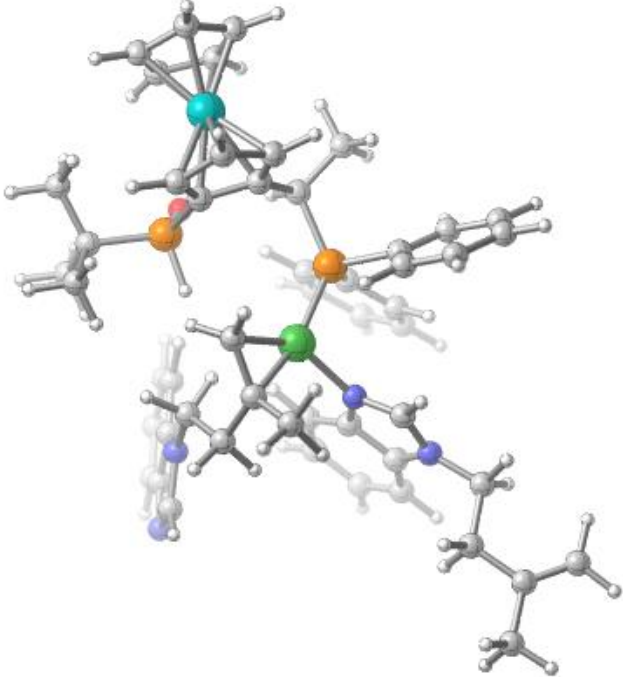
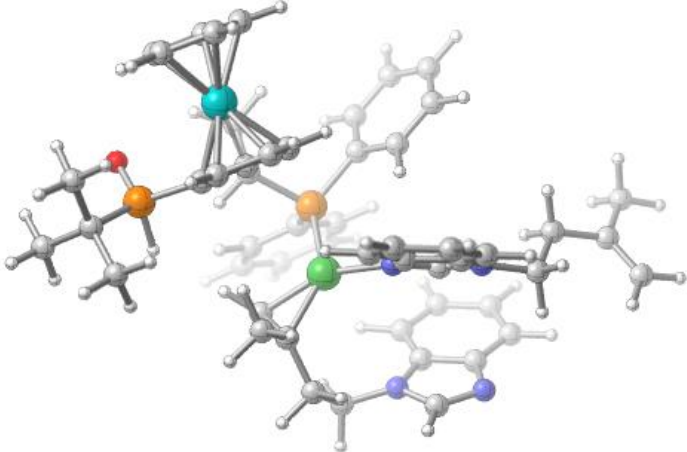
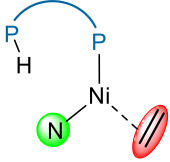
Table S2. Geometries and relative energies of the different substrate-coordinated complexes.

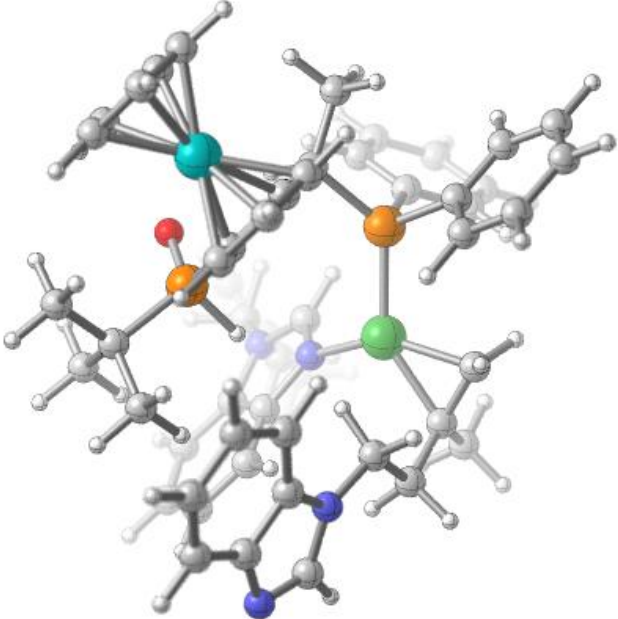
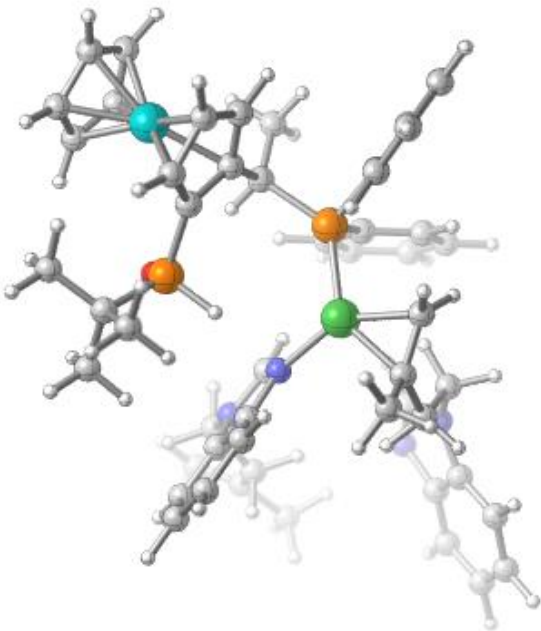
complex	geometry	ΔG_{sol} (kcal/mol)
		
c1		2.3
c1-2		4.2

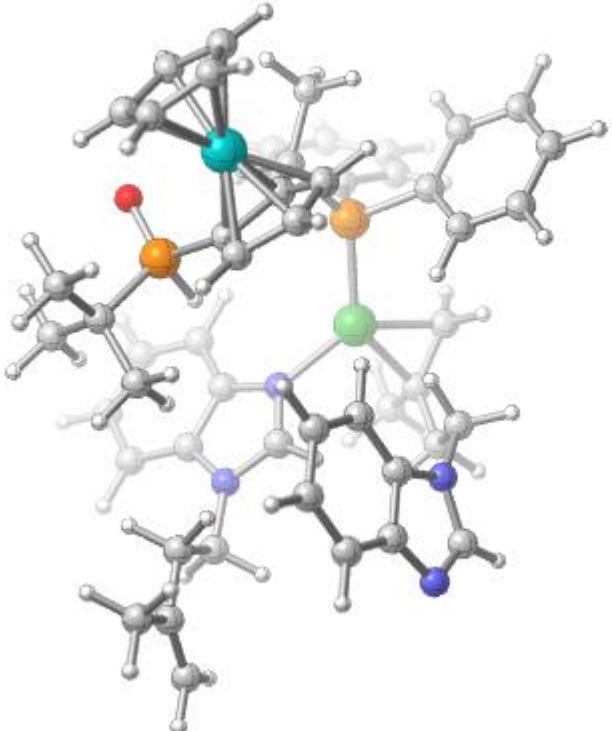
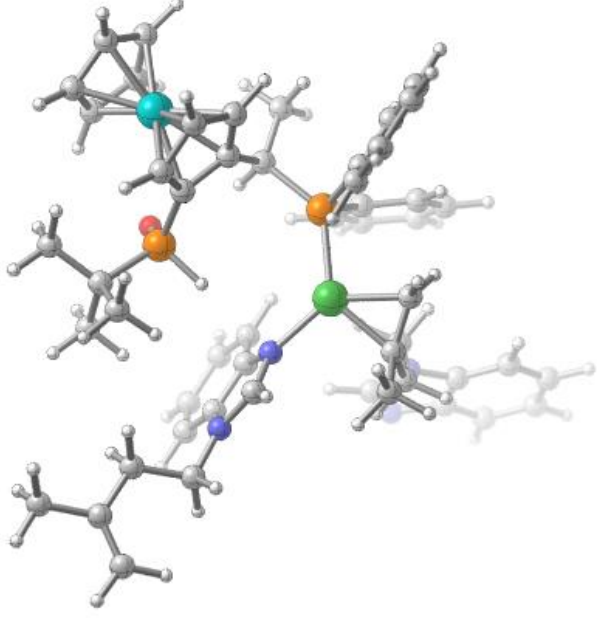
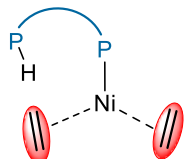
<p>c1-3</p>	 <p>ORTEP diagram showing the displacement of a green nitrogen atom (N) in a nickel complex. The nickel atom (Ni) is coordinated to two phosphorus atoms (P, orange) and a hydrogen atom (H, white). The nitrogen atom (N, green) is shown in two positions, with a displacement of 1.3 Å between them. The displacement is indicated by a dashed line and a curved arrow.</p>	<p>1.3</p>
<p>c1-4</p>	 <p>ORTEP diagram showing the displacement of a green nitrogen atom (N) in a nickel complex. The nickel atom (Ni) is coordinated to two phosphorus atoms (P, orange) and a hydrogen atom (H, white). The nitrogen atom (N, green) is shown in two positions, with a displacement of 0.0 Å between them. The displacement is indicated by a dashed line and a curved arrow.</p>	<p>0.0</p>
	 <p>Schematic diagram showing the nickel atom (Ni) coordinated to two phosphorus atoms (P) and a hydrogen atom (H). A nitrogen atom (N) is also shown, with a curved arrow indicating its displacement.</p>	

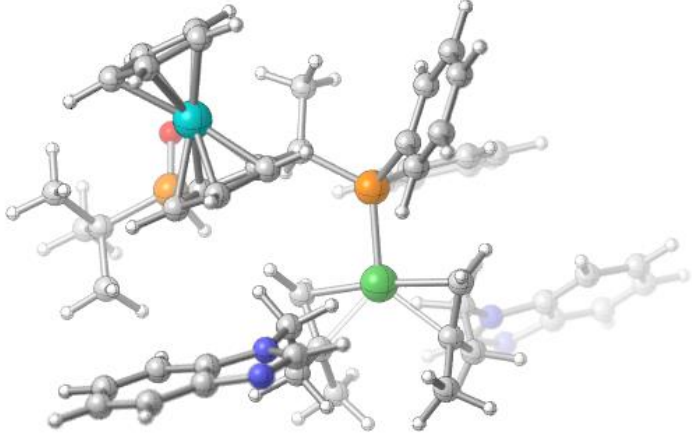
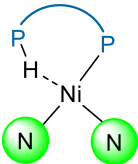
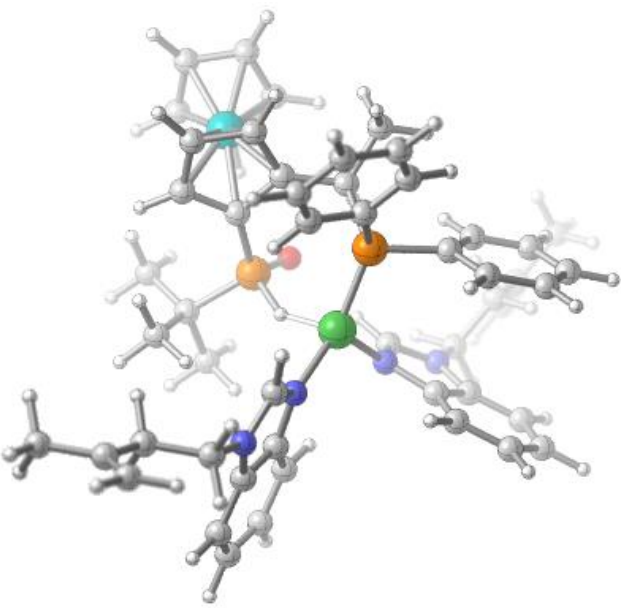
c2		7.2
c2-2		7.7
		

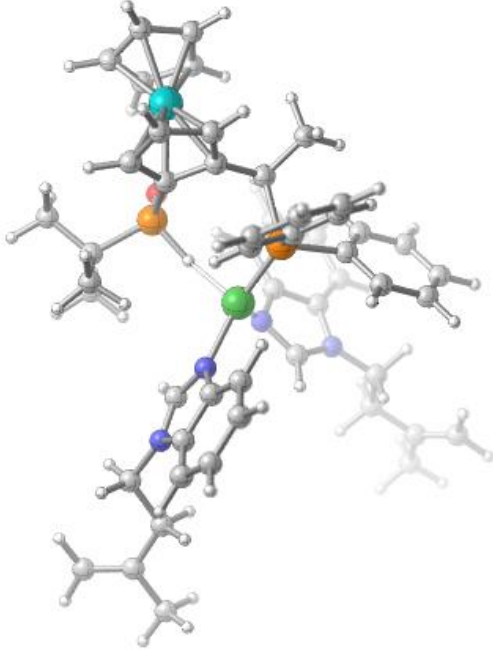
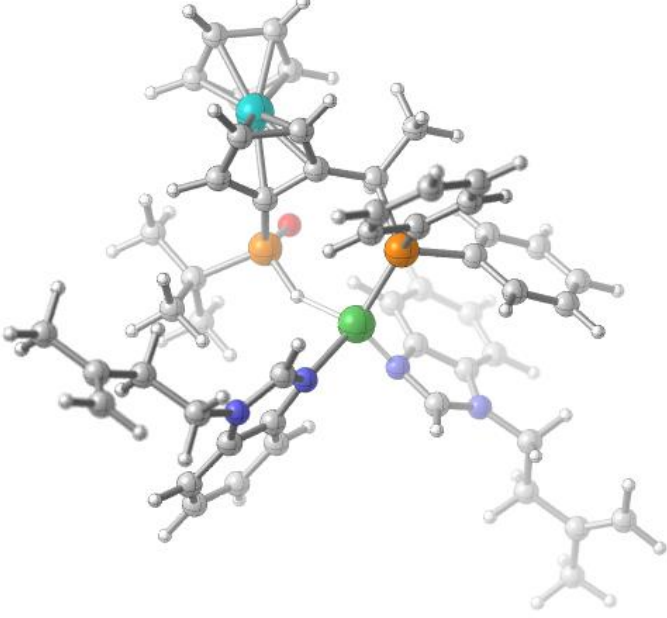
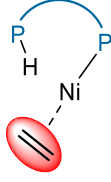
c3	 <p>A 3D ball-and-stick model of a complex organic molecule. The structure features a central core with several substituents. Key atoms are highlighted in different colors: a cyan atom at the top, an orange atom below it, a green atom in the center, and a blue atom at the bottom. The molecule is composed of carbon (grey), hydrogen (white), oxygen (red), and nitrogen (blue) atoms.</p>	-6.7
c3-2	 <p>A 3D ball-and-stick model of a complex organic molecule, similar to the one above. It features a central core with several substituents. Key atoms are highlighted in different colors: a cyan atom at the top, an orange atom below it, a green atom in the center, and a blue atom at the bottom. The molecule is composed of carbon (grey), hydrogen (white), oxygen (red), and nitrogen (blue) atoms.</p>	-6.2

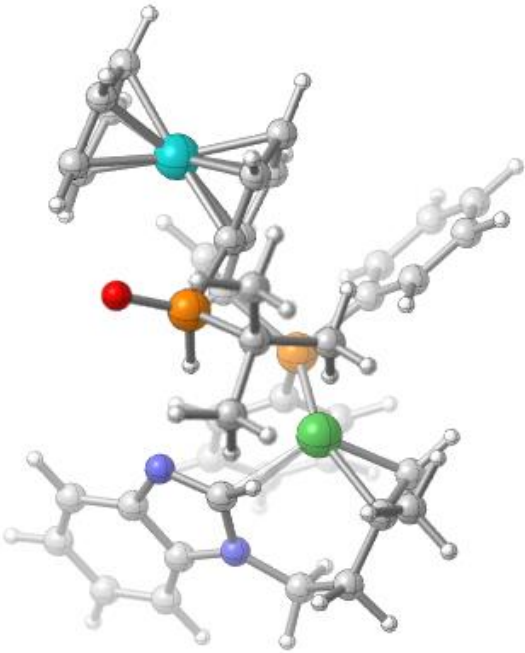
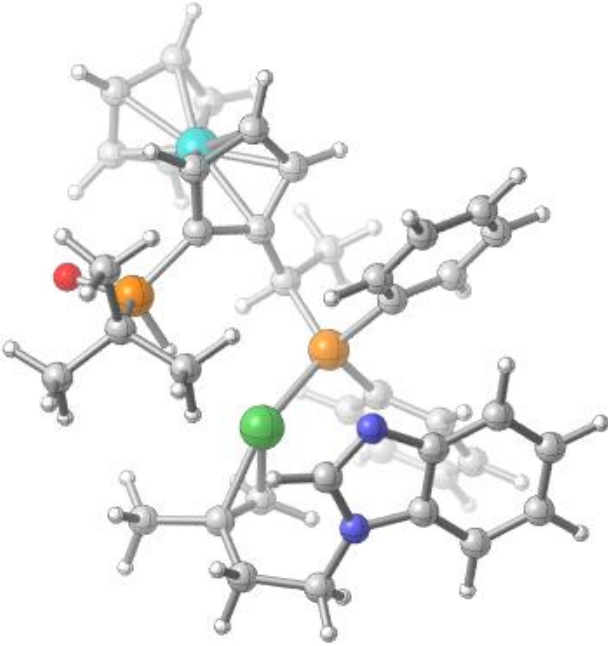
c3-3		-4.8
c3-4		-0.3
		

c4	 A 3D ball-and-stick model of a complex organic molecule. The structure features a central core with several substituents. A cyan atom is highlighted at the top left, an orange atom at the top center, a green atom at the bottom center, and a red atom at the top left. The molecule is shown in a perspective view with semi-transparent grey atoms for the rest of the structure.	-6.5
c4-2	 A 3D ball-and-stick model of a complex organic molecule, similar to the one above. The structure features a central core with several substituents. A cyan atom is highlighted at the top left, an orange atom at the top center, and a green atom at the bottom center. The molecule is shown in a perspective view with semi-transparent grey atoms for the rest of the structure.	-5.0

c4-3		-3.2
c4-4		-1.7
		

<p>c5</p>		<p>2.4</p>
		
<p>c6</p>		<p>0.7</p>

c6-2		4.0
c6-3		2.4
		

<p>c7</p>		<p>8.0</p>
<p>c7-2</p>		<p>9.3</p>

5. Additional result for nickel(0)-promoted hydroarylation *via* the OA mechanism.

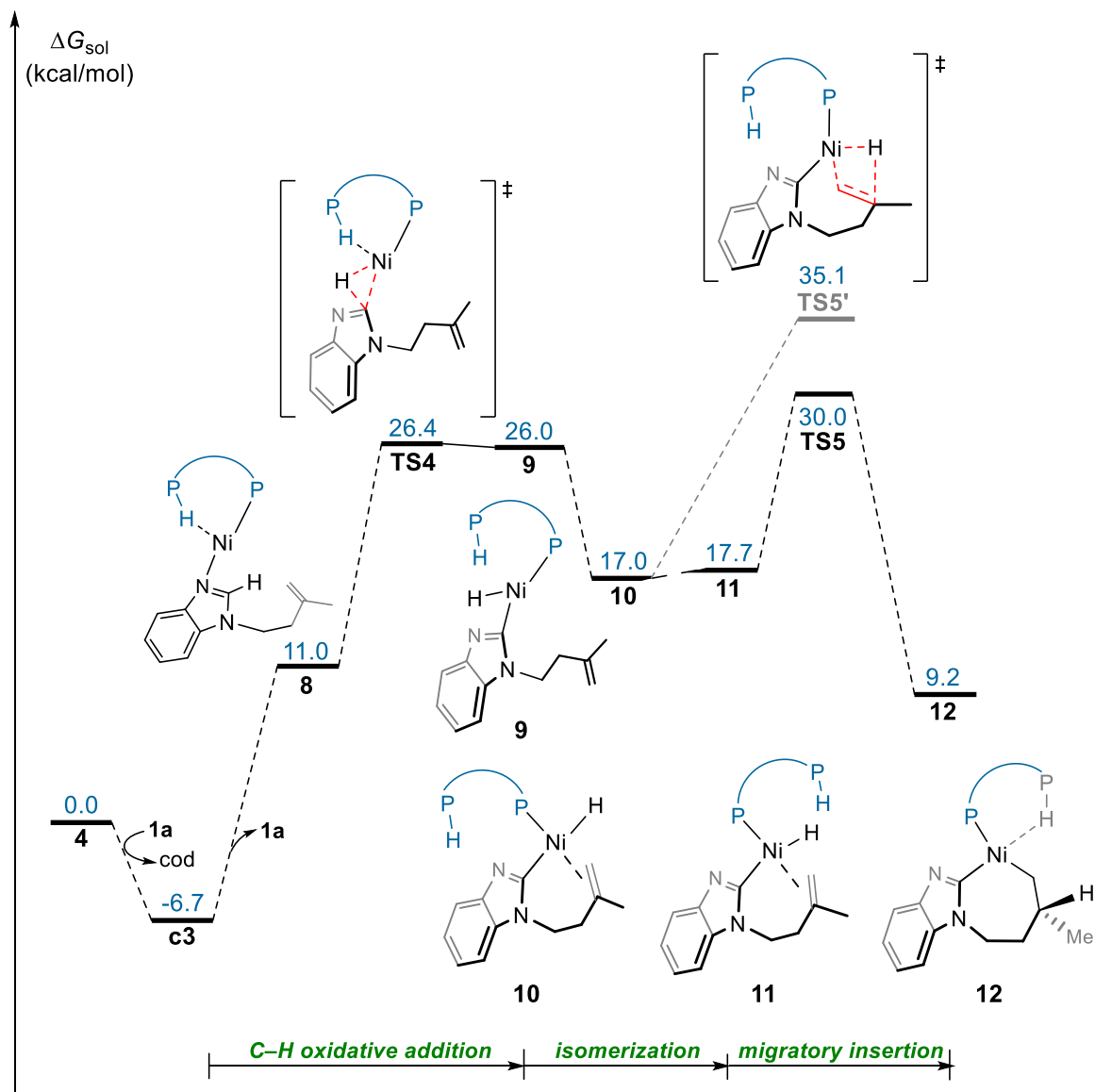


Fig. S8 The alternative migratory insertion from 10 in the OA mechanism.

6. The formation of the (*S*)-product via the LLHT mechanism.

The free energy profile for the formation of the (*S*)-product via the LLHT mechanism is shown in Fig. S9. The LLHT transition state **TS7'** in the formation of the (*S*)-product is 4.1 kcal/mol higher in free energy than its counterpart in the formation of the (*R*)-product. It should be noted that the orientation of the substrate in the formation of the (*S*)-product (Fig. S9) is different from that of the (*R*)-product. Besides **TS7** and **TS7'**, we also located another two possible transition states (see **TS7s** and **TS7s'** in Fig. S10), while they are less stable.

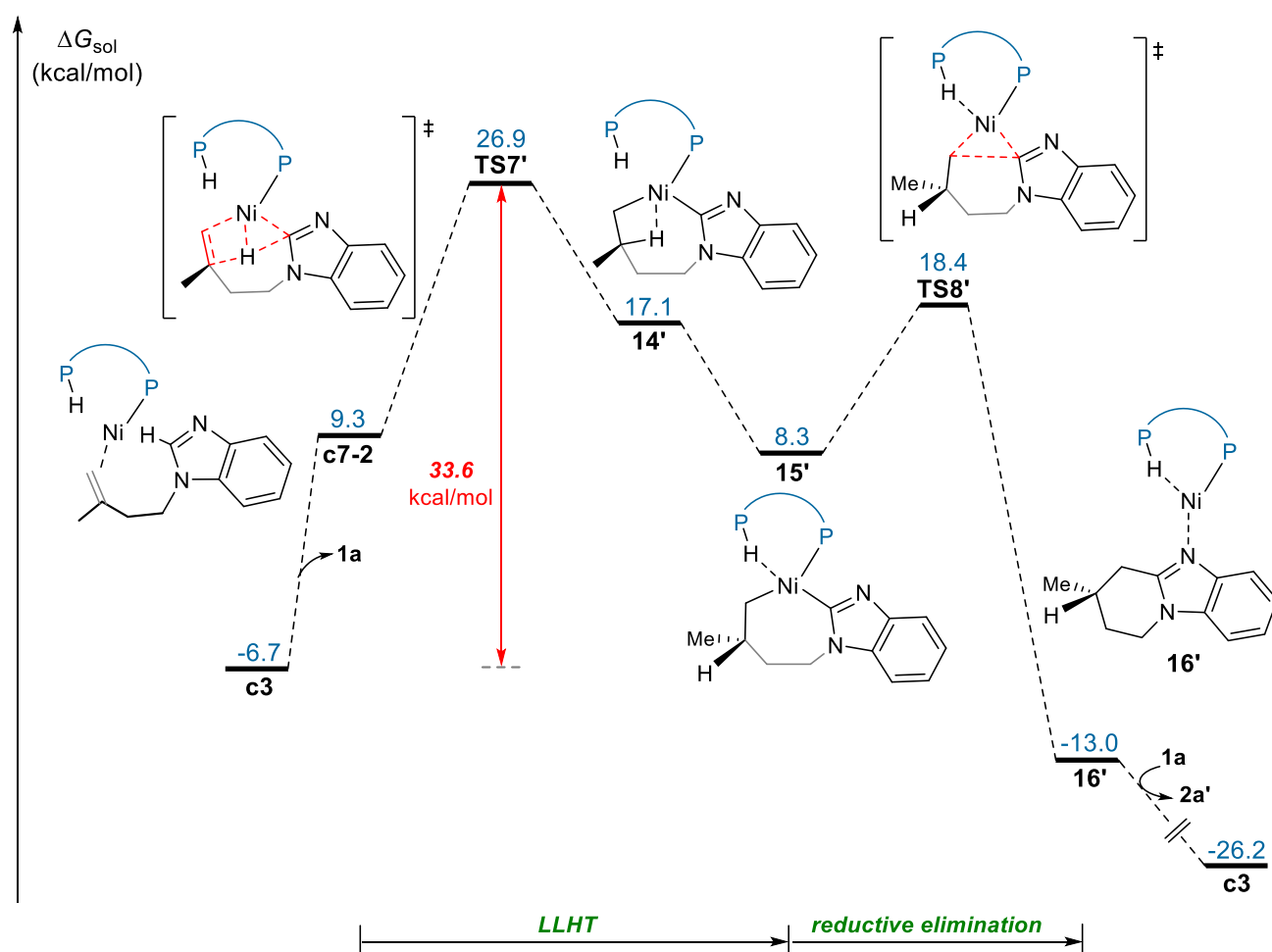


Fig. S9 Free energy profile for the formation of the (*S*)-product via the LLHT mechanism.

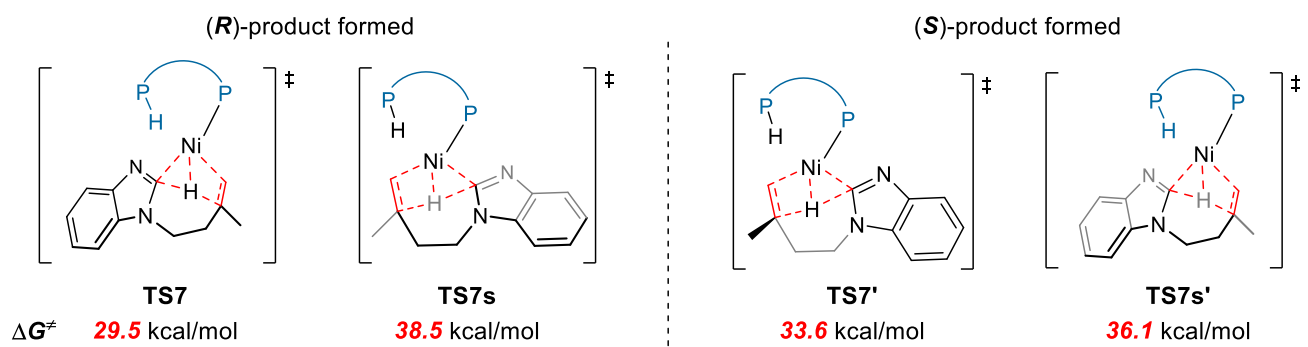


Fig. S10 A comparison of the four possible LLHT transition states.

7. The formation of the (*S*)-product via the new σ -CAM mechanism.

The free energy profile for the formation of the (*S*)-product via the new σ -CAM mechanism is shown in Fig. S11. It should be noted that, different from the results of (*R*)-product, the structure of intermediate **15''** in the σ -CAM mechanism is different from that in the LLHT mechanism (**15'** in Fig. S9) due to the different orientation of the substrate.

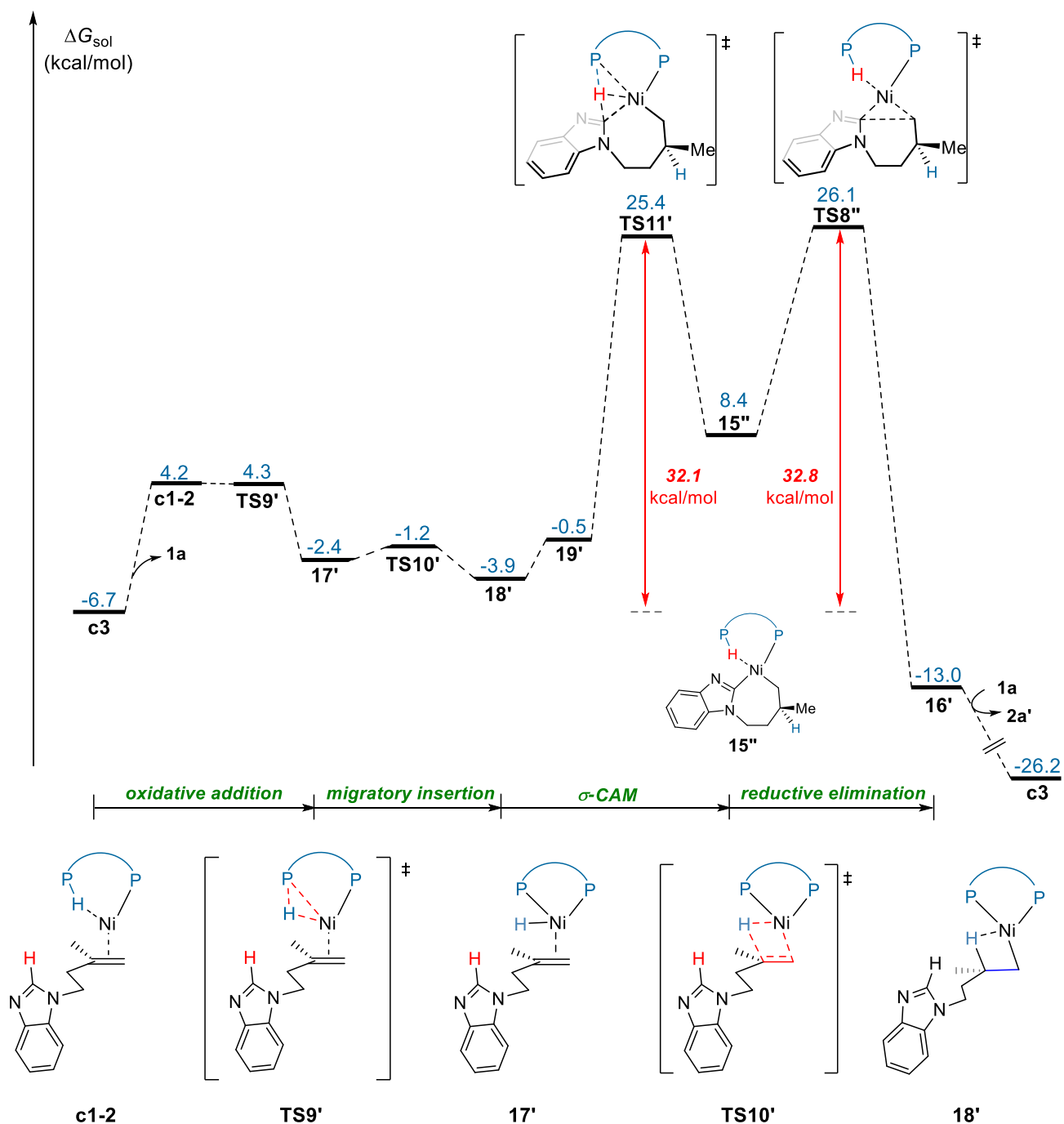


Fig. S11 Free energy profile for the formation of the (*S*)-product via the new σ -CAM mechanism.

8. GC-FID analysis of the solution resulting from nickel-catalyzed cyclization of **1a**.

Catalytic reaction: In a nitrogen filled glove box a vial was loaded with a stir-bar, substrate **1a** (93.1 mg, 0.50 mmol, 1.0 equiv), [Ni(1,5-cod)₂] (6.9 mg, 25 μmol, 5.0 mol %), ligand (6.3 mg, 12.5 μmol, 2.5 mol %) and toluene (1.0 mL). The resulted solution was stirred at 95 °C for 20 h. Subsequently, it was diluted with ethyl acetate (2 mL), passed through a pipette filled with silica, and subjected to a GC-FID analysis.

Stoichiometric reaction between complex **3 and **1a**:** In a nitrogen filled glove box a vial was loaded with a stir-bar, substrate **1a** (9.3 mg, 0.05 mmol), complex **3** (34.3 mg, 0.05 mmol), and toluene (2.0 mL). The resulted solution was stirred at 95 °C for 20 h. Subsequently, it was diluted with ethyl acetate (2 mL), passed through a pipette filled with silica, and subjected to a GC-FID analysis.

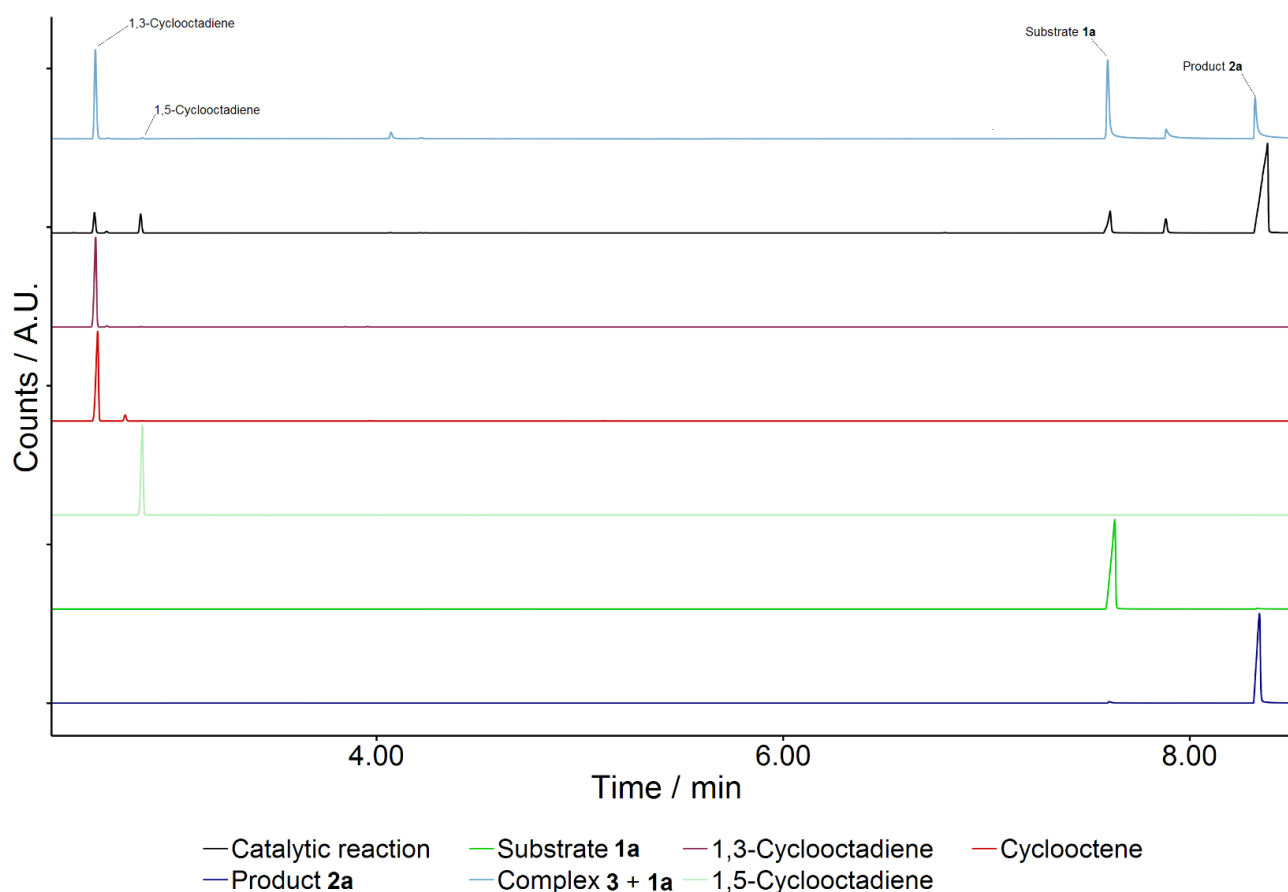


Fig. S12 GC-FID analysis of the solution resulting from the Ni(cod)₂-catalyzed cyclization of **1a** in presence of JoSPOphos (black line, second from top) and the solution resulting from the stoichiometric reaction between complex **3** and **1a** (sky blue line, top) both in toluene at 95 °C and 20 h reaction time

demonstrating formation of 1,3-cyclooctadiene by the end of catalysis. Chromatograms are normalized to the highest peak.

References

- [1] (a) Y. Zhao and D. G. Truhlar, *J. Chem. Phys.*, 2006, **125**, 194101; (b) Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc.*, 2008, **120**, 215–241.

9. Calculated energies and imaginary frequencies.

Table S3. Calculated energies and imaginary frequencies.

Stationary point	Corrected thermal correction to Gibbs free energy at B3LYP-D3(BJ)/6-31G(d,p)/LANL2DZ(Ni) (in a.u.)	Single-point energy including solvation energy at B3LYP-D3(BJ)/def2-TZVP (in a.u.)	Imaginary frequencies (in cm^{-1})
Ni(cod)₂	0.314824	-2132.827871	
L	0.453915	-3108.669612	
L-PA	0.454305	-3108.645063	
cod	0.147348	-312.1919693	
coe	0.170998	-313.4234814	
1a	0.194351	-575.4870022	
2a	0.199475	-575.5159716	
2a'	0.199639	-575.5233913	
2a''	0.175900	-574.2993386	
4	0.623785	-4929.318620	
4'	0.624215	-4929.314150	
4''	0.627193	-4929.331201	
TS0	0.449529	-3108.568539	1628.47 <i>i</i>
TS0'	0.619664	-4929.261917	701.51 <i>i</i>
5	0.846930	-5504.856941	
TS1	0.844207	-5504.806578	1004.65 <i>i</i>
6	0.654990	-5191.404993	
6'	0.845249	-5504.837911	
TS2	0.656777	-5191.362793	352.97 <i>i</i>
TS2'	0.849254	-5504.797983	348.49 <i>i</i>
7	0.656073	-5191.420247	
7'	0.848407	-5504.851849	
7_{coe}	0.852264	-5504.857959	
TS3	0.846094	-5504.784323	1376.40 <i>i</i>

TS3'	0.870911	-5766.835151	961.83 <i>i</i>
8	0.671781	-5192.597182	
TS4	0.667931	-5192.568698	566.22 <i>i</i>
9	0.665679	-5192.567183	
10	0.671813	-5192.587513	
11	0.667879	-5192.582499	
TS5	0.669666	-5192.564758	739.74 <i>i</i>
TS5'	0.670671	-5192.557543	708.51 <i>i</i>
12	0.671125	-5192.599346	
TS6	0.673042	-5192.586104	287.92 <i>i</i>
13	0.674686	-5192.635578	
TS7	0.670717	-5192.577317	549.14 <i>i</i>
14	0.673660	-5192.588879	
15	0.672850	-5192.598428	
TS8	0.671909	-5192.576776	330.61 <i>i</i>
16	0.673440	-5192.638065	
TS7'	0.668926	-5192.568996	799.56 <i>i</i>
14'	0.672643	-5192.588328	
15'	0.673266	-5192.602868	
TS8'	0.672667	-5192.586183	
16'	0.674452	-5192.637975	
TS7s	0.668788	-5192.560905	880.11 <i>i</i>
TS7s'	0.668937	-5192.564880	829.79 <i>i</i>
TS9	0.672143	-5192.611174	20.56 <i>i</i>
17	0.671630	-5192.620712	
TS10	0.671218	-5192.619652	431.53 <i>i</i>
18	0.674727	-5192.626411	
19	0.675170	-5192.604339	
TS11	0.674478	-5192.580442	1101.26 <i>i</i>

TS9'	0.674865	-5192.610952	31.33 <i>i</i>
17'	0.670659	-5192.617292	
TS10'	0.671274	-5192.616085	442.96 <i>i</i>
18'	0.673191	-5192.622212	
19'	0.673831	-5192.617455	
TS11'	0.674577	-5192.577043	1073.79 <i>i</i>
15''	0.673260	-5192.602759	
TS8''	0.673010	-5192.574303	322.35 <i>i</i>
16'	0.674452	-5192.637975	
20	0.624945	-4929.326943	
TS12	0.621488	-4929.321226	442.34 <i>i</i>
21	0.622151	-4929.322294	
TS13	0.620752	-4929.312162	26.69 <i>i</i>
22	0.624645	-4929.319903	
TS14	0.623111	-4929.311275	84.18 <i>i</i>
23	0.624147	-4929.313633	
TS15	0.623730	-4929.312096	555.89 <i>i</i>
24	0.629165	-4929.326137	
25	0.626823	-4929.319914	
TS16	0.622567	-4929.312339	467.34 <i>i</i>
26	0.622766	-4929.313157	
27	0.623812	-4929.310494	
TS17	0.622345	-4929.310054	428.12 <i>i</i>
28	0.625151	-4929.318600	
29	0.625042	-4929.323457	
TS18	0.623053	-4929.316879	589.00 <i>i</i>
30	0.621359	-4929.320634	
TS19	0.650767	-5191.414669	674.51 <i>i</i>
31	0.655803	-5191.429614	

32	0.848868	-5504.848296	
TS20	0.841394	-5504.784763	1103.26 <i>i</i>
c1	0.675172	-5192.614440	
c1-2	0.674840	-5192.610983	
c1-3	0.674510	-5192.615266	
c1-4	0.673101	-5192.615974	
c2	0.666989	-5192.598418	
c2-2	0.669237	-5192.599844	
c3	0.889496	-5768.131671	
c3-2	0.892651	-5768.134080	
c3-3	0.889820	-5768.128958	
c3-4	0.894766	-5768.126736	
c4	0.889389	-5768.131329	
c4-2	0.890695	-5768.130271	
c4-3	0.890782	-5768.127369	
c4-4	0.892152	-5768.126337	
c5	0.895288	-5768.122942	
c6	0.883639	-5768.114053	
c6-2	0.884139	-5768.109338	
c6-3	0.884494	-5768.112265	
c7	0.673661	-5192.603737	
c7-2	0.674388	-5192.602362	

Stationary point	Corrected thermal correction to Gibbs free energy at B3LYP-D3(BJ)/def2-TZVP (in a.u.)	Single-point energy including solvation energy at B3LYP-D3(BJ)/def2-QZVP (in a.u.)	Imaginary frequencies (in cm^{-1})
4	0.622114	-4929.515508	
4'	0.622198	-4929.511146	

Stationary point	Corrected thermal correction to Gibbs free energy at M06/def2-TZVP (in a.u.)	Single-point energy including solvation energy at M06/def2-QZVP (in a.u.)	Imaginary frequencies (in cm^{-1})
4	0.620923	-4927.961966	
4'	0.618402	-4927.953576	

10. Cartesian coordinates of all optimized structures.

Ni(cod)₂

H	-3.12168500	2.40203300	-0.33179100
C	-2.21864600	1.83388300	-0.60655100
H	-0.75464300	2.36531000	0.95311300
H	-3.52953200	-0.13819300	0.99721100
C	-1.37605400	1.53912000	0.61467100
H	-1.63482100	2.49576400	-1.25707100
C	-1.52305500	0.47265300	1.48017700
H	-2.87829400	-0.88640600	2.43204600
C	-2.61930600	-0.57885300	1.41273600
H	-0.98320600	0.52908700	2.42122000
H	-3.52903800	0.13795600	-0.99831900
C	-2.61853900	0.57880600	-1.41306900
H	-2.87683700	0.88655900	-2.43249200
C	-2.21859500	-1.83397800	0.60670400
Ni	-0.00003400	-0.00042700	-0.00074500
H	-3.12134300	-2.40242400	0.33157900
C	-1.52203300	-0.47258900	-1.47992400
C	-1.37535300	-1.53913500	-0.61406400
H	-1.63496200	-2.49556700	1.25771300
H	-0.98283800	-0.52989800	-2.42129900
H	-0.75470200	-2.36582800	-0.95274300
H	3.12084300	2.40272100	0.33224700
C	2.21805200	1.83418800	0.60703900
H	0.75428400	2.36556200	-0.95276400
H	3.52950300	-0.13738200	-0.99735000
C	1.37536900	1.53921400	-0.61407000
H	1.63408500	2.49575200	1.25776800
C	1.52263200	0.47279000	-1.47984400
H	2.87811400	-0.88599300	-2.43189500
C	2.61929000	-0.57838400	-1.41256200
H	0.98342900	0.52971700	-2.42123400
H	3.52908700	0.13863700	0.99823800
C	2.61857300	0.57914900	1.41330300
H	2.87702600	0.88680200	2.43271800
C	2.21925800	-1.83359300	-0.60631600
H	3.12229000	-2.40158500	-0.33120300
C	1.52247700	-0.47257400	1.48025600
C	1.37605600	-1.53905300	0.61454900
H	1.63583800	-2.49552500	-1.25714800
H	0.98258100	-0.52943800	2.42124700
H	0.75499100	-2.36557200	0.95284900

L

Fe	2.18927200	-1.22065900	-0.81673900
P	1.58479200	1.71945000	0.77158000
P	-1.98590800	0.54606600	0.62708200
O	1.45692300	2.39531600	-0.57417300
C	1.41316100	-0.07695000	0.69711700
C	0.34483300	-0.71124900	-0.04589100
C	0.52989300	-2.12143700	0.06043900
H	-0.08653200	-2.87053500	-0.41354800
C	1.69433900	-2.37263500	0.84122900
H	2.11794800	-3.34380500	1.05643400
C	2.24094400	-1.12100700	1.23854800
H	3.14338700	-0.98933000	1.81456900
C	-0.78138300	-0.00079200	-0.74156200
H	-0.37716700	0.93802700	-1.13176700
C	-1.40464700	-0.80922100	-1.87832200
H	-1.82754500	-1.75114900	-1.52109300
H	-0.64778000	-1.04455200	-2.63286800
H	-2.20603300	-0.24656600	-2.36262700
C	3.27528600	0.02960300	-2.05703800
H	3.35368700	1.09032100	-1.87194100
C	2.22196100	-0.59633100	-2.78597500
H	1.40096300	-0.08424100	-3.26680100
C	2.41259500	-2.01008400	-2.71581800
H	1.75862800	-2.76210900	-3.13513300
C	3.58616600	-2.25770800	-1.94142000
H	3.97798200	-3.22992000	-1.67596200
C	4.11933500	-0.99629000	-1.53397300
H	4.98799900	-0.84765300	-0.90827800
C	-2.74138400	-1.07580800	1.07056000
C	-2.20442900	-1.73040600	2.19035800
H	-1.42850200	-1.24074900	2.77212500
C	-2.65169600	-2.99953100	2.56044100
H	-2.22159500	-3.49223600	3.42760300
C	-3.65624100	-3.62743700	1.82333200
H	-4.01200300	-4.61172500	2.11370700
C	-4.20772000	-2.98237100	0.71375500
H	-4.99137500	-3.46572100	0.13716900
C	-3.75115000	-1.71952700	0.33680400
H	-4.18408400	-1.23003700	-0.52866700
C	-3.30508800	1.41027200	-0.32229600
C	-2.97710700	2.23898600	-1.40862000
H	-1.95089800	2.30525400	-1.75583700

C	-3.95757100	2.99547500	-2.05095600
H	-3.68242200	3.62360200	-2.89340300
C	-5.28250600	2.94807700	-1.61550400
H	-6.04525200	3.53578600	-2.11757200
C	-5.61752900	2.14539100	-0.52366700
H	-6.64386800	2.10735500	-0.16957600
C	-4.63878000	1.38893300	0.12018900
H	-4.91567000	0.77283600	0.97004500
C	3.09083900	2.19761900	1.74217800
C	4.37249000	1.70862800	1.05154900
H	4.42736800	0.61955100	1.00094400
H	5.24660400	2.06613200	1.60812400
H	4.44429200	2.09867200	0.03234600
C	2.98293600	1.66527200	3.17976200
H	2.05398100	1.99223200	3.65925600
H	3.81577300	2.05422400	3.77683500
H	3.01949000	0.57520900	3.22969200
C	3.07741600	3.73873700	1.76523100
H	3.12143500	4.15153100	0.75435300
H	3.94422100	4.10276800	2.32841200
H	2.17553300	4.12663200	2.25173200
H	0.56194100	2.09280100	1.67769200

L-PA

Fe	2.17813900	-1.27586500	-0.73700000
P	1.50543600	1.82724600	0.88748100
P	-2.01648700	0.55677200	0.66509000
O	1.74446500	2.27086600	-0.73478800
C	1.44470200	0.01105400	0.70997900
C	0.35619800	-0.65380400	0.02479800
C	0.50991100	-2.06028800	0.21401100
H	-0.12776000	-2.82430600	-0.20520700
C	1.67364700	-2.28495300	1.00229100
H	2.07858300	-3.24848000	1.27970500
C	2.24907900	-1.01950200	1.30877400
H	3.15668800	-0.87473800	1.87264900
C	-0.78218300	0.02350600	-0.68450500
H	-0.40323100	0.96504500	-1.09195100
C	-1.38357600	-0.81020400	-1.81665700
H	-1.76976000	-1.76384700	-1.45045200
H	-0.62462700	-1.02428400	-2.57463000
H	-2.20999000	-0.28243400	-2.29856600
C	3.31927700	-0.18630800	-2.08248100
H	3.45917700	0.87866100	-1.98437200

C	2.22886000	-0.81421000	-2.75274000
H	1.43418900	-0.30324800	-3.27689400
C	2.34668000	-2.22567300	-2.56780700
H	1.65305200	-2.97500600	-2.92366400
C	3.51198200	-2.46903000	-1.77954500
H	3.85423000	-3.43473800	-1.43342100
C	4.11217200	-1.20799400	-1.47906900
H	4.99223200	-1.05274200	-0.87109300
C	-2.82069700	-1.06053500	1.04178500
C	-2.32175100	-1.76477400	2.14911300
H	-1.53703900	-1.31914900	2.75385800
C	-2.81953500	-3.02657600	2.47755000
H	-2.41905600	-3.55845700	3.33572800
C	-3.83705900	-3.59621700	1.71133900
H	-4.23235100	-4.57432100	1.96981000
C	-4.35139200	-2.90033100	0.61463500
H	-5.14536600	-3.33822900	0.01619700
C	-3.84469200	-1.64499200	0.27925300
H	-4.24839200	-1.11462100	-0.57625500
C	-3.30712700	1.44852400	-0.30305600
C	-2.99013600	2.20148600	-1.44513900
H	-1.98196300	2.18749900	-1.84646100
C	-3.95828400	2.97663700	-2.08554000
H	-3.69025500	3.54428600	-2.97224000
C	-5.26288900	3.02052400	-1.59427700
H	-6.01682200	3.62132500	-2.09406500
C	-5.58938600	2.28895500	-0.45026900
H	-6.60046500	2.31979400	-0.05416900
C	-4.62193000	1.51771700	0.19130600
H	-4.89172500	0.95757300	1.08167900
C	3.19546900	2.23441500	1.62077100
C	4.38818600	1.63020100	0.87128800
H	4.37817500	0.53996100	0.87832300
H	5.32596900	1.96387000	1.33432100
H	4.39759700	1.95927200	-0.17107900
C	3.18356800	1.81672800	3.10127100
H	2.32130400	2.24038100	3.62822400
H	4.08932800	2.18506800	3.59827900
H	3.15199500	0.73273200	3.23256400
C	3.28884700	3.77140700	1.54258200
H	3.27882900	4.11804400	0.50440700
H	4.22638300	4.11061100	1.99903300
H	2.46242800	4.25594700	2.07399800
H	1.20941100	3.05926400	-0.90049500

cod

H	-2.71093100	0.33352000	0.69415700
C	-1.92068100	0.01341600	-0.00215600
H	-1.78810300	1.82837200	-1.20445200
H	0.64538400	0.71796300	1.59779500
C	-1.19593500	1.23389700	-0.50782600
H	-2.45526200	-0.42831200	-0.85447800
C	0.03270600	1.68818100	-0.23597800
H	1.77378900	1.88904900	0.97115000
C	1.08370700	1.09227800	0.67117600
H	0.34007900	2.59562300	-0.75533700
H	-0.64533800	-0.71796200	1.59783200
C	-1.08368800	-1.09227400	0.67122300
H	-1.77376500	-1.88904100	0.97121800
C	1.92068100	-0.01340900	-0.00223100
H	2.71096900	-0.33350000	0.69404300
C	-0.03271100	-1.68818600	-0.23595500
C	1.19592000	-1.23390200	-0.50785000
H	2.45521400	0.42831500	-0.85458600
H	-0.34009300	-2.59564200	-0.75528200
H	1.78806800	-1.82839300	-1.20447800

coe

C	-0.38752500	1.74987100	-0.08196900
H	-0.83643800	2.67243700	-0.44880500
C	0.88118000	1.52347400	-0.44683100
H	1.34987500	2.29360200	-1.06164600
C	1.81411800	0.37358400	-0.14987900
H	2.17552600	-0.02334000	-1.11154100
C	1.32160000	-0.79259600	0.71843400
H	0.89295500	-0.40188900	1.64423700
H	2.20227300	-1.36848500	1.02892600
C	0.35238100	-1.77354400	0.02858900
H	0.94249400	-2.40801800	-0.64624800
H	-0.06254000	-2.44871900	0.78923000
C	-0.79319100	-1.17430100	-0.80083600
H	-0.37273700	-0.55115900	-1.59782900
H	-1.30845900	-2.00052600	-1.30738200
C	-1.84472100	-0.36028700	-0.03925200
H	-2.37298400	-1.00947400	0.67171500
H	-2.59690000	-0.01863900	-0.76187300
C	-1.30390500	0.86624700	0.73267500
H	-2.15906800	1.46167500	1.07119700

H	-0.80414900	0.52584700	1.64178400
H	2.71052700	0.80199900	0.32264900

1a

C	-1.08261400	-0.03876100	0.40952600
C	-1.82115100	0.89040000	-0.36630700
C	-3.09361700	0.54930200	-0.84011100
C	-3.59308900	-0.70982400	-0.52456500
C	-2.84763700	-1.62151800	0.24956100
C	-1.58086100	-1.30348400	0.73241400
C	0.03457700	1.84324500	0.11234300
H	-3.66321900	1.25588600	-1.43493900
H	-4.57733100	-0.99996900	-0.87911600
H	-3.27179800	-2.59445900	0.47787500
H	-1.01798000	-2.00895000	1.33489900
H	0.85055200	2.54796300	0.19382900
N	0.11455900	0.60022000	0.69539300
N	-1.08945900	2.06010700	-0.53041800
C	1.21015700	0.07871600	1.50937400
H	1.20432100	0.57994200	2.48336500
H	1.00357700	-0.97779400	1.68990900
C	2.58658900	0.23942500	0.86537000
H	2.78591100	1.30366400	0.68056400
H	3.33136800	-0.05403100	1.61866200
C	4.19783900	-0.24764400	-1.02753800
H	4.36773400	-0.85223800	-1.92194400
H	4.27936100	0.80988400	-1.31050200
H	5.01407800	-0.44481000	-0.32036500
C	2.85621000	-0.53627100	-0.40535900
C	2.00481100	-1.41231100	-0.94546400
H	2.26318800	-1.94928600	-1.85379100
H	1.02725700	-1.62573200	-0.52873400

2a

H	-3.04478200	-0.61043800	1.49987200
C	-2.91265200	-0.19665900	0.49474900
C	-4.29113500	-0.10348800	-0.16488600
C	-2.25493500	1.20386400	0.66121700
C	-2.01737100	-1.19540300	-0.29850200
H	-4.73747100	-1.09551200	-0.29439400
H	-4.97887500	0.49741800	0.43907300
H	-4.22181300	0.36066800	-1.15628900
C	-1.13687100	1.48521000	-0.34925700
H	-1.81527100	1.28557100	1.66042800

H	-3.01491000	1.98801200	0.58111800
C	-0.56049800	-0.91036100	-0.16509700
H	-2.27869300	-1.12141000	-1.36414600
H	-2.21695700	-2.22590400	0.00132100
N	-0.16574300	0.40514300	-0.26310200
H	-0.63384400	2.42796600	-0.12440500
H	-1.52791700	1.55092800	-1.37218500
N	0.44342300	-1.74486900	0.00556200
C	1.21242500	0.42713500	-0.14007800
C	1.57650800	-0.93661700	0.02471300
C	2.15176200	1.45825900	-0.15274100
C	2.92461000	-1.27749300	0.18166100
C	3.48719000	1.09334100	0.00696600
H	1.86241400	2.49597600	-0.28537800
C	3.86735600	-0.25289200	0.17080100
H	3.21500900	-2.31552500	0.30822300
H	4.25163200	1.86436400	0.00192700
H	4.91939200	-0.49339800	0.29032400

2a'

C	1.23844900	0.42685400	0.00893200
C	1.58554100	-0.94801000	0.02155400
C	2.93394600	-1.32116300	-0.00011400
C	3.89297100	-0.31209800	-0.03810300
C	3.52914600	1.04826800	-0.05571100
C	2.19260500	1.44353500	-0.03422000
C	-0.56324200	-0.87111300	0.05931300
H	3.21291300	-2.36991200	0.01110900
H	4.94591400	-0.57668900	-0.05574700
H	4.30626700	1.80579900	-0.08781800
H	1.91373500	2.49223100	-0.05129800
N	-0.14584900	0.44541100	0.04506200
N	0.43615800	-1.72867300	0.05105800
C	-1.00716300	1.61868800	-0.05061400
H	-0.61165800	2.39635200	0.61007200
H	-0.96878600	2.00425600	-1.07750700
C	-2.44240200	1.25639000	0.32935600
H	-2.51509200	1.12751200	1.41698400
H	-3.09508400	2.09283900	0.05930500
C	-4.38207000	-0.32307100	-0.10135800
H	-4.69473400	-1.25537700	-0.58336500
H	-4.57903400	-0.42103000	0.97281600
H	-5.01603300	0.48262200	-0.48595800
C	-2.90407000	-0.03586400	-0.36101300

C	-2.02140800	-1.20310300	0.11557900
H	-2.20052900	-2.10768800	-0.47272600
H	-2.28814800	-1.45054200	1.15306900
H	-2.75570800	0.08660100	-1.44338100

2a''

C	-1.18690700	0.43146800	-0.01690300
C	-1.52717400	-0.94887400	0.01518500
C	-2.87387200	-1.32808400	0.06187100
C	-3.83893200	-0.32466300	0.06450700
C	-3.48293400	1.03746800	0.02354100
C	-2.14926900	1.44098300	-0.01823200
C	0.61895200	-0.86288100	-0.05485200
H	-3.14538900	-2.37836900	0.09049400
H	-4.89011100	-0.59437700	0.09749100
H	-4.26482100	1.79075300	0.02392500
H	-1.87838700	2.49134600	-0.05200300
N	0.19455100	0.45368800	-0.03560600
N	-0.37969400	-1.72823300	-0.01230000
C	1.09662600	1.56904900	-0.28286200
H	1.17668300	1.73421400	-1.36546700
H	0.67573000	2.47238200	0.16480000
C	2.47401200	1.26050200	0.31219000
H	3.19619000	1.98547500	-0.07712600
H	2.44712100	1.40517400	1.40182700
C	4.42136800	-0.39333700	0.01832700
H	4.66051900	-1.45232500	-0.10757700
H	4.90098500	0.16864600	-0.79359800
H	4.88255200	-0.04437800	0.95183100
C	2.94311200	-0.15374700	0.03415600
C	2.03865600	-1.14144600	-0.11382600
H	2.33309500	-2.17535100	-0.25786400

4

Ni	-1.48319600	1.22641200	0.17834400
Fe	3.44456700	-0.96505200	-0.25018900
P	1.24203100	1.64916500	-0.32077200
P	-1.28021900	-0.92139900	-0.07298800
O	1.17750300	1.58606000	-1.82848400
C	1.87637000	0.15402400	0.45840300
C	1.42627100	-1.17233300	0.09431800
C	2.14408000	-2.10123000	0.90558700
H	2.05496900	-3.17576000	0.85415600
C	3.03607200	-1.38240700	1.74865300

H	3.74658700	-1.81522700	2.43901900
C	2.87701800	0.00395300	1.48053900
H	3.43977000	0.79553200	1.94828800
C	0.33694700	-1.50642800	-0.88282600
H	0.43824000	-0.84684600	-1.74959100
C	0.36145100	-2.96924600	-1.32375000
H	0.21277900	-3.64768500	-0.48001800
H	1.32815800	-3.20918600	-1.77844700
H	-0.41971700	-3.17389200	-2.05810700
C	4.14257300	-0.05807800	-1.96988400
H	3.67031900	0.82125500	-2.38300500
C	3.75438100	-1.40283000	-2.24386600
H	2.96764200	-1.70553700	-2.92015200
C	4.54203900	-2.26856200	-1.42534300
H	4.45860600	-3.34543000	-1.37380000
C	5.41959300	-1.45722100	-0.64452400
H	6.11702700	-1.81240600	0.10156800
C	5.17328500	-0.09112800	-0.98184300
H	5.65283700	0.76846200	-0.53580000
C	-1.27937200	-1.92874800	1.46962000
C	-0.89061700	-1.26909700	2.64470200
H	-0.68179800	-0.20386200	2.59626100
C	-0.76619400	-1.96560400	3.84692000
H	-0.45928100	-1.44077700	4.74704500
C	-1.04264500	-3.33304800	3.89170700
H	-0.95362000	-3.87717200	4.82750800
C	-1.44061800	-3.99937600	2.73032800
H	-1.66137400	-5.06259500	2.76175500
C	-1.55506400	-3.30377800	1.52620400
H	-1.86979000	-3.83033200	0.63166500
C	-2.59097600	-1.67171100	-1.11050100
C	-2.50689700	-1.56234500	-2.50890000
H	-1.61467000	-1.14564500	-2.96667800
C	-3.56493600	-1.96924800	-3.32034000
H	-3.47904600	-1.88050900	-4.39947500
C	-4.73184600	-2.48288500	-2.74979500
H	-5.55679700	-2.79707700	-3.38210700
C	-4.83251800	-2.58197700	-1.36137100
H	-5.73887400	-2.97219300	-0.90712600
C	-3.77370300	-2.17621900	-0.54782100
H	-3.87159600	-2.24529300	0.53027200
C	2.13061400	3.15512700	0.31987100
C	3.62693100	3.10007000	-0.02049200
H	4.13918200	2.28466200	0.49278000

H	4.10373500	4.04042000	0.28033600
H	3.78256000	2.97629700	-1.09585900
C	1.89842100	3.31141000	1.83039600
H	0.83078100	3.31039200	2.07236800
H	2.31387600	4.26823000	2.16703900
H	2.37320300	2.52064300	2.41460400
C	1.48275000	4.34100400	-0.42132900
H	1.60366100	4.24623400	-1.50297500
H	1.95748800	5.27402000	-0.09699700
H	0.41335500	4.41534400	-0.20367900
H	-0.00170900	1.91483400	0.40300600
H	-2.87145500	4.47648700	1.92702500
C	-2.19721000	3.86687600	1.30360200
H	-1.50945100	2.23559200	2.62529200
H	-4.72516600	2.68837200	0.81530900
C	-2.16986800	2.42776500	1.77999700
H	-1.19538600	4.28349300	1.45638100
C	-3.10398800	1.44674200	1.47367200
H	-5.13591500	0.99655900	0.96698600
C	-4.34793500	1.67818200	0.62810800
H	-3.10567300	0.55129200	2.09059300
H	-3.66915100	4.11047100	-0.28285300
C	-2.58171500	4.04226200	-0.18688600
H	-2.19126200	5.00533800	-0.53644900
C	-4.15566300	1.46356100	-0.90155100
H	-4.93179600	2.03238300	-1.43682100
C	-2.06361200	2.93667100	-1.08768400
C	-2.78298000	1.81577500	-1.43459200
H	-4.33864400	0.41238800	-1.13397400
H	-1.15712400	3.13945600	-1.65285300
H	-2.44455000	1.22656400	-2.28291300

4'

Ni	1.54572400	1.06942400	-0.64849400
Fe	-3.47879500	-0.78165200	-0.15654500
P	-1.22837400	2.09538100	-0.11374400
P	1.32264600	-0.89709900	0.22225500
O	0.08033800	2.01333700	0.66118700
C	-1.86253200	0.48372000	-0.61036600
C	-1.38786200	-0.79832200	-0.14441000
C	-1.90167000	-1.78393200	-1.03898000
H	-1.74396900	-2.84814300	-0.95181800
C	-2.69250600	-1.14003700	-2.03379500
H	-3.24788200	-1.63228100	-2.81980400

C	-2.67865700	0.25573100	-1.76992800
H	-3.18989900	1.01806500	-2.34115400
C	-0.42139300	-1.05345600	0.97612200
H	-0.46864200	-0.20692300	1.66507700
C	-0.69542000	-2.35263100	1.73351500
H	-0.67160500	-3.22172800	1.07218200
H	-1.68326100	-2.31452700	2.20208000
H	0.04809900	-2.51116300	2.51827300
C	-4.94128600	0.00051500	1.13182200
H	-4.99545600	1.01510700	1.49300100
C	-4.24528800	-1.07533800	1.75910000
H	-3.66860700	-1.01365800	2.67124300
C	-4.42931400	-2.24059900	0.95583100
H	-3.99637300	-3.21411300	1.13789200
C	-5.23088400	-1.88003900	-0.16876300
H	-5.51006200	-2.53361600	-0.98352400
C	-5.54415400	-0.49161600	-0.06111500
H	-6.11263600	0.08990000	-0.77376000
C	1.38758100	-2.40761700	-0.82946100
C	1.15574800	-2.23282300	-2.20148900
H	1.01341000	-1.22596100	-2.57953000
C	1.09964100	-3.32982000	-3.06195100
H	0.91785100	-3.17604200	-4.12183900
C	1.28221300	-4.61992200	-2.56131700
H	1.24489800	-5.47540400	-3.22970500
C	1.52033600	-4.80694500	-1.19740400
H	1.66646800	-5.80855600	-0.80275100
C	1.57017200	-3.70964500	-0.33707700
H	1.75840400	-3.86584800	0.71952300
C	2.41653200	-1.30959700	1.64263600
C	2.14854700	-0.77344500	2.91382800
H	1.22910800	-0.22342400	3.08833300
C	3.05912800	-0.92152600	3.95933100
H	2.82799700	-0.50490500	4.93568500
C	4.26477800	-1.59583300	3.75328000
H	4.97544000	-1.70758800	4.56667900
C	4.55159600	-2.11684700	2.49081900
H	5.48952800	-2.63637000	2.31574400
C	3.63823000	-1.97410200	1.44559300
H	3.87712600	-2.38261900	0.46909300
C	-2.45070400	3.13701400	0.79302500
C	-2.65244500	2.54121700	2.19437500
H	-2.98180800	1.50164000	2.14741900
H	-3.40855600	3.11690400	2.74054500

H	-1.72074100	2.57513600	2.76542600
C	-3.75764200	3.21386000	-0.00835600
H	-3.59399300	3.67082500	-0.99102600
H	-4.48218000	3.83940300	0.52563600
H	-4.20283800	2.22932600	-0.16040000
C	-1.81915500	4.53727300	0.90517800
H	-0.86678700	4.50294500	1.44065100
H	-2.49788200	5.20244400	1.45096400
H	-1.64115000	4.98049100	-0.08098200
H	-1.13391000	2.76896000	-1.35379100
H	2.33851200	4.38097200	-2.62552500
C	2.12095600	3.74840100	-1.74758300
H	0.86324400	2.29211300	-2.77420700
H	4.58086400	2.16020600	-2.46521700
C	1.77245700	2.33196200	-2.16657100
H	1.22654000	4.18645800	-1.28202400
C	2.64145300	1.21448500	-2.30287500
H	4.60797900	0.42828100	-2.65279700
C	4.15200700	1.23427200	-2.06513600
H	2.32709300	0.46112100	-3.02501700
H	4.24379000	3.75831300	-1.27786500
C	3.29582900	3.89025300	-0.75136700
H	3.30017800	4.91996000	-0.37271800
C	4.61078700	1.03723500	-0.59706100
H	5.66577700	1.34158900	-0.50977500
C	3.21365100	2.93525600	0.40961300
C	3.78383200	1.71680400	0.47101600
H	4.59444100	-0.03435700	-0.37354600
H	2.61591400	3.25818200	1.25962000
H	3.66982700	1.15362500	1.39407300

4''

Fe	3.49093800	0.82461000	0.25543500
P	0.84432400	-1.60894400	0.12904900
P	-1.21471900	0.97687800	0.08184000
O	1.17045200	-1.57145700	1.79274100
C	1.83760800	-0.19897000	-0.46272900
C	1.49439400	1.16208700	-0.11151100
C	2.28955600	2.03612000	-0.91348600
H	2.28784300	3.11456500	-0.86071000
C	3.13077200	1.24577900	-1.74498700
H	3.88127500	1.61789800	-2.42863800
C	2.85653300	-0.12387400	-1.47199600
H	3.35780600	-0.95847400	-1.93584500

C	0.41808800	1.57912700	0.85155900
H	0.51327800	0.97412100	1.75858700
C	0.47946200	3.06045800	1.21759800
H	0.35251300	3.69579700	0.33767200
H	1.44988300	3.29992000	1.66576800
H	-0.30032700	3.32352100	1.93539000
C	4.13331900	-0.08982000	1.99630500
H	3.62150900	-0.93609100	2.42885500
C	3.81913600	1.28007400	2.24127700
H	3.04970700	1.64337700	2.90816700
C	4.65700300	2.08388900	1.40914600
H	4.63409200	3.16246700	1.33548900
C	5.48985200	1.20850500	0.64844900
H	6.20809000	1.50847100	-0.10214700
C	5.16571500	-0.13432200	1.01126700
H	5.59991300	-1.02811300	0.58629000
C	-1.21660200	1.95311200	-1.47943900
C	-0.80154100	1.28103400	-2.63935100
H	-0.57270800	0.22112800	-2.57211100
C	-0.67261400	1.96160300	-3.85007400
H	-0.34484300	1.42752500	-4.73728600
C	-0.96736000	3.32421700	-3.91999400
H	-0.87260200	3.85554100	-4.86258300
C	-1.38749200	4.00248700	-2.77379900
H	-1.61934100	5.06270500	-2.82285300
C	-1.50727400	3.32381300	-1.56052900
H	-1.83400300	3.86301600	-0.67798800
C	-2.49562800	1.76944900	1.12784500
C	-2.38278400	1.69782800	2.52689900
H	-1.48085100	1.29307300	2.97724500
C	-3.41878200	2.13364700	3.35190000
H	-3.30861800	2.07389900	4.43094500
C	-4.59345500	2.64399600	2.79488000
H	-5.40115300	2.98219900	3.43688300
C	-4.72291500	2.70965700	1.40651400
H	-5.63514900	3.09786200	0.96243200
C	-3.68729200	2.27196200	0.58051100
H	-3.80979700	2.31111500	-0.49654500
C	1.80169000	-3.16849100	-0.31696000
C	3.27364200	-3.12766400	0.11315600
H	3.84035700	-2.35564400	-0.40707500
H	3.74709900	-4.09494700	-0.09933000
H	3.35963900	-2.94210200	1.18668300
C	1.66554200	-3.40789700	-1.82927000

H	0.61411000	-3.45302200	-2.12747000
H	2.13500400	-4.36209100	-2.09794800
H	2.14388400	-2.62540900	-2.42333200
C	1.10354400	-4.31615800	0.43523300
H	1.18975300	-4.18821600	1.51767600
H	1.57163900	-5.27086700	0.16708900
H	0.04381700	-4.37496400	0.17972800
H	0.30695000	-1.51020600	2.22517800
Ni	-1.23019000	-1.17432700	-0.22483300
H	-3.02159600	-4.40243400	-1.91868400
C	-2.33842200	-3.85233200	-1.25007400
H	-1.48399700	-2.31940800	-2.57695700
H	-4.79204700	-2.44586800	-0.89773900
C	-2.16691900	-2.42802700	-1.73564300
H	-1.37114900	-4.35560300	-1.34252700
C	-3.03045400	-1.36827000	-1.48113500
H	-5.02345600	-0.72387200	-1.04630600
C	-4.32070300	-1.48132200	-0.68080300
H	-2.95063300	-0.50065800	-2.13033300
H	-3.94200200	-3.98330800	0.21282100
C	-2.84927800	-4.01823600	0.20423300
H	-2.58041100	-5.02373600	0.54829600
C	-4.19559700	-1.29394400	0.85352500
H	-5.07636600	-1.74363400	1.33868800
C	-2.32164600	-3.00324700	1.19448800
C	-2.93323500	-1.82818400	1.48878800
H	-4.24518400	-0.22752100	1.07809400
H	-1.45717100	-3.29657600	1.78500600
H	-2.54670200	-1.24001400	2.31939700

TS0

Fe	2.19357400	-1.24128200	-0.77357700
P	1.57704400	1.72893500	0.78029400
P	-1.99590000	0.53343500	0.64919200
O	1.63020100	2.35729400	-0.71831200
C	1.41734800	-0.06579600	0.71833600
C	0.34691000	-0.70870500	-0.01724000
C	0.52395700	-2.11708300	0.11206600
H	-0.09414200	-2.87089100	-0.35217000
C	1.68312700	-2.36194300	0.90321900
H	2.09985300	-3.33235500	1.13506200
C	2.23600600	-1.10828700	1.28173800
H	3.13664800	-0.97267800	1.85930000
C	-0.78151300	-0.00631300	-0.71521400

H	-0.38712000	0.93301300	-1.11246200
C	-1.39733800	-0.81993900	-1.85302900
H	-1.80741300	-1.76722100	-1.49566400
H	-0.63973200	-1.04439700	-2.60999300
H	-2.20772900	-0.26758300	-2.33421300
C	3.29455600	-0.03020900	-2.05238900
H	3.37028700	1.03626400	-1.90300800
C	2.24376500	-0.68011600	-2.76392100
H	1.42844600	-0.18301800	-3.26942000
C	2.43121100	-2.09080700	-2.64455300
H	1.77950700	-2.85577500	-3.04358100
C	3.59757800	-2.31332100	-1.85171700
H	3.98487800	-3.27633500	-1.54861000
C	4.12878400	-1.03903900	-1.48292000
H	4.99217200	-0.86954000	-0.85535100
C	-2.79515200	-1.08238700	1.03874100
C	-2.28240900	-1.78286300	2.14215200
H	-1.49521200	-1.33200000	2.73991400
C	-2.77009000	-3.04709300	2.47634400
H	-2.35922900	-3.57580700	3.33156100
C	-3.79101500	-3.62319800	1.71962100
H	-4.17855500	-4.60319200	1.98255100
C	-4.31856800	-2.93156100	0.62652200
H	-5.11501000	-3.37470300	0.03532500
C	-3.82191600	-1.67377300	0.28518400
H	-4.23586400	-1.14696000	-0.56760100
C	-3.28718200	1.43567000	-0.30568600
C	-2.95296100	2.22938600	-1.41542500
H	-1.93565000	2.24343100	-1.79318000
C	-3.91672200	3.01415900	-2.05013300
H	-3.63617200	3.61398600	-2.91126100
C	-5.23181300	3.02827700	-1.58497500
H	-5.98176900	3.63713000	-2.08102800
C	-5.57390400	2.25782100	-0.47177500
H	-6.59301700	2.26616500	-0.09563100
C	-4.61155600	1.47545700	0.16468800
H	-4.89329900	0.88490800	1.03123200
C	3.10929000	2.20401800	1.73505900
C	4.37194200	1.67679700	1.03750100
H	4.42596700	0.58708000	1.04331400
H	5.26156200	2.06401400	1.54893900
H	4.41326200	2.01451600	-0.00209000
C	2.99852900	1.70826400	3.18447700
H	2.07923900	2.06924200	3.65796700

H	3.84496500	2.08871700	3.76837000
H	3.00672400	0.61888300	3.25890700
C	3.12697300	3.74387700	1.71768000
H	3.16316000	4.12793600	0.69479500
H	4.01192400	4.10513100	2.25389800
H	2.24094800	4.16051100	2.20818300
H	0.66165200	2.75321600	0.23704400

TS0'

Ni	-1.17853600	0.74334500	-0.02565600
H	-4.32446400	4.95798600	0.32735900
C	-4.30197500	3.97069100	0.81393800
H	-6.45031500	3.75424800	1.11272800
H	-4.28372300	1.95203800	-1.57003900
C	-5.62321600	3.28848400	0.57525600
H	-4.22791400	4.18663000	1.88945800
C	-5.93083300	2.23133400	-0.18559900
H	-5.62866700	0.86313800	-1.78662600
C	-5.02219800	1.36327100	-1.02326200
H	-6.97504500	1.91845400	-0.17805600
H	-3.00978000	3.10792200	-0.70727000
C	-3.01729600	3.24216600	0.37450900
H	-2.17391000	3.90278500	0.59523200
C	-4.31811500	0.26298400	-0.20716600
H	-3.81555800	-0.42073600	-0.90098500
C	-2.78418400	1.93584700	1.10504800
C	-3.34363700	0.70222300	0.86779900
H	-5.09013600	-0.34201500	0.28851600
H	-2.25734600	2.04073900	2.05419700
H	-3.17612200	-0.04842300	1.63819200
Fe	3.75032200	-0.11197500	0.09841900
P	0.75652500	1.72715300	-0.42702500
P	-0.78773200	-1.37656500	-0.13378200
O	0.87412800	1.26416700	-1.95340400
C	1.88502200	0.66448300	0.54532300
C	1.84482100	-0.78547800	0.44501400
C	2.72817200	-1.31482100	1.43655600
H	2.94797100	-2.36085600	1.58986200
C	3.33418900	-0.23039100	2.13102700
H	4.08702600	-0.31132700	2.90310600
C	2.81480900	0.98033400	1.59115200
H	3.10732200	1.97247600	1.89792900
C	1.04065700	-1.60644200	-0.53470200
H	1.14464600	-1.13045400	-1.51350500

C	1.47794000	-3.06791500	-0.60413500
H	1.34213200	-3.57467600	0.35477300
H	2.53680300	-3.13369700	-0.87140200
H	0.90247400	-3.61294500	-1.35601700
C	4.25786100	0.55326100	-1.79363000
H	3.56929800	1.14016100	-2.38334000
C	4.28586600	-0.87195800	-1.74326900
H	3.65517800	-1.53465600	-2.31916200
C	5.24276100	-1.26586400	-0.75864500
H	5.46951300	-2.28054100	-0.46122900
C	5.80757000	-0.08078800	-0.19753400
H	6.53833900	-0.04021000	0.59858300
C	5.19896200	1.04205700	-0.83641400
H	5.39411000	2.08011900	-0.61026000
C	-0.93810200	-2.20064100	1.49493200
C	-0.83341100	-1.38337800	2.63177300
H	-0.72593000	-0.30977900	2.50513600
C	-0.85690200	-1.94093200	3.90983600
H	-0.77186800	-1.29787200	4.78072400
C	-0.99324800	-3.32140800	4.06649000
H	-1.01827200	-3.75646300	5.06116400
C	-1.09666400	-4.14242800	2.94151000
H	-1.19896100	-5.21723700	3.05963400
C	-1.06346900	-3.58795700	1.66169200
H	-1.13836600	-4.23349300	0.79340700
C	-1.68043700	-2.42612000	-1.33465100
C	-1.25295800	-2.47169800	-2.67185300
H	-0.34369800	-1.96079000	-2.97205100
C	-1.99479200	-3.16213400	-3.62915400
H	-1.64607600	-3.19309000	-4.65713500
C	-3.18023500	-3.80723600	-3.27089800
H	-3.75680400	-4.34409700	-4.01805500
C	-3.62413700	-3.74964000	-1.94903100
H	-4.54962900	-4.24053000	-1.66240900
C	-2.88395500	-3.06083600	-0.98785600
H	-3.24437300	-3.01832900	0.03459600
C	1.34005600	3.50652700	-0.28802900
C	2.81672000	3.68364900	-0.65950300
H	3.48082700	3.17445400	0.04026200
H	3.07637300	4.75038400	-0.65897100
H	3.01574800	3.29320100	-1.66112300
C	1.05512600	4.02235100	1.13015400
H	0.00898400	3.85562200	1.40775300
H	1.25024000	5.10057000	1.18424900

H	1.67951700	3.53688900	1.88484000
C	0.47207700	4.27887400	-1.29822500
H	0.64833500	3.92315700	-2.31643500
H	0.71226000	5.34812700	-1.25405400
H	-0.59421900	4.16059000	-1.08187300
H	-0.37725300	0.56522200	-1.35361700

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Ni	0.08686700	1.04861500	0.14871000
Fe	-4.67611400	-0.90431300	-0.58295500
P	-2.03166500	1.19314200	0.77336500
P	-0.10996900	-1.23681400	0.31358900
O	-2.11722800	0.47285400	2.13532700
C	-2.91475000	0.20884700	-0.50773300
C	-2.64835900	-1.20846400	-0.60288900
C	-3.22040900	-1.69472900	-1.81721800
H	-3.21793400	-2.72247400	-2.15082100
C	-3.87122000	-0.60484900	-2.46523600
H	-4.44646400	-0.65965200	-3.37950700
C	-3.67989300	0.56174900	-1.66696000
H	-4.07656700	1.53752000	-1.89560400
C	-1.83618500	-1.97050500	0.40187600
H	-2.17047100	-1.66075600	1.39414200
C	-1.90998400	-3.48689700	0.26420200
H	-1.56071800	-3.83044600	-0.71266400
H	-2.94669800	-3.81747400	0.38606800
H	-1.30527800	-3.97513100	1.03380000
C	-5.68666700	-0.71247000	1.21666000
H	-5.28271900	-0.17206300	2.05922100
C	-5.45137700	-2.08766900	0.92462000
H	-4.85910700	-2.76712500	1.52175200
C	-6.08726400	-2.39301700	-0.31776900
H	-6.05914100	-3.34502000	-0.82984800
C	-6.71697300	-1.20339400	-0.79385700
H	-7.25049500	-1.09700600	-1.72837300
C	-6.46749100	-0.16407100	0.15313800
H	-6.78804500	0.86424300	0.06283800
C	0.58056900	-2.00083400	-1.20193200
C	0.58732100	-1.21062100	-2.36243800
H	0.26740100	-0.17439700	-2.30058000
C	1.00918900	-1.74019000	-3.58226300
H	1.00585000	-1.11564200	-4.47086500
C	1.43000700	-3.06937500	-3.65723900
H	1.75619000	-3.48576600	-4.60590800

C	1.42835300	-3.86421100	-2.50828300
H	1.75506800	-4.89839300	-2.56162400
C	1.00480300	-3.33549100	-1.28884400
H	1.00422700	-3.96303300	-0.40485700
C	0.76967600	-1.95106600	1.74347900
C	0.16344900	-1.81334100	3.00446800
H	-0.81279800	-1.34332800	3.07995900
C	0.84370900	-2.21048800	4.15415400
H	0.36631700	-2.10071800	5.12366900
C	2.13957400	-2.72389900	4.06532800
H	2.67137000	-3.02143400	4.96436500
C	2.75511800	-2.83555800	2.81840900
H	3.77088200	-3.21189900	2.74284300
C	2.07659200	-2.45230500	1.66169200
H	2.57869800	-2.52800500	0.70407500
C	1.65484000	2.78598400	-2.68426700
H	1.54792400	2.50836200	-3.73283500
C	0.55306800	2.68165000	-1.90389800
H	-0.34385500	2.30882300	-2.40473500
C	0.33696300	2.96414100	-0.47051700
H	-0.62480200	3.45580700	-0.35883000
C	1.38592800	3.71905200	0.34389400
H	2.34987300	3.21479300	0.29782600
H	1.09547600	3.66944700	1.40116100
C	1.56047900	5.21374100	-0.01138100
H	0.67721400	5.75960500	0.34786400
H	2.41291200	5.60740100	0.56161000
C	1.73826300	5.56429000	-1.49660500
H	0.82786000	5.28634000	-2.03763100
H	1.81783900	6.65657000	-1.57830600
C	2.94473600	4.95345600	-2.22265600
H	3.87632900	5.29860200	-1.75274300
H	2.95198500	5.34942400	-3.24667500
C	2.97692800	3.40355200	-2.29473600
H	3.74316300	3.11441600	-3.02549300
H	3.32001800	3.01407000	-1.33443000
C	-2.95299800	2.83427600	0.97516000
C	-4.29974800	2.53462100	1.65126800
H	-4.93669100	1.93100000	1.00256800
H	-4.82381600	3.47499300	1.86594600
H	-4.14955100	1.99483000	2.58883200
C	-3.20660000	3.59982000	-0.33610500
H	-2.38438400	3.53106500	-1.05186500
H	-3.36433600	4.66366400	-0.11906200

H	-4.11087300	3.24022000	-0.83246500
C	-2.10375600	3.67639400	1.94687400
H	-1.86914900	3.10395800	2.84896800
H	-2.66744800	4.56860000	2.24657000
H	-1.16430200	4.00882700	1.50199900
C	4.16483100	0.42396200	1.12588200
C	2.80894800	0.71231500	1.39555400
C	2.35732400	0.90664500	2.70303900
C	3.29556700	0.79823700	3.72270200
C	4.64945300	0.51356500	3.44895200
C	5.11138900	0.32383300	2.14899700
C	2.98405200	0.44912600	-0.75210600
H	1.31021700	1.11040900	2.89733300
H	2.98055200	0.92812400	4.75293400
H	5.35162400	0.44009500	4.27363100
H	6.15595900	0.10933400	1.94934800
H	2.75048300	0.40203100	-1.80339400
N	4.24088700	0.25361900	-0.25468300
N	2.10770800	0.72557500	0.19397500
C	5.44038000	-0.02297100	-1.04516200
H	5.68922700	0.87012900	-1.62723900
H	6.25790600	-0.19158300	-0.34239200
C	5.29270400	-1.21946200	-1.98428700
H	4.43125200	-1.06405000	-2.64750000
H	6.16481000	-1.21387700	-2.65291700
C	5.05850000	-3.71122100	-2.35705400
H	4.95165000	-4.68215300	-1.86641200
H	4.19046400	-3.55922800	-3.00790300
H	5.94155400	-3.75142600	-3.00840400
C	5.17988600	-2.59138700	-1.35689700
C	5.20264700	-2.82241300	-0.04033600
H	5.13257100	-3.83623000	0.34409500
H	5.29022100	-2.03574500	0.69938600

TS1

Ni	0.14831900	1.01430700	0.14574100
Fe	-4.73416300	-0.80126700	-0.50534400
P	-2.03881800	1.27739500	0.63802900
P	-0.15819200	-1.20446000	0.26836800
O	-2.18151700	0.66150600	2.04301600
C	-2.95433900	0.27397400	-0.59447900
C	-2.72079000	-1.14947000	-0.63583800
C	-3.37399800	-1.68023900	-1.78876900
H	-3.41043100	-2.72184200	-2.07302700

C	-4.04172400	-0.60769600	-2.44909900
H	-4.66979000	-0.69326300	-3.32539300
C	-3.78400200	0.59084700	-1.71976900
H	-4.18162800	1.56239800	-1.96638100
C	-1.90301500	-1.87992800	0.38597200
H	-2.22464400	-1.53086600	1.36926700
C	-2.00181300	-3.40016000	0.30288700
H	-1.67714500	-3.78025200	-0.66860800
H	-3.04167900	-3.70739700	0.45429400
H	-1.39194300	-3.87387400	1.07657600
C	-5.61763000	-0.46343400	1.33527700
H	-5.14829400	0.14424400	2.09358200
C	-5.39369400	-1.85788100	1.14099300
H	-4.75232200	-2.48360300	1.74602200
C	-6.11474500	-2.26679900	-0.02221000
H	-6.11706900	-3.25845600	-0.45349100
C	-6.78572800	-1.12187400	-0.54821500
H	-7.38888700	-1.09526600	-1.44538500
C	-6.47826100	-0.00752900	0.28990200
H	-6.81553700	1.00821300	0.14013300
C	0.47389300	-1.96089300	-1.26778200
C	0.46856800	-1.16795400	-2.42431800
H	0.18215500	-0.12377800	-2.34896600
C	0.83765400	-1.70774500	-3.65526600
H	0.83029000	-1.08205600	-4.54272900
C	1.22282400	-3.04670800	-3.74183700
H	1.51199400	-3.46951400	-4.69959100
C	1.23908800	-3.84214000	-2.59365900
H	1.54186300	-4.88299800	-2.65595200
C	0.86559600	-3.30410600	-1.36226300
H	0.88031900	-3.92935000	-0.47693600
C	0.70550100	-1.96847800	1.67699700
C	0.09134500	-1.89897000	2.93832000
H	-0.88749900	-1.44090200	3.03870000
C	0.76408700	-2.35867100	4.06905200
H	0.28277700	-2.29886500	5.04075800
C	2.05793400	-2.87128800	3.95681900
H	2.58521700	-3.21670900	4.84114300
C	2.67874100	-2.92095400	2.70855300
H	3.69355600	-3.29494500	2.61762600
C	2.00968100	-2.47122400	1.57148600
H	2.51802300	-2.48835900	0.61455800
C	-2.86949000	2.97812100	0.67922400
C	-4.31493300	2.79910100	1.17010800

H	-4.90087400	2.19539500	0.47599900
H	-4.79557400	3.78175000	1.25995900
H	-4.33345000	2.31746300	2.15039900
C	-2.88072600	3.69879900	-0.68367700
H	-2.00025300	3.49755500	-1.29885200
H	-2.93389500	4.78379600	-0.53315400
H	-3.75557800	3.41700900	-1.27383700
C	-2.11931800	3.80168400	1.74477900
H	-2.08393000	3.25637200	2.69147200
H	-2.64867600	4.74749000	1.91233400
H	-1.09393000	4.04469900	1.46067600
C	0.59536900	3.09853400	-0.39246000
H	-0.41056400	3.46052500	-0.24433300
C	0.84970200	2.65570000	-1.69068300
H	-0.03866300	2.40939900	-2.27512600
C	2.10809800	2.39312600	-2.33641700
H	1.98477000	2.24646400	-3.41326700
C	3.36870400	3.19659800	-1.99023000
H	3.69259400	2.95200100	-0.97592200
H	4.17285900	2.83207600	-2.64245800
C	3.29195900	4.72771000	-2.14113600
H	3.23240300	4.97821400	-3.20894100
H	4.24386000	5.14581100	-1.78444600
C	2.13129700	5.44018500	-1.43020100
H	1.19317200	5.18128400	-1.93413000
H	2.25966800	6.51964000	-1.58326500
C	1.96552200	5.19656400	0.07795700
H	2.87409400	5.50891600	0.60975700
H	1.16323700	5.85856200	0.42890400
C	1.62525700	3.74328300	0.50565100
H	1.23979000	3.76763300	1.53142300
H	2.52878500	3.14002800	0.55016600
C	4.09070000	0.29671800	1.17497700
C	2.73524300	0.56571800	1.46510600
C	2.30229800	0.74209200	2.78070600
C	3.25012000	0.61831100	3.79395900
C	4.59896700	0.34099600	3.50243200
C	5.04354400	0.17986100	2.18936500
C	2.89034500	0.34170000	-0.74930800
H	1.25815500	0.94180900	2.99642900
H	2.94298600	0.73319800	4.82884700
H	5.31204900	0.25502600	4.31691200
H	6.08771100	-0.02395600	1.97441400
H	2.44608900	1.24091000	-1.88078000

N	4.14681900	0.16939100	-0.21157400
N	2.04527600	0.59849800	0.25815600
C	5.34423900	-0.10151600	-1.00012800
H	6.16542000	-0.29769900	-0.30693600
H	5.60591500	0.79932400	-1.56577700
C	5.17616100	-1.26889100	-1.97108600
H	6.03033800	-1.25392900	-2.66320000
H	4.29121300	-1.08208200	-2.59158800
C	4.90291300	-3.74721900	-2.40624600
H	4.80045400	-4.73133700	-1.94074700
H	5.76417000	-3.77787900	-3.08688100
H	4.01688400	-3.56576400	-3.02488400
C	5.06669300	-2.65633200	-1.38007700
C	5.11775900	-2.92556800	-0.07140000
H	5.04506200	-3.94890100	0.28747300
H	5.22874100	-2.15802100	0.68539000

6

Ni	-1.00090900	0.47356500	-0.51976500
Fe	3.52308500	-1.87822600	0.18705900
P	0.02966600	-1.44790900	0.07049300
P	0.66080300	1.73062400	0.37159800
O	0.08941700	-1.70805600	1.57262600
C	1.74098300	-1.11478000	-0.54954700
C	2.53693400	-0.09788800	0.09870200
C	3.77924400	0.01750300	-0.59413200
H	4.59390700	0.67428600	-0.32609200
C	3.78519600	-0.94203600	-1.64759200
H	4.60697200	-1.14405100	-2.32087300
C	2.53765000	-1.63258400	-1.62579900
H	2.27092600	-2.43746900	-2.29247700
C	2.01297700	0.75065000	1.21566200
H	1.47674500	0.09998700	1.91203900
C	3.05673500	1.57717400	1.95689900
H	3.59418800	2.25561900	1.29001000
H	3.78927600	0.91184100	2.42525500
H	2.58893500	2.17371600	2.74543000
C	3.05578100	-3.25747500	1.65217500
H	2.02998600	-3.43905100	1.93569500
C	3.87778300	-2.22327300	2.18838200
H	3.59151400	-1.53596900	2.97173200
C	5.11195100	-2.21591800	1.46853800
H	5.92716400	-1.51965700	1.60991700
C	5.05237100	-3.24912800	0.48496500

H	5.81761400	-3.47663300	-0.24438800
C	3.78267900	-3.89338700	0.60014500
H	3.42223400	-4.69794600	-0.02438900
C	1.62034400	2.99646100	-0.53301100
C	1.99076100	2.67775900	-1.84929900
H	1.65324400	1.74303600	-2.28391700
C	2.80488100	3.53647000	-2.58707700
H	3.08480900	3.27392100	-3.60283300
C	3.25734700	4.72793500	-2.01797000
H	3.88493400	5.40229200	-2.59283900
C	2.91015600	5.04573300	-0.70349300
H	3.27345600	5.96368000	-0.25117000
C	2.10523100	4.18214200	0.04020700
H	1.86811800	4.42704800	1.06895900
C	-0.31084700	2.51943900	1.69960400
C	-0.84189000	1.64008900	2.66123200
H	-0.61759100	0.57744500	2.61269300
C	-1.71038300	2.11913000	3.63919000
H	-2.12047200	1.43007300	4.37079000
C	-2.07162400	3.46803000	3.66182900
H	-2.75278300	3.83663700	4.42306600
C	-1.57111300	4.33781200	2.69179100
H	-1.86286300	5.38404400	2.69376600
C	-0.69818100	3.86702100	1.71007100
H	-0.33624000	4.54821700	0.94857000
C	-0.55329900	-2.98572600	-0.86247600
C	0.46115000	-4.12270400	-0.64748600
H	1.45545600	-3.88807200	-1.02280800
H	0.10514900	-5.02023800	-1.16819400
H	0.54700900	-4.36579800	0.41438300
C	-0.71773600	-2.66728200	-2.35257000
H	-1.37934600	-1.80924200	-2.48933500
H	-1.16415100	-3.52289800	-2.87388600
H	0.23165300	-2.43834700	-2.84250100
C	-1.89404500	-3.45373300	-0.27037000
H	-1.86110400	-3.46616800	0.82119200
H	-2.09737900	-4.47274100	-0.62192400
H	-2.72633400	-2.82611700	-0.58166600
C	-4.79683600	-1.05336700	-0.36213900
C	-4.33346900	-1.04721700	0.97831500
C	-5.19660900	-1.42475800	2.01421600
C	-6.49983900	-1.79063100	1.68546000
C	-6.94656700	-1.78580000	0.34974900
C	-6.10154600	-1.41842700	-0.69796100

C	-2.64566400	-0.39468700	-0.23642600
H	-4.84615000	-1.42849600	3.04184400
H	-7.18767200	-2.08806700	2.47181300
H	-7.96937100	-2.07732200	0.12917400
H	-6.45341700	-1.42259100	-1.72547400
N	-3.69880600	-0.65533300	-1.11760500
N	-3.00607900	-0.64604800	1.01457700
C	-3.74305300	-0.24671100	-2.50511600
H	-2.99644600	-0.79120800	-3.09095300
H	-4.72267800	-0.51427400	-2.90490700
C	-3.53394300	1.26864800	-2.62370800
H	-3.81737500	1.57851100	-3.63832800
H	-4.21585600	1.76277400	-1.92568000
C	-1.11490800	1.38860500	-3.46393100
H	-0.19391900	1.96113400	-3.35261200
H	-0.85984700	0.32305800	-3.43200500
H	-1.53002100	1.58934000	-4.45897400
C	-2.11823600	1.74101000	-2.39406300
C	-1.81120200	2.58472600	-1.37477900
H	-0.87258100	3.12504900	-1.36659100
H	-2.55763600	2.87511700	-0.64193200

6'

Ni	0.37592900	1.63063800	-0.37248300
Fe	2.75139000	-2.86723300	-1.13248000
P	0.18861800	-0.44814200	-1.22517400
P	1.69863700	0.89480600	1.31886500
O	-0.56191700	-1.42340000	-0.31949600
C	1.96550200	-0.95147400	-1.28293100
C	2.67581900	-1.15249600	-0.04015700
C	4.03700200	-1.45845100	-0.34076900
H	4.80882300	-1.68370300	0.38061600
C	4.17676800	-1.49216000	-1.75877100
H	5.07354500	-1.75340100	-2.30401200
C	2.91114100	-1.17981100	-2.33798500
H	2.70798200	-1.16357300	-3.39702800
C	2.04259700	-0.94377200	1.30048700
H	1.04925200	-1.39842200	1.27165600
C	2.83453700	-1.47384100	2.48924700
H	3.83027900	-1.02882500	2.55425700
H	2.95433600	-2.55793300	2.39683400
H	2.30833000	-1.26956600	3.42628100
C	1.16535800	-4.19226100	-1.09432900
H	0.14527800	-3.83961800	-1.11618900

C	1.95409300	-4.32927100	0.08496600
H	1.61297100	-4.14311300	1.09352900
C	3.28046300	-4.68925600	-0.30467700
H	4.12323700	-4.82773900	0.35865900
C	3.31081500	-4.77677200	-1.72930300
H	4.18015900	-4.99737000	-2.33361100
C	2.00380500	-4.47060100	-2.21681400
H	1.71124700	-4.42427600	-3.25593000
C	3.34018800	1.57334200	1.75357700
C	4.20633700	1.84927600	0.68309400
H	3.85507000	1.71593500	-0.33439000
C	5.51703200	2.26377300	0.91759200
H	6.17527800	2.46942500	0.07889800
C	5.97839500	2.41076800	2.22665100
H	6.99639500	2.73998900	2.41184400
C	5.13114400	2.12154400	3.29789400
H	5.49094400	2.21729000	4.31797000
C	3.82319200	1.69507900	3.06550100
H	3.18790300	1.44170000	3.90585300
C	0.51594200	1.17834800	2.68114400
C	-0.66487500	0.41461300	2.61985500
H	-0.80114200	-0.31889300	1.82934900
C	-1.69159900	0.64366400	3.53249400
H	-2.59961300	0.05297000	3.46957500
C	-1.56463200	1.64122900	4.50145600
H	-2.36938400	1.81960000	5.20845100
C	-0.40907000	2.42244100	4.54588700
H	-0.31166100	3.21190400	5.28550300
C	0.62628900	2.19812600	3.63712600
H	1.50729400	2.82854700	3.67031700
C	-0.44909300	-0.57874300	-2.99783900
C	-0.18322200	-2.00385700	-3.51410600
H	0.87206600	-2.27011900	-3.50874200
H	-0.55047900	-2.08323900	-4.54472700
H	-0.72243500	-2.73799000	-2.91079900
C	0.22754600	0.46366200	-3.89409100
H	0.07021400	1.46994000	-3.50216500
H	-0.20574800	0.42728700	-4.90106400
H	1.30417500	0.30398900	-3.99065800
C	-1.97378400	-0.37024800	-2.99745700
H	-2.44855700	-0.93889600	-2.19502800
H	-2.37674000	-0.72244600	-3.95496000
H	-2.25253700	0.67635900	-2.88964100
C	-3.17551100	3.05090500	-1.80194100

C	-3.52498500	2.12398800	-0.78759700
C	-4.86548500	1.97581300	-0.41169900
C	-5.81996700	2.75977400	-1.05582500
C	-5.45673800	3.67940600	-2.05842700
C	-4.12698600	3.84091200	-2.44892800
C	-1.35788700	1.99718900	-0.98937200
H	-5.13985800	1.27101500	0.36572200
H	-6.86640900	2.66259200	-0.78124200
H	-6.22685000	4.27575200	-2.53903600
H	-3.85683200	4.55294600	-3.22320400
N	-1.79453600	2.93167300	-1.93119500
N	-2.38309600	1.48779300	-0.31970200
C	-0.93693900	3.89006400	-2.59404600
H	-0.21262800	3.37417000	-3.23054500
H	-1.55616900	4.50859900	-3.24600400
C	-0.21984000	4.77107900	-1.55957500
H	0.19684200	5.64578500	-2.07533600
H	-0.96381600	5.13233500	-0.84391600
C	2.16923800	3.86070700	-1.64739200
H	3.00686600	3.56255600	-1.01722200
H	2.01334400	3.08202700	-2.40381200
H	2.44837600	4.77518900	-2.18442000
C	0.91862000	4.09005600	-0.83748200
C	0.87076400	3.84055600	0.49634300
H	1.76917500	3.58122100	1.04299000
H	-0.01817700	4.06301400	1.07837600
C	-4.24724400	-4.76194100	1.29739700
H	-4.24247500	-5.83824800	1.47021400
C	-3.15370800	-4.08954000	1.68293500
H	-2.35324800	-4.69049700	2.12036400
C	-2.80350200	-2.62398100	1.60829300
H	-2.54580800	-2.29247600	2.62823500
C	-3.79888000	-1.63364400	0.98909700
H	-4.10607700	-2.00172100	0.00663100
H	-3.25218000	-0.70816100	0.78053900
C	-5.02693100	-1.28427600	1.85291100
H	-4.70893900	-0.56008100	2.61619800
H	-5.75933400	-0.75369900	1.22871500
C	-5.73199000	-2.43560300	2.58622500
H	-5.00989000	-2.94467400	3.23440000
H	-6.48593200	-2.00243300	3.25716700
C	-6.43040100	-3.47910100	1.70698000
H	-7.25095200	-3.00346200	1.15254300
H	-6.89477500	-4.22450100	2.36627400

C	-5.51836700	-4.20910700	0.69383100
H	-6.08940500	-5.03409600	0.25221900
H	-5.28850600	-3.53239500	-0.13143600
H	-1.87075600	-2.53208300	1.03898500

TS2

Ni	-0.98882200	0.92125900	0.41120000
Fe	2.46955000	-2.80457000	-0.62216200
P	-0.24085400	-1.15662300	1.09725800
P	1.14639500	1.60080400	0.18884700
O	0.66952300	-1.01730900	2.33293700
C	0.77872500	-1.60422900	-0.37041400
C	1.95895900	-0.82594900	-0.65784300
C	2.46059400	-1.21569300	-1.93681100
H	3.35126000	-0.83277900	-2.41403900
C	1.62553000	-2.25981900	-2.43338600
H	1.77455900	-2.80919800	-3.35309400
C	0.59393400	-2.49721000	-1.47534100
H	-0.17522700	-3.24891100	-1.56177200
C	2.45311100	0.24651700	0.25845800
H	2.36398100	-0.12761000	1.28042000
C	3.87290700	0.73021500	-0.01202700
H	3.99718400	1.10870400	-1.02908200
H	4.57005400	-0.10202100	0.12362200
H	4.15438500	1.52409700	0.68596000
C	2.90925100	-3.75189100	1.16814200
H	2.34658900	-3.56809500	2.07052200
C	4.02825600	-2.98840700	0.72429900
H	4.46908700	-2.15432600	1.25131100
C	4.42367700	-3.48204800	-0.55637800
H	5.21810600	-3.08552800	-1.17374400
C	3.54840300	-4.55547400	-0.90274500
H	3.56565100	-5.11608600	-1.82733200
C	2.61262000	-4.72181700	0.16232300
H	1.80289200	-5.43666200	0.18597200
C	1.58868400	2.40044900	-1.39660300
C	0.92360100	1.91904200	-2.53423700
H	0.15140100	1.16893500	-2.41498400
C	1.25805300	2.37865100	-3.80713400
H	0.73296800	1.99116500	-4.67504800
C	2.26548800	3.33214000	-3.96123900
H	2.52259500	3.69979000	-4.95000200
C	2.95147200	3.80026500	-2.83951600
H	3.75059200	4.52663700	-2.95356000

C	2.62684900	3.32941800	-1.56660100
H	3.19805300	3.67627400	-0.71497600
C	1.58193300	2.66205200	1.61770400
C	1.51436400	2.01389600	2.86617500
H	1.23511100	0.96077400	2.91281900
C	1.78548700	2.72338500	4.03520100
H	1.73249600	2.21287200	4.99229600
C	2.11496500	4.07945800	3.98055800
H	2.32477600	4.62809200	4.89402600
C	2.16369800	4.72921500	2.74726400
H	2.40608100	5.78666000	2.69569200
C	1.89546700	4.02746300	1.57072700
H	1.90994700	4.55854000	0.62790000
C	-1.39463900	-2.62226300	1.38128900
C	-0.55428500	-3.89076200	1.59654700
H	0.03267700	-4.14574300	0.71406500
H	-1.22464900	-4.73185000	1.81625000
H	0.12534400	-3.77051100	2.44356300
C	-2.36012500	-2.83611700	0.19829600
H	-2.56432900	-1.92082100	-0.35736900
H	-3.32063300	-3.22457500	0.55191000
H	-1.95964700	-3.56544600	-0.51164700
C	-2.14244800	-2.33333000	2.69635500
H	-1.42824200	-2.17244900	3.50863800
H	-2.76456500	-3.20051400	2.95311100
H	-2.78913000	-1.45983700	2.61350200
C	-4.59812400	-0.15163600	-0.90413500
C	-4.83210300	-0.48344600	0.46091600
C	-6.01599300	-1.14767800	0.82077200
C	-6.92519900	-1.45675500	-0.18412700
C	-6.67495000	-1.12409000	-1.53301200
C	-5.50494900	-0.47415600	-1.91727000
C	-2.88883100	0.47023300	0.40991500
H	-6.20037300	-1.41047200	1.85754800
H	-7.84838000	-1.96969100	0.06870900
H	-7.40984600	-1.38497000	-2.28858400
H	-5.31127600	-0.23238100	-2.95771900
N	-3.36116700	0.45773900	-0.91027100
N	-3.77219300	-0.07979300	1.23799900
C	-2.68457300	1.11190600	-2.01690800
H	-1.77897200	0.54864500	-2.25880400
H	-3.33938900	1.07008300	-2.88975700
C	-2.33737400	2.57967800	-1.68477000
H	-1.63439800	2.94535900	-2.43870300

H	-3.25514400	3.17847700	-1.78847000
C	-0.98812500	4.06910400	-0.09569600
H	-0.62389100	4.16912000	0.92751600
H	-0.14672400	4.16538100	-0.78519300
H	-1.65507700	4.92358900	-0.28778000
C	-1.76331200	2.79032300	-0.29314200
C	-2.58988200	2.33690200	0.78012500
H	-2.24792800	2.53788700	1.79657000
H	-3.67173500	2.39783100	0.69882100

TS2'

Ni	1.83227300	0.59765400	-0.63295000
Fe	-1.70815100	-1.71736300	2.39982200
P	0.48165600	-1.27233000	-0.41793600
P	0.14768200	1.89157900	0.10375600
O	-0.77671700	-1.10651800	-1.29607700
C	0.00471500	-1.14219300	1.35687600
C	-0.77968400	-0.00895500	1.78690000
C	-0.85843900	-0.02373500	3.21277300
H	-1.40489000	0.67891100	3.82488200
C	-0.16707500	-1.18113300	3.67655700
H	-0.09564400	-1.51039500	4.70432600
C	0.36193200	-1.86635000	2.54204000
H	0.90420100	-2.79785300	2.58155700
C	-1.33646600	1.00005500	0.83386200
H	-1.74418000	0.46132500	-0.02306000
C	-2.39240800	1.92894600	1.42185200
H	-2.02968900	2.45979800	2.30484000
H	-3.26783000	1.34196500	1.71087700
H	-2.71609500	2.67012200	0.68608700
C	-2.94262500	-2.77175600	1.11820800
H	-2.69121000	-2.92994600	0.08143900
C	-3.62428700	-1.62927400	1.63051700
H	-3.99381600	-0.80305100	1.04018000
C	-3.67197000	-1.74505900	3.05313600
H	-4.08759400	-1.01694600	3.73630400
C	-3.02057000	-2.96191000	3.41974300
H	-2.86100300	-3.31922600	4.42792900
C	-2.56963800	-3.59690700	2.22270600
H	-2.01512700	-4.52263800	2.16744200
C	0.55173200	3.03792900	1.47212200
C	1.49093700	2.56222700	2.39996600
H	1.96467900	1.60359200	2.22564800
C	1.80076300	3.29502800	3.54465100

H	2.52732400	2.90732800	4.25238600
C	1.17597500	4.52115500	3.77684800
H	1.42145000	5.09990100	4.66212300
C	0.22158000	4.99263700	2.87430200
H	-0.28486500	5.93505800	3.06007300
C	-0.10147400	4.25116300	1.73702600
H	-0.87687400	4.61394800	1.07499700
C	-0.57786900	2.75125900	-1.34204700
C	-1.06001900	1.87836100	-2.33684100
H	-0.98763800	0.80042200	-2.18803300
C	-1.62099500	2.39315700	-3.50481000
H	-1.99412900	1.71014400	-4.26203200
C	-1.70013000	3.77352600	-3.70235300
H	-2.13895500	4.17092000	-4.61268600
C	-1.20309100	4.64030500	-2.72892800
H	-1.24671800	5.71473900	-2.88112100
C	-0.64086900	4.13478200	-1.55507400
H	-0.23331300	4.82592000	-0.82909100
C	1.10652000	-3.03902500	-0.65942400
C	0.01272100	-4.02336000	-0.21749500
H	-0.21756300	-3.93889600	0.84483100
H	0.35206100	-5.04860500	-0.41388600
H	-0.90621100	-3.85888600	-0.78450600
C	2.39866500	-3.32515500	0.11901400
H	3.14679300	-2.54541700	-0.00191200
H	2.84210000	-4.26310000	-0.23619100
H	2.21015800	-3.44152600	1.18882400
C	1.31284300	-3.21995900	-2.17479300
H	0.38061500	-3.01901200	-2.70933000
H	1.60686800	-4.25843500	-2.37530600
H	2.09179600	-2.56251100	-2.56239400
C	5.39688500	-1.18767400	-0.49383300
C	4.98119700	-1.78530600	-1.71866200
C	5.77315800	-2.78532500	-2.30638500
C	6.94886000	-3.15234400	-1.66290800
C	7.34363800	-2.55194300	-0.44754100
C	6.57102100	-1.56742600	0.16239100
C	3.43724500	-0.35645600	-1.20432100
H	5.46154500	-3.25197400	-3.23540000
H	7.57952600	-3.92152700	-2.09863900
H	8.26875700	-2.86892300	0.02435200
H	6.87190100	-1.11815900	1.10381600
N	4.40176100	-0.28353600	-0.18945600
N	3.78370500	-1.24801300	-2.12932200

C	4.36405300	0.69644600	0.88237900
H	3.54072700	0.44521000	1.55722700
H	5.29208000	0.61860700	1.45226700
C	4.19584300	2.13168100	0.33488900
H	3.93803600	2.78939500	1.16991300
H	5.17230700	2.46734300	-0.04654300
C	2.64250100	3.66437000	-1.00667900
H	1.92491100	3.70025900	-1.82734600
H	2.18764000	4.10480800	-0.11711000
H	3.48730200	4.31212500	-1.28616100
C	3.15998700	2.26651400	-0.77023600
C	3.37696000	1.43441400	-1.91086800
H	2.69727500	1.55210200	-2.75587100
H	4.38941600	1.20762600	-2.23376100
C	-5.47456700	0.76466800	-0.57935200
H	-5.60131400	1.74846500	-0.12759400
C	-4.38931100	0.59803000	-1.35029900
H	-3.72640300	1.45921600	-1.43808300
C	-3.88911800	-0.59190900	-2.13053500
H	-3.73921600	-0.26329000	-3.17189100
C	-4.70660600	-1.89143900	-2.13103600
H	-4.92202300	-2.19052700	-1.10317500
H	-4.05877800	-2.68276700	-2.52892400
C	-5.99234100	-1.87666900	-2.98078600
H	-5.69813100	-1.94928800	-4.03663800
H	-6.56836300	-2.78738100	-2.76570200
C	-6.90919600	-0.65052200	-2.85101400
H	-6.34659500	0.24721300	-3.13042600
H	-7.71038200	-0.74789100	-3.59528800
C	-7.56300800	-0.41854900	-1.48398700
H	-8.22984700	-1.25772800	-1.24432400
H	-8.20235700	0.47063800	-1.56132900
C	-6.58348200	-0.22436600	-0.30195100
H	-7.15789300	0.12125900	0.56526100
H	-6.17152700	-1.19360700	-0.01366300
H	-2.87657600	-0.81919700	-1.76978100

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Fe	-2.84710100	-2.61800900	0.70429600
P	-0.29260700	-1.18201700	-1.22784500
P	-1.12285900	1.68632800	0.03171700
O	-1.36367200	-1.11315100	-2.33584700
C	-1.07636200	-1.60625400	0.38210100
C	-2.09636800	-0.71835000	0.88973400

C	-2.51373000	-1.19097700	2.17093400
H	-3.29020900	-0.75866800	2.78564300
C	-1.77592600	-2.37562600	2.46334900
H	-1.89505200	-2.99859200	3.33934800
C	-0.89361500	-2.63039900	1.37094700
H	-0.23709700	-3.48306900	1.29661300
C	-2.57003900	0.48578900	0.13683800
H	-2.70271200	0.18435700	-0.90573300
C	-3.85445600	1.11266100	0.66752900
H	-3.75210400	1.44502900	1.70338500
H	-4.66256300	0.37595300	0.62756300
H	-4.14956400	1.97264000	0.05918100
C	-3.44951000	-3.30755000	-1.14724800
H	-2.87773800	-3.05851100	-2.02950300
C	-4.46113700	-2.48309500	-0.57099700
C	-4.86705200	-3.07089000	0.66661900
C	-4.10250000	-4.26193600	0.85751000
H	-4.14873400	-4.91586500	1.71751000
C	-3.22801000	-4.40703500	-0.26333000
H	-2.49582300	-5.19086000	-0.39729700
C	-1.16246400	2.51579900	1.65588900
C	-0.35048200	1.96325400	2.65836400
H	0.30133100	1.13267100	2.41212600
C	-0.38942700	2.45950100	3.96085100
H	0.24343200	2.01869600	4.72511700
C	-1.23996000	3.51970200	4.27691400
H	-1.26667800	3.91406400	5.28817000
C	-2.06648500	4.06397200	3.29200500
H	-2.74322800	4.87689700	3.53735500
C	-2.03926400	3.55957800	1.99178000
H	-2.71270000	3.96982500	1.24912800
C	-1.62388900	2.82984600	-1.30167500
C	-1.87777400	2.21971400	-2.54561700
H	-1.80973900	1.13644600	-2.64721500
C	-2.18108700	3.00539000	-3.65599000
H	-2.37720900	2.52649400	-4.61073700
C	-2.22390300	4.39772100	-3.54659700
H	-2.45971000	5.00570800	-4.41494500
C	-1.95030400	5.00499700	-2.32118300
H	-1.96625400	6.08724200	-2.23239100
C	-1.64609900	4.22670900	-1.20285400
H	-1.40886900	4.71587000	-0.26602100
C	0.93105600	-2.56861400	-1.58308000
C	0.18549500	-3.90303500	-1.73049700

H	-0.32795100	-4.19214300	-0.81150700
H	0.89221600	-4.70128500	-1.99092300
H	-0.56137900	-3.83970900	-2.52697600
C	2.00068700	-2.63821700	-0.48393100
H	2.43948500	-1.65543200	-0.29213500
H	2.81830800	-3.30048700	-0.79210900
H	1.60792400	-3.01486300	0.46221000
C	1.60210000	-2.22626100	-2.92460600
H	0.85680800	-2.04260600	-3.70380800
H	2.23756100	-3.06098700	-3.24355500
H	2.24821800	-1.34599700	-2.84777600
Ni	0.69953000	0.78636800	-0.70228300
C	5.03182000	-0.42035000	0.86278800
C	5.51424000	-0.80062000	-0.41806900
C	6.61808600	-1.65566500	-0.51747600
C	7.20225600	-2.10874200	0.66208700
C	6.70866100	-1.72211900	1.92443500
C	5.61363600	-0.86947500	2.04875100
C	3.83544500	0.49066200	-0.76446000
H	6.99530600	-1.95329400	-1.49058700
H	8.05691900	-2.77667600	0.61259400
H	7.19064600	-2.10026900	2.82090400
H	5.23144500	-0.57774200	3.02179700
N	3.95993100	0.41673500	0.60253800
N	4.73783900	-0.21656600	-1.41251800
C	3.06302800	1.09297500	1.52973100
H	2.21160500	0.43654700	1.74869000
H	3.60263000	1.27347400	2.46278700
C	2.59556300	2.40680000	0.90274800
H	1.86341400	2.87546300	1.56587000
H	3.45991700	3.08942500	0.85573800
C	1.70299300	3.55979200	-1.17018800
H	1.19853000	3.41967200	-2.13035500
H	1.05694200	4.18410700	-0.54655800
H	2.62683000	4.13088600	-1.35480700
C	2.00579800	2.24135900	-0.49106000
C	2.68774300	1.22575700	-1.35913500
H	1.94679600	0.32806400	-1.65410900
H	2.91517400	1.57124000	-2.36991500
H	-5.59469800	-2.66561200	1.35646500
H	-4.81924300	-1.54942600	-0.98189000

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Fe	-1.82632100	-1.46048200	-2.92792300
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P	-0.64106900	0.54634200	-0.28360800
P	0.92938100	-2.05868000	0.82147000
O	-1.94169000	0.14257800	0.44073400
C	-0.41014600	-0.49203400	-1.78193500
C	-0.33267700	-1.92348000	-1.60170300
C	-0.04946300	-2.52470900	-2.86539400
H	0.02929300	-3.58455200	-3.06107600
C	0.03467600	-1.48505900	-3.83782800
H	0.18855100	-1.61990500	-4.89988400
C	-0.18269900	-0.23896100	-3.17625700
H	-0.21848100	0.72130900	-3.66620300
C	-0.51359700	-2.58477400	-0.27098700
H	-1.36353500	-2.10240000	0.21889000
C	-0.73601800	-4.09190500	-0.32628000
H	0.09743000	-4.61617500	-0.79995700
H	-1.64065200	-4.30309500	-0.90488300
H	-0.87309300	-4.50360900	0.67782600
C	-3.66319700	-0.76611500	-2.28547800
H	-3.75374600	-0.04692800	-1.48632600
C	-3.58124800	-2.18014400	-2.11726700
C	-3.35699900	-2.77084900	-3.39888700
C	-3.29867900	-1.71800100	-4.36239100
H	-3.10640400	-1.83493100	-5.42014000
C	-3.48984800	-0.48085100	-3.67331200
H	-3.46692900	0.50373300	-4.11887700
C	2.26304900	-3.19620300	0.31355700
C	3.13962700	-2.73469000	-0.68080200
H	3.03838100	-1.72003600	-1.04862900
C	4.12144700	-3.57206000	-1.20932600
H	4.78996900	-3.19953600	-1.97953900
C	4.24181900	-4.88330400	-0.74748200
H	5.01037100	-5.53518400	-1.15157500
C	3.36224200	-5.35923800	0.22670700
H	3.43917700	-6.38442800	0.57609200
C	2.37093400	-4.52728200	0.74686400
H	1.67463700	-4.92346400	1.47577800
C	0.33949100	-2.45087800	2.50590200
C	-0.85537600	-1.80673800	2.88317700
H	-1.37597500	-1.16200900	2.17443600
C	-1.35064300	-1.96335500	4.17638700
H	-2.27350400	-1.46499600	4.45830700
C	-0.66333500	-2.74650700	5.10730300
H	-1.05284800	-2.86485100	6.11406000
C	0.53210100	-3.36573400	4.74293500

H	1.08017100	-3.96278200	5.46584400
C	1.03656800	-3.21556200	3.44980400
H	1.98108400	-3.67938800	3.19316000
C	-0.76086700	2.32405100	-0.88631100
C	-1.98870900	2.47993800	-1.79505500
H	-1.89746700	1.89190100	-2.71102200
H	-2.11542900	3.53230800	-2.07934300
H	-2.89466000	2.15657800	-1.27602200
C	0.53339900	2.74652900	-1.59434100
H	1.41165300	2.53751000	-0.97640200
H	0.52429900	3.82647500	-1.78426300
H	0.67403500	2.24330400	-2.55278700
C	-0.95400800	3.19509800	0.36721400
H	-1.77954000	2.82657800	0.98093800
H	-1.17719500	4.22678800	0.07093200
H	-0.05268200	3.22934600	0.98778600
Ni	1.25255100	0.07966200	0.86067800
C	4.52433700	3.24576200	-0.59022100
C	3.90176000	4.35631600	0.04017500
C	4.20513400	5.65492100	-0.38540400
C	5.11546800	5.80558600	-1.42767500
C	5.72240600	4.69180300	-2.04230200
C	5.43847300	3.38998100	-1.63464700
C	3.14147800	2.60358900	1.01743800
H	3.73579400	6.51082700	0.08887500
H	5.36497300	6.80228700	-1.77888000
H	6.42539100	4.85157600	-2.85424400
H	5.90351900	2.53360100	-2.11257300
N	4.01983200	2.13722900	0.06872100
N	3.03798000	3.91633400	1.03695900
C	4.28199300	0.72181000	-0.15275800
H	3.54547100	0.32700400	-0.86392600
H	5.27485500	0.61843700	-0.59683500
C	4.19604300	-0.01447400	1.18447900
H	4.31910400	-1.08669500	1.00944300
H	5.04845800	0.30393100	1.80696500
C	2.87681300	-0.34881200	3.32450000
H	1.89679500	-0.24963100	3.79998600
H	3.12445200	-1.41336200	3.30246000
H	3.61764200	0.14463800	3.97344800
C	2.89538200	0.24173100	1.93116200
C	2.35455900	1.63583500	1.82628200
H	1.28832100	1.65637400	1.26889500
H	2.03754600	2.07449500	2.77477300

H	-3.21578700	-3.82412100	-3.59977000
H	-3.63024100	-2.70461600	-1.17316900
C	-5.58373100	2.24490300	-0.23985300
H	-6.10683800	2.39634700	-1.18395400
C	-5.55979000	0.99167100	0.23571300
H	-6.04814900	0.23594300	-0.38178300
C	-4.93493500	0.40828100	1.47957400
H	-5.69619900	-0.21304000	1.97732100
C	-4.28908100	1.34379000	2.51011700
H	-3.52780000	1.94304000	2.01070900
H	-3.72918600	0.71396200	3.21354000
C	-5.24597600	2.22079900	3.34026700
H	-5.74320600	1.57701400	4.07927400
H	-4.64570000	2.93495700	3.92159000
C	-6.35040100	2.98093600	2.58955100
H	-7.00231200	2.25854300	2.08642100
H	-6.97859900	3.48542200	3.33560800
C	-5.89702500	4.03099800	1.56840500
H	-5.33694600	4.82682300	2.07802400
H	-6.79500500	4.50534400	1.15113700
C	-5.03005600	3.49321000	0.40533000
H	-4.94459300	4.27896200	-0.35399900
H	-4.01538300	3.32001300	0.76452200
H	-4.15039700	-0.27904100	1.13876500

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Ni	-0.13602500	-0.22159200	-0.66076200
C	-2.05904600	0.14325000	-0.69329200
C	-1.91584100	-0.63985600	-1.98193100
C	-2.89167600	-0.55176800	0.37525400
C	-2.52758100	1.58426100	-0.87567100
H	-2.11759400	-0.05202900	-2.88050700
H	-0.84495300	-1.02132000	-2.16799300
H	-2.48013900	-1.57456800	-2.00273500
C	-4.36768200	-0.64223200	-0.03521400
H	-2.82137900	0.00255600	1.31428600
H	-2.51788900	-1.55832700	0.56255400
C	-4.01885800	1.66287700	-1.02915300
H	-2.05984100	2.06729600	-1.73745200
H	-2.24525800	2.18593100	-0.00444600
N	-4.82320900	0.63714400	-0.56932200
H	-4.99451700	-0.90785400	0.82251100
H	-4.51073200	-1.41414700	-0.80269700
N	-4.70401200	2.65752200	-1.55529400

C	-6.13164100	1.00242900	-0.83966500
C	-6.03739600	2.27869500	-1.45178300
C	-7.35120000	0.36150800	-0.61969100
C	-7.20322600	2.94334300	-1.84895300
C	-8.49922500	1.04194300	-1.02396700
H	-7.40904600	-0.61907700	-0.15772100
C	-8.42562200	2.31261700	-1.62763200
H	-7.14483200	3.92109700	-2.31679300
H	-9.47086500	0.58158100	-0.87158500
H	-9.34422300	2.80821800	-1.92763600
H	-1.78493100	2.66475100	2.15290900
C	-1.63355300	1.79648800	2.78319900
C	-0.60576000	0.88516100	2.49741900
C	-2.47321100	1.59310900	3.87940200
P	0.43415900	1.01095000	1.00387900
C	-0.44230100	-0.23650400	3.32651500
C	-2.29814000	0.48040000	4.70250500
H	-3.26477600	2.30690600	4.08641200
C	0.48718100	2.76966100	0.52226200
H	0.33509900	-0.96261700	3.11162200
C	-1.27868400	-0.43289400	4.42412600
H	-2.95123600	0.32467600	5.55565800
C	0.61379900	3.05805400	-0.84471800
C	0.52440700	3.82078800	1.45060600
H	-1.13580900	-1.30230300	5.05839800
H	0.60645200	2.24006800	-1.55880000
C	0.76799700	4.37300400	-1.27827700
C	0.67201900	5.13715300	1.01328600
H	0.43343000	3.61545200	2.51142300
H	0.86651200	4.58352600	-2.33876000
C	0.79369600	5.41493600	-0.34942900
H	0.69357100	5.94544500	1.73808300
H	0.90768400	6.44085000	-0.68632400
C	2.19923600	0.67948400	1.58637900
C	3.06683000	1.11933000	0.44423500
H	2.25253700	-0.41129800	1.66174900
C	2.56471900	1.33501300	2.91558000
C	3.06616200	0.49495500	-0.85656700
C	3.93261500	2.25503100	0.40153900
H	2.46312000	2.42234500	2.87012900
H	3.60836500	1.10721500	3.15418000
H	1.93917900	0.96978300	3.73198400
P	1.97891100	-0.96522700	-1.11970300
C	3.95406100	1.26443000	-1.68110700

H	4.16521300	2.90875500	1.22888500
C	4.48421000	2.33859700	-0.90788600
O	2.42166400	-2.12578800	-0.20701000
H	4.22099600	1.05494900	-2.70479200
H	5.21427900	3.06164000	-1.24527200
C	2.23281200	-1.44639100	-2.92761200
C	3.70109600	-1.82067800	-3.17958100
C	1.75982500	-0.31280000	-3.84694100
C	1.37476900	-2.69790700	-3.17889500
H	4.37673000	-0.97301100	-3.06113500
H	3.82287100	-2.21006700	-4.19864600
H	4.01670100	-2.59902000	-2.47904300
H	0.71462800	-0.05290600	-3.64241800
H	1.82374600	-0.62131000	-4.89804900
H	2.35295200	0.59715700	-3.73149900
H	1.66895700	-3.51532800	-2.51526800
H	1.50093800	-3.03491400	-4.21515900
H	0.30875200	-2.50347100	-3.02423000
Fe	4.96194900	0.51175000	-0.04276300
C	6.37161700	-0.84435600	-0.71530300
C	5.48900600	-1.46956400	0.21674400
C	7.01927900	0.24589500	-0.05619900
H	6.49374400	-1.11947300	-1.75348100
H	4.76133000	-2.24036600	0.00408400
C	5.59195500	-0.76317900	1.45235900
C	6.53749700	0.29530400	1.28690100
H	7.72212600	0.93468500	-0.50468500
H	5.01963100	-0.97246500	2.34552100
H	6.81296500	1.02733300	2.03375500
C	-0.57722000	-3.46859400	-0.10835300
H	0.35993600	-3.19463200	-0.58352200
C	-0.61505300	-3.25359400	1.21530100
H	0.28520600	-2.79986800	1.62893200
C	-1.68234700	-3.53649800	2.24404600
H	-1.21957000	-4.12301100	3.05325500
C	-2.98436300	-4.22883500	1.81249100
H	-3.42907600	-3.68773600	0.97333200
H	-3.70279200	-4.12271500	2.63525700
C	-2.87012600	-5.73284700	1.49113600
H	-2.78772400	-6.27324300	2.44371400
H	-3.81450100	-6.06493200	1.03833200
C	-1.69484200	-6.18438600	0.61051500
H	-0.75371500	-5.91208300	1.10008700
H	-1.70772800	-7.28119800	0.57194100

C	-1.67019200	-5.66366000	-0.83119300
H	-2.54730700	-6.03656800	-1.37701000
H	-0.79067400	-6.09059800	-1.32927400
C	-1.61987400	-4.12460400	-0.97912700
H	-1.40288000	-3.89154600	-2.02778300
H	-2.61252400	-3.71281300	-0.78084200
H	-1.94272600	-2.57798000	2.71354900

TS3

Ni	0.15261100	0.70729200	-0.41202900
C	2.34522200	0.75946800	-0.67984100
C	2.05142700	0.53136600	-2.16236100
C	3.44360000	1.82546700	-0.47583900
C	2.81944800	-0.51044400	0.03257900
H	2.84516400	-0.05115800	-2.64726500
H	1.12569900	-0.04594900	-2.30998100
H	1.94373000	1.47618400	-2.70223600
C	4.76671000	1.42892400	-1.13939300
H	3.61375900	1.95981900	0.59802900
H	3.14246500	2.79307600	-0.88049100
C	4.23372000	-0.88085600	-0.30138900
H	2.19459000	-1.37145900	-0.20977000
H	2.75608800	-0.36458600	1.11379800
N	5.11248400	0.05617000	-0.79812900
H	5.57002200	2.09065600	-0.80025400
H	4.69842200	1.52292200	-2.22999700
N	4.77752800	-2.07188000	-0.15016800
C	6.32315900	-0.58923000	-0.99347100
C	6.09441500	-1.92521300	-0.57240800
C	7.55563400	-0.15336800	-1.47981200
C	7.13703200	-2.85671400	-0.63279700
C	8.57921400	-1.09911900	-1.53116400
H	7.71484500	0.87018100	-1.80423600
C	8.37254100	-2.42837500	-1.11358000
H	6.97625800	-3.88146700	-0.31289400
H	9.55641400	-0.80436900	-1.90176700
H	9.19689800	-3.13315400	-1.17001000
H	1.98776500	-2.82051500	1.84463900
C	1.74473900	-2.10719100	2.62346300
C	0.68895400	-1.19970900	2.44972600
C	2.51611100	-2.08168300	3.78637500
P	-0.28750700	-1.08477900	0.90082900
C	0.42759700	-0.26627400	3.46823600
C	2.24647600	-1.15266200	4.79117000

H	3.33457600	-2.78627700	3.89744400
C	-0.24191300	-2.74577700	0.13969600
H	-0.38222800	0.44795000	3.35638100
C	1.19772600	-0.24414100	4.62897900
H	2.84944600	-1.13399600	5.69391100
C	-0.27901100	-2.80043500	-1.26086200
C	-0.27612300	-3.94214100	0.87228500
H	0.97778400	0.48217700	5.40562700
H	-0.26892700	-1.87416600	-1.82582800
C	-0.35598900	-4.02585900	-1.92063900
C	-0.34558700	-5.16737600	0.21059500
H	-0.24081300	-3.91733500	1.95559400
H	-0.39010600	-4.05424000	-3.00551100
C	-0.38796100	-5.21120200	-1.18476700
H	-0.36740000	-6.08875700	0.78488600
H	-0.44311000	-6.16742900	-1.69628600
C	-2.07468200	-0.95351900	1.51203500
C	-2.91096200	-1.31494700	0.32291000
H	-2.20454700	0.11162200	1.73032100
C	-2.41585300	-1.78718200	2.74615400
C	-2.95802000	-0.56074200	-0.90372100
C	-3.69237100	-2.49882800	0.15803700
H	-2.23079200	-2.85088200	2.57644500
H	-3.47850700	-1.66447700	2.97876000
H	-1.83791900	-1.48095000	3.61838400
P	-2.01442100	1.00861900	-1.07712000
C	-3.80309400	-1.29862500	-1.80410600
H	-3.86849900	-3.25281200	0.91033800
C	-4.24550600	-2.48415700	-1.15199400
O	-2.66904100	2.15952700	-0.29351500
H	-4.09687000	-1.00146800	-2.79714500
H	-4.92509700	-3.21740200	-1.56420000
C	-2.12463300	1.39615500	-2.92830900
C	-3.57443400	1.78750200	-3.26158900
C	-1.62145300	0.24398800	-3.80771500
C	-1.23288200	2.62181700	-3.17071600
H	-4.27946800	0.96680200	-3.12294700
H	-3.64053600	2.11718300	-4.30642500
H	-3.89746200	2.61109700	-2.61946400
H	-0.58309800	-0.01020200	-3.57217800
H	-1.64650900	0.54616400	-4.86250000
H	-2.21588000	-0.66515600	-3.71078000
H	-1.51669600	3.45062800	-2.51722900
H	-1.32972200	2.95771900	-4.21060600

H	-0.18161300	2.38194500	-2.99194000
Fe	-4.84685200	-0.79419000	-0.10457900
C	-6.41390500	0.43168900	-0.66744100
C	-5.56596800	1.10945200	0.25925300
C	-6.91626800	-0.74724000	-0.03388100
H	-6.60692200	0.73417900	-1.68724700
H	-4.93646800	1.96345600	0.05085200
C	-5.54170200	0.34704300	1.46538300
C	-6.37704600	-0.79891900	1.28749800
H	-7.55817700	-1.49004400	-0.48752500
H	-4.95672300	0.57878700	2.34469300
H	-6.53945800	-1.58768100	2.00943500
C	1.71480900	5.02528600	-0.48633400
H	1.88115300	5.72224400	-1.30722600
C	0.94746000	3.95433200	-0.76824900
H	0.58772100	3.89308800	-1.79089700
C	0.44853900	2.85617000	0.09979700
H	-0.64063000	2.80915900	0.00027900
C	0.82016400	2.82719200	1.58721400
H	1.89459000	2.96090500	1.72113200
H	0.61542500	1.82041400	1.96173100
C	0.03153500	3.81845800	2.46534500
H	-0.99504000	3.44130400	2.55717700
H	0.46290300	3.80157400	3.47620000
C	-0.05472800	5.26608000	1.96374100
H	-0.57272200	5.27499600	0.99905200
H	-0.69804100	5.82470800	2.65552600
C	1.26690800	6.03320800	1.82895500
H	1.74541800	6.12887700	2.81311400
H	1.02778200	7.05355000	1.50338700
C	2.30250500	5.43564300	0.84155700
H	3.07783800	6.19018400	0.66689700
H	2.81490700	4.59517200	1.31498800
H	1.34120400	1.75425400	-0.25937100

TS3'

Ni	-0.09909300	-0.29133800	-1.15967500
N	0.96386200	1.25126700	-1.21322700
C	1.02427700	2.64076700	-1.32368000
C	2.22655600	0.75307900	-1.07675100
C	2.39078700	3.00056700	-1.24310300
C	0.04311500	3.62498700	-1.48180000
H	1.77971800	-0.72961000	-0.91319300
N	3.09516900	1.80589500	-1.09794200

C	2.80962400	4.33070200	-1.30095300
C	0.46366400	4.95246800	-1.54583900
H	-1.00220700	3.34371000	-1.53169200
C	4.54658500	1.64139500	-1.08061400
C	1.82338500	5.30311800	-1.45393100
H	3.85692800	4.59377900	-1.20151400
H	-0.27888400	5.73671300	-1.66338700
H	4.76159000	0.69506000	-1.58212400
H	4.98070600	2.44744600	-1.67927500
C	5.19114200	1.62213300	0.31510800
H	2.11088100	6.34945900	-1.49917300
H	4.74543800	0.80634400	0.89397900
H	6.24495900	1.36285700	0.16172700
C	5.08741500	2.93704700	1.05759000
C	3.90175700	3.10100000	1.96566800
C	6.00374100	3.89832200	0.89347500
H	3.88543800	4.08497700	2.44129700
H	2.95958700	2.97023900	1.42595300
H	3.91344100	2.33659800	2.75193900
H	5.92358400	4.85552800	1.40237200
H	6.86858000	3.76013000	0.24830100
C	1.43073400	-1.95640500	-0.87672200
C	-0.00091700	-2.48085900	-0.78401400
C	2.13322500	-2.40524100	-2.17488700
C	2.20585300	-2.30339200	0.42803600
H	-0.37766100	-2.51118500	0.23462900
H	-0.77376700	-1.91044400	-1.39078800
H	-0.12574500	-3.47165600	-1.24028700
C	3.14082900	-3.54462900	-1.97605100
H	2.69434300	-1.55454900	-2.58516200
H	1.39300500	-2.69391600	-2.92881700
C	3.66713000	-2.46821200	0.19421600
H	1.81315900	-3.23414500	0.86261900
H	2.05935000	-1.51951500	1.17597500
N	4.07794800	-3.12880300	-0.94244400
H	3.70082300	-3.73464000	-2.89485900
H	2.64743900	-4.47998500	-1.68316700
N	4.66814300	-2.05659700	0.94621800
C	5.46290900	-3.14160600	-0.92759000
C	5.81394600	-2.46376400	0.27141500
C	6.41825500	-3.64660300	-1.80986700
C	7.16356900	-2.28397800	0.59570100
C	7.75570700	-3.45502200	-1.46563300
H	6.13950700	-4.16750800	-2.72053900

C	8.12212500	-2.78456300	-0.28206000
H	7.44250700	-1.76568300	1.50774000
H	8.53196200	-3.83315400	-2.12414000
H	9.17580400	-2.65782300	-0.05176900
H	0.83584900	0.69568000	4.12431200
C	0.58320800	1.59730500	3.57656600
C	-0.28249200	1.53107800	2.47239500
C	1.10849800	2.81984800	3.99524100
P	-0.92228800	-0.06281000	1.81559600
C	-0.55178400	2.71217100	1.76017100
C	0.80441800	3.99216700	3.30148500
H	1.76324700	2.85289200	4.86131700
C	-1.11636800	-1.12974600	3.31155700
H	-1.16559200	2.68646600	0.86695900
C	-0.01349000	3.93012200	2.17298000
H	1.21914500	4.94211100	3.62493200
C	-0.99106800	-2.51655600	3.13660900
C	-1.42443900	-0.64817800	4.59567300
H	-0.22653400	4.82660000	1.59920700
H	-0.74727600	-2.91411900	2.15719200
C	-1.17633100	-3.39835200	4.20276900
C	-1.59941400	-1.52591000	5.66442000
H	-1.52345200	0.41799900	4.76185800
H	-1.07517400	-4.46784300	4.04269100
C	-1.47839300	-2.90400600	5.47118200
H	-1.83434500	-1.13293300	6.64946900
H	-1.61479600	-3.58602300	6.30524600
C	-2.72744200	0.39232900	1.43724600
C	-3.26815500	-0.69250200	0.55539600
H	-2.63172400	1.28175400	0.81209500
C	-3.59726300	0.72551600	2.64573600
C	-3.08069700	-0.75641700	-0.87689400
C	-3.94183000	-1.88304500	0.95776200
H	-3.73861200	-0.13389400	3.30551400
H	-4.58266200	1.06168500	2.31216000
H	-3.14521200	1.53031900	3.23193300
P	-2.07008200	0.49010300	-1.73507200
C	-3.65169300	-1.99630100	-1.32914900
H	-4.25850000	-2.11169200	1.96507500
C	-4.18561400	-2.68042000	-0.19927500
O	-2.48824300	1.89749000	-1.32852100
H	-3.72131800	-2.33066500	-2.35284800
H	-4.72763600	-3.61582800	-0.22329000
C	-2.17792000	0.26168000	-3.59232400

C	-3.63721700	0.39161500	-4.05163900
C	-1.57599100	-1.08194300	-4.02758000
C	-1.33953800	1.40460900	-4.19264100
H	-4.26887200	-0.40337600	-3.64813200
H	-3.68260600	0.34159600	-5.14651900
H	-4.05531800	1.35265300	-3.74174800
H	-0.52567500	-1.15959000	-3.72698300
H	-1.61344000	-1.16229000	-5.12042600
H	-2.11074400	-1.94127700	-3.61659700
H	-1.72978100	2.38141100	-3.89816400
H	-1.36281600	1.33804200	-5.28665700
H	-0.29544900	1.34741600	-3.86966100
Fe	-5.09100200	-0.83169200	-0.42175400
C	-6.68424800	-0.61636900	-1.73380700
C	-6.13836000	0.66275800	-1.41655800
C	-7.12058300	-1.22326900	-0.51609900
H	-6.73028600	-1.06351000	-2.71708500
H	-5.68568900	1.35547400	-2.10917400
C	-6.23489400	0.84814400	-0.00662700
C	-6.84211600	-0.31718600	0.55178100
H	-7.54812100	-2.21140000	-0.41608200
H	-5.87821600	1.71000700	0.53796400
H	-7.01777600	-0.49959700	1.60282100

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Ni	-0.88516200	-0.75437100	-0.48636800
H	-2.08371900	-0.58429900	-2.80068300
C	-2.29769100	-1.18782300	-1.92579700
N	-3.63665100	-1.38144000	-1.56849800
N	-1.51517600	-2.24351800	-1.52807100
C	-3.69708200	-2.54159200	-0.82047800
C	-4.75477600	-0.59314300	-2.05807600
C	-2.37704600	-3.06230200	-0.78316000
C	-4.75336700	-3.18117100	-0.16820100
H	-4.85019500	-0.74652600	-3.14139700
H	-5.66312000	-0.98627900	-1.59669400
C	-4.64054400	0.90685000	-1.78419000
C	-2.10980900	-4.24976900	-0.09998600
C	-4.46480500	-4.36325100	0.51799600
H	-5.76292400	-2.78410400	-0.19231400
H	-3.68375600	1.28098500	-2.17040400
H	-5.40799600	1.40432900	-2.39384100
C	-4.79386600	1.37005700	-0.35425000
C	-3.16430200	-4.89165200	0.55212900

H	-1.10641800	-4.66137000	-0.08903900
H	-5.26668900	-4.88466600	1.03211700
C	-4.89121300	2.86643700	-0.20486100
C	-4.83888800	0.55121000	0.70103400
H	-2.97717400	-5.81464000	1.09250600
H	-4.99166900	3.16398300	0.84249500
H	-4.00538800	3.36075100	-0.61958600
H	-5.75677000	3.26168000	-0.75315100
H	-4.95180800	0.94444700	1.70636800
H	-4.74622800	-0.52493300	0.61966100
P	-0.52957700	1.16477100	0.41691700
C	1.30630300	1.54417100	0.73432400
C	-1.08879100	2.64303200	-0.52210200
C	-1.20833000	1.31806400	2.11940400
C	2.08566200	0.99565000	-0.42132200
H	1.53878400	0.92086900	1.60095700
C	1.62424900	2.99670300	1.07729100
C	-1.27494200	2.48036500	-1.90299100
C	-1.25946100	3.92189800	0.03232600
C	-0.62118700	0.51898400	3.11793100
C	-2.33727200	2.08098900	2.44326500
C	2.35569700	-0.40927900	-0.63914500
C	2.64425300	1.71444300	-1.51696600
H	1.39649100	3.67647500	0.25311200
H	2.68716200	3.09889900	1.31445100
H	1.05032800	3.31946800	1.95044800
H	-1.13553600	1.49419100	-2.33351800
C	-1.63153700	3.56149200	-2.71039300
C	-1.62650700	5.00098800	-0.77178600
H	-1.10606900	4.07833100	1.09328200
H	0.23463600	-0.11213100	2.88881100
C	-1.13750500	0.51584200	4.41258500
C	-2.85097400	2.07449900	3.74151400
H	-2.82650300	2.67296300	1.68151700
P	1.84301000	-1.65762300	0.55533400
C	3.08754900	-0.52313800	-1.87021500
H	2.64195100	2.78911900	-1.62714700
C	3.26473300	0.78451500	-2.40194800
H	-1.77061600	3.41581400	-3.77771200
C	-1.81498800	4.82385700	-2.14447300
H	-1.76198200	5.98203300	-0.32588900
H	-0.66927000	-0.10316300	5.17242100
C	-2.25117800	1.29657600	4.73134200
H	-3.72475900	2.67671300	3.97502100

O	2.17991100	-1.30233700	1.98803100
C	2.37368200	-3.35429300	0.03262900
H	0.41690300	-1.75201300	0.34406900
H	3.47713100	-1.43077800	-2.30274200
H	3.81746000	1.03132900	-3.29783600
H	-2.10102100	5.66574700	-2.76804100
H	-2.65143400	1.29173800	5.74093700
C	3.90521100	-3.46603800	0.04258100
C	1.79067000	-3.69596800	-1.34851300
C	1.77798200	-4.29199400	1.10116300
H	4.36823500	-2.80965200	-0.69750600
H	4.19647500	-4.49688200	-0.19091200
H	4.31478600	-3.21678700	1.02560600
H	0.72535700	-3.45985300	-1.41970100
H	1.91832500	-4.76844300	-1.53761400
H	2.29706100	-3.15891500	-2.15300500
H	2.16855300	-4.06090800	2.09535900
H	2.03439700	-5.32940700	0.85848400
H	0.68684300	-4.21389400	1.14226100
Fe	4.11422100	0.63564700	-0.51067300
C	6.14226800	1.03571100	-0.66778200
C	5.93871600	-0.26684200	-0.11727100
C	5.51588500	1.98234800	0.19816100
H	6.64679100	1.26166000	-1.59716800
H	6.26611300	-1.19926800	-0.55531900
C	5.18707900	-0.12429500	1.08796200
C	4.92635500	1.26360800	1.28288100
H	5.46028900	3.05004800	0.03646400
H	4.80946200	-0.91911200	1.71361500
H	4.34290800	1.68377100	2.08936900

TS4

Ni	-0.75938800	-1.12314500	-0.71377200
H	-1.48198900	-2.28570400	-1.31852600
C	-2.51532900	-1.59845100	-0.37161700
N	-3.63931900	-1.18280600	-1.08821600
N	-2.84867700	-2.16532700	0.78153400
C	-4.75298100	-1.49999000	-0.32086500
C	-3.62528000	-0.69640500	-2.45921600
C	-4.22930900	-2.09320500	0.85937000
C	-6.12359500	-1.32407400	-0.51451300
H	-3.08232100	-1.42986300	-3.06723700
H	-4.65700400	-0.67538400	-2.81768400
C	-2.96358800	0.67054900	-2.66188300

C	-5.09773500	-2.49625300	1.87958400
C	-6.97366800	-1.73905400	0.51417600
H	-6.52431500	-0.88626200	-1.42346800
H	-1.98949200	0.66002400	-2.15087800
H	-2.72649800	0.75986200	-3.73132700
C	-3.72470300	1.90889300	-2.24471300
C	-6.46766200	-2.31101100	1.69478400
H	-4.70094600	-2.93920700	2.78765800
H	-8.04648100	-1.61726400	0.39587500
C	-3.16000000	3.19462600	-2.79080600
C	-4.79963400	1.90319300	-1.44946400
H	-7.15953200	-2.61694000	2.47451900
H	-3.70778500	4.06641700	-2.42290200
H	-2.10776900	3.30948400	-2.51284100
H	-3.19685900	3.20428300	-3.88852400
H	-5.29884200	2.83280400	-1.18727700
H	-5.21141100	0.99961200	-1.01947400
P	-0.35600500	0.68478500	0.52550900
C	1.27693700	0.67159500	1.47811000
C	-0.26384100	2.30879700	-0.31312800
C	-1.67935300	0.80089200	1.77248100
C	2.37490700	0.83604900	0.46191300
H	1.33224300	-0.34283800	1.88327000
C	1.35503900	1.70889100	2.59858700
C	0.33048700	2.33483100	-1.58456500
C	-0.64150500	3.51866200	0.28631900
C	-1.59002100	0.06965700	2.96506500
C	-2.89968500	1.40091900	1.42965400
C	2.75894800	-0.10970400	-0.56825100
C	3.19635000	1.99035300	0.29488600
H	1.21823400	2.72328200	2.21401300
H	2.33347800	1.66078800	3.08726600
H	0.58792200	1.53437400	3.35392700
H	0.61898100	1.40035100	-2.05601300
C	0.56620500	3.54605300	-2.23374300
C	-0.42342200	4.72915300	-0.37311600
H	-1.10947500	3.51367300	1.26479800
H	-0.67503000	-0.45473700	3.22019400
C	-2.69130300	-0.02840800	3.81419500
C	-4.00128800	1.28972600	2.27515800
H	-3.00784800	1.92409300	0.48672900
P	2.00459900	-1.72848300	-0.72502300
C	3.82730400	0.48264000	-1.32837700
H	3.17846300	2.86549900	0.92629800

C	4.08901500	1.77138200	-0.79120600
H	1.03399100	3.55168400	-3.21365700
C	0.18807500	4.74636200	-1.62835600
H	-0.72650700	5.65984500	0.09730600
H	-2.60993300	-0.60169300	4.73280400
C	-3.89978000	0.57867000	3.47151700
H	-4.94487400	1.74220400	1.98544100
O	1.77755400	-2.42813900	0.58823100
C	2.78729400	-2.75669600	-2.05467100
H	0.78752200	-1.44313900	-1.48947200
H	4.36660100	0.02229400	-2.14077300
H	4.86506500	2.44771000	-1.12117200
H	0.36136400	5.69045600	-2.13613200
H	-4.76336100	0.48021100	4.12198200
C	4.26467600	-3.02642400	-1.73206900
C	2.61714000	-2.07305200	-3.42042800
C	1.99735100	-4.07979700	-2.04032600
H	4.86435200	-2.11436200	-1.74493500
H	4.67781800	-3.71450600	-2.47809700
H	4.37499200	-3.49439900	-0.75003200
H	1.56122100	-1.88378300	-3.64248900
H	3.00447400	-2.73338300	-4.20415300
H	3.15341100	-1.12418900	-3.49138100
H	2.09319400	-4.59137100	-1.07999100
H	2.38330300	-4.73678600	-2.82753900
H	0.93132800	-3.91350500	-2.22926300
Fe	4.34642400	0.29818900	0.65966900
C	6.31256100	0.34963800	1.31688100
C	5.99082400	-0.95505200	0.83368300
C	5.42244300	0.65336500	2.39064200
H	7.06946500	1.00856600	0.91427500
H	6.46601600	-1.45960100	0.00454400
C	4.90069400	-1.45651400	1.60775500
C	4.54922000	-0.46279800	2.56839600
H	5.38868800	1.58276700	2.94207200
H	4.37625200	-2.38862000	1.45680400
H	3.73162100	-0.52811400	3.27227600
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Ni	-0.23791600	-0.21884100	-1.11655400
H	-0.21857800	-0.99066100	-2.36790500
C	-1.82244200	-1.13614300	-0.94470200
N	-3.01899600	-1.00063600	-1.62697700
N	-1.89089700	-2.08289200	-0.01776300

C	-3.90499800	-1.93935700	-1.10545200
C	-3.27097600	-0.09530500	-2.73769500
C	-3.17781300	-2.60024900	-0.08170500
C	-5.23212500	-2.25769800	-1.39566800
H	-2.56074100	-0.33136400	-3.53772100
H	-4.27562300	-0.30360400	-3.11251400
C	-3.13058100	1.38909200	-2.39370800
C	-3.79440300	-3.59894900	0.67816700
C	-5.82827700	-3.26242300	-0.62991400
H	-5.78649500	-1.75197500	-2.18020000
H	-2.13078700	1.54881200	-1.96956200
H	-3.13132700	1.94068300	-3.34448800
C	-4.15366200	2.02267000	-1.47656700
C	-5.12101000	-3.92060500	0.39235400
H	-3.24536400	-4.10084400	1.46913500
H	-6.85950500	-3.53882600	-0.82933700
C	-4.11609700	3.52949800	-1.45802400
C	-5.02402600	1.34477400	-0.72000400
H	-5.62048800	-4.69378000	0.96925200
H	-4.84063200	3.94295000	-0.75107700
H	-3.12246500	3.89430600	-1.18219100
H	-4.33568800	3.94003200	-2.45278300
H	-5.72984700	1.87510800	-0.08506500
H	-5.07463900	0.26422500	-0.69207000
P	-0.39123200	1.14915200	0.72250300
C	1.41615000	1.24913500	1.24997500
C	-0.80454400	2.89682800	0.39201600
C	-1.39382700	0.59398400	2.13329800
C	2.10998900	0.88311300	-0.03365300
H	1.58010900	0.42894100	1.95362700
C	1.86537800	2.55996200	1.88559800
C	-0.43231400	3.41425200	-0.85947500
C	-1.34416000	3.75971700	1.35546900
C	-0.86049700	-0.28994400	3.08203900
C	-2.76996800	0.87260900	2.14777700
C	2.15859000	-0.47973700	-0.55899900
C	2.63407600	1.75399900	-1.03629800
H	1.73093700	3.41115800	1.21405200
H	2.92517100	2.49824400	2.15021200
H	1.29508500	2.76099600	2.79664900
H	-0.02931200	2.74770100	-1.61589300
C	-0.57386300	4.77450900	-1.13301000
C	-1.50628800	5.11567100	1.07088600
H	-1.63457300	3.37263500	2.32615600

H	0.18834700	-0.56749600	3.05924700
C	-1.68903700	-0.85900600	4.04904000
C	-3.59169800	0.29613400	3.11362900
H	-3.20659300	1.51573700	1.39091500
P	1.74860700	-1.91065800	0.50414700
C	2.78005300	-0.40183800	-1.86015300
H	2.73906600	2.82469600	-0.94220800
C	3.05114500	0.96411700	-2.14955600
H	-0.27809900	5.16393200	-2.10253300
C	-1.11313600	5.62733400	-0.16762400
H	-1.93183000	5.77514800	1.82129800
H	-1.26564500	-1.54242800	4.77889000
C	-3.05301200	-0.56713600	4.06939200
H	-4.65573400	0.51278300	3.10958200
O	2.37974200	-1.79668900	1.87758900
C	2.06649600	-3.51156600	-0.37516500
H	0.33680000	-1.89483400	0.54476300
H	3.00828100	-1.23654100	-2.50299400
H	3.53370000	1.33389700	-3.04341700
H	-1.23433700	6.68474800	-0.38235800
H	-3.69608700	-1.02077100	4.81759100
C	3.56345600	-3.70793800	-0.64834500
C	1.23896100	-3.59429500	-1.66664700
C	1.56672500	-4.58464400	0.61424600
H	3.95507900	-2.96517700	-1.34734200
H	3.72584300	-4.69962900	-1.08626100
H	4.14708300	-3.65157200	0.27465100
H	0.17912400	-3.41138500	-1.47304600
H	1.33974700	-4.60138500	-2.08917800
H	1.56753500	-2.87946800	-2.42297500
H	2.10930700	-4.54118900	1.56224800
H	1.71393600	-5.57782800	0.17508300
H	0.49823300	-4.46264900	0.82178600
Fe	4.04531600	0.38022700	-0.42734000
C	6.06989600	0.69979300	-0.71582100
C	5.82853500	-0.68342600	-0.45092500
C	5.60379500	1.45030200	0.40587400
H	6.49165300	1.10983700	-1.62317900
H	6.04148700	-1.50406700	-1.12115600
C	5.21298700	-0.78554300	0.83190500
C	5.07164800	0.53043200	1.36023100
H	5.60853500	2.52802300	0.49383600
H	4.82609600	-1.67815500	1.29829400
H	4.60261100	0.78075400	2.30051200

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Ni	-1.98987200	-1.83789800	-0.82868200
H	-3.41101700	-1.40208900	-1.03098300
C	-0.17470700	-2.35570100	-0.37682900
N	0.78930400	-2.66298100	-1.33599400
N	0.32323900	-2.58331900	0.84489500
C	1.91931100	-3.15319800	-0.70043200
C	0.57344700	-2.58287100	-2.76428900
C	1.60588300	-3.08478400	0.68200200
C	3.13842000	-3.65210900	-1.16231700
H	0.31407000	-1.55428900	-3.03440300
H	1.51167700	-2.82771600	-3.26628200
C	-0.52630800	-3.56004200	-3.21570400
C	2.54769600	-3.50664100	1.62921900
C	4.05479900	-4.08697800	-0.20326600
H	3.37113300	-3.70855100	-2.22153900
H	-0.45797700	-3.67623500	-4.30455300
H	-0.32050400	-4.53509600	-2.76480200
C	-1.93451300	-3.11403800	-2.88865700
C	3.76578900	-4.01008500	1.17289200
H	2.31819200	-3.45285600	2.68940000
H	5.01284200	-4.48421700	-0.52532900
C	-2.53072100	-2.09510000	-3.82628100
C	-2.67055200	-3.71775800	-1.91201800
H	4.50727300	-4.35070200	1.88979400
H	-3.52674700	-1.78428200	-3.50781500
H	-1.89384700	-1.20575300	-3.90003100
H	-2.59729300	-2.51882100	-4.83700900
H	-3.73434400	-3.53723100	-1.81172800
H	-2.24360800	-4.52237700	-1.32012900
P	-2.12864000	-0.16735700	0.50963400
C	-0.47788200	0.51275200	1.06620700
C	-3.10604700	1.28785100	-0.03739300
C	-2.90108800	-0.76349100	2.05734400
C	0.38835700	0.86971500	-0.12380100
H	-0.03003100	-0.39299700	1.49220900
C	-0.56628900	1.57042000	2.17238900
C	-3.47639600	1.39896400	-1.38457600
C	-3.43635500	2.33394600	0.84038400
C	-2.18166500	-1.68773400	2.83443000
C	-4.19840000	-0.39918500	2.44053000
C	1.83264200	0.96858800	-0.09707600
C	-0.01266700	1.03272000	-1.48591100

H	-1.03069500	2.48677300	1.81313800
H	0.43658800	1.81856500	2.52637100
H	-1.14598100	1.18649400	3.01713300
H	-3.26356000	0.57554100	-2.05817600
C	-4.11860900	2.54323600	-1.85684900
C	-4.08926300	3.47381400	0.37008200
H	-3.20408800	2.25514900	1.89476400
H	-1.20079600	-2.02375600	2.50479100
C	-2.74727600	-2.20253800	3.99994900
C	-4.75803100	-0.92451900	3.60598600
H	-4.77388800	0.29074300	1.83408500
P	2.83125000	0.81426400	1.40202900
C	2.28013400	1.19348600	-1.44331800
H	-1.02700100	1.06053700	-1.84664900
C	1.14295400	1.22772100	-2.29299800
H	-4.39173900	2.61361800	-2.90555600
C	-4.41945600	3.58763700	-0.98145600
H	-4.34154200	4.27128200	1.06252500
H	-2.18350600	-2.91211400	4.59855800
C	-4.03161900	-1.81925300	4.39241300
H	-5.76284400	-0.63251100	3.89715400
O	2.62859600	1.89592200	2.43931800
C	4.61595600	0.56425800	0.96871800
H	2.45654500	-0.47512900	1.85109900
H	3.29836300	1.35298700	-1.75894500
H	1.14994300	1.42753300	-3.35565400
H	-4.92238400	4.47823600	-1.34618100
H	-4.46783000	-2.22328500	5.30130800
C	5.21156900	1.88380700	0.45400000
C	4.79476900	-0.58679900	-0.02874700
C	5.29153200	0.18489700	2.30257800
H	4.77675900	2.19203700	-0.50011600
H	6.29138100	1.76631100	0.30660400
H	5.05189700	2.69073400	1.17489800
H	4.31806800	-1.50101100	0.32952600
H	5.86357400	-0.79998800	-0.15041100
H	4.38626000	-0.36177400	-1.01511000
H	5.14513800	0.95907300	3.06021800
H	6.36801500	0.05651000	2.14170800
H	4.89784500	-0.75961100	2.69366000
Fe	1.02934900	2.71217000	-0.85534600
C	1.42667000	4.52634000	-1.76809300
C	2.15590000	4.41525200	-0.54536000
C	0.03590800	4.42828100	-1.46092600

H	1.85379300	4.61732800	-2.75754300
H	3.23211600	4.40795700	-0.44446100
C	1.21715100	4.25194500	0.51864900
C	-0.09118300	4.26590600	-0.04880500
H	-0.77951700	4.43421100	-2.17100300
H	1.47074900	4.05307500	1.54964400
H	-1.02301200	4.13327400	0.48009300

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Ni	1.19020200	1.09039200	-0.94022800
H	-0.26930500	1.36671100	-0.93054100
C	3.05455900	0.53974300	-0.92693100
N	3.99158000	1.23957700	-0.16611100
N	3.63144600	-0.51711500	-1.49953500
C	5.21687400	0.60526200	-0.27126600
C	3.71737800	2.50246200	0.48276100
C	4.96720300	-0.50545800	-1.12132800
C	6.47345100	0.84965900	0.28526800
H	2.98909100	2.36075600	1.28925400
H	4.64316900	2.86473600	0.93419800
C	3.20718700	3.53388200	-0.54344300
C	6.00700700	-1.39381400	-1.42287700
C	7.49514200	-0.04723800	-0.03060100
H	6.65560400	1.69505100	0.94230100
H	3.31135900	4.53466800	-0.10667300
H	3.85831200	3.48501200	-1.42059400
C	1.75760100	3.36494400	-0.94897300
C	7.26452300	-1.15292900	-0.87170300
H	5.82479200	-2.24838800	-2.06795300
H	8.48674900	0.10902600	0.38453200
C	0.75376600	3.95205900	0.00866400
C	1.39107100	2.88705700	-2.17810000
H	8.08446400	-1.83123700	-1.09043800
H	-0.26955500	3.79894600	-0.33261300
H	0.85301900	3.51534300	1.00902700
H	0.93543400	5.02997400	0.11254900
H	0.36935800	2.97595700	-2.52975100
H	2.14560000	2.60400100	-2.90607100
P	0.69209400	-0.60533000	0.31157100
C	-1.05053700	-0.81657500	1.00807500
C	1.03917600	-2.21120300	-0.47916000
C	1.73702500	-0.50352500	1.81476300
C	-2.03498900	-0.81803500	-0.12410600
H	-1.22368800	0.08036500	1.60831200

C	-1.16780500	-2.03645500	1.92875100
C	0.94822300	-2.28008300	-1.87610700
C	1.32211200	-3.37425000	0.25011800
C	1.31268400	0.26266400	2.91191500
C	3.03002300	-1.04752400	1.82178800
C	-2.84741700	0.30044900	-0.53935700
C	-2.27250000	-1.88708000	-1.03884300
H	-1.09512700	-2.97161300	1.37035900
H	-2.13789000	-2.01390900	2.42760900
H	-0.38870900	-2.03140500	2.69475700
H	0.75808100	-1.37445700	-2.44226400
C	1.11051600	-3.49812200	-2.53232100
C	1.49523200	-4.59088500	-0.41010200
H	1.41911700	-3.33085500	1.32890100
H	0.32336900	0.70921800	2.92367600
C	2.16138300	0.46557400	4.00094500
C	3.87567200	-0.83902000	2.90976200
H	3.38533600	-1.60808200	0.96556100
P	-2.93580600	1.81262500	0.44726700
C	-3.56574500	-0.10160200	-1.71704700
H	-1.83475200	-2.87213100	-0.97885500
C	-3.20643200	-1.44545600	-2.01824600
H	1.03937700	-3.54052500	-3.61484600
C	1.38224100	-4.65550100	-1.80010900
H	1.71972200	-5.48643000	0.16166000
H	1.81804000	1.05521100	4.84588100
C	3.44460600	-0.08406200	4.00224500
H	4.87787900	-1.25582300	2.89168300
O	-3.37889400	1.60854300	1.87761400
C	-3.85836700	3.12655400	-0.47787500
H	-1.61197700	2.29242200	0.35024900
H	-4.28899700	0.48552200	-2.26061700
H	-3.61400600	-2.04330200	-2.82162200
H	1.51684800	-5.60383100	-2.31208000
H	4.10605800	0.07917700	4.84789600
C	-5.35004100	2.77227400	-0.57655300
C	-3.22678400	3.34104100	-1.86246200
C	-3.69545300	4.40730100	0.36420600
H	-5.52489700	1.84527200	-1.12700600
H	-5.88633800	3.57745000	-1.09202500
H	-5.78929200	2.66124000	0.41898800
H	-2.15366700	3.54718600	-1.78584200
H	-3.69503100	4.20499600	-2.34829800
H	-3.35014300	2.47850200	-2.51960100

H	-4.08991600	4.27212400	1.37466200
H	-4.23846200	5.23133300	-0.11245200
H	-2.64399100	4.70485500	0.44722400
Fe	-4.05506400	-1.30641300	-0.12766100
C	-5.50616300	-2.77292200	0.07183100
C	-6.12000100	-1.49040700	-0.06397900
C	-4.67383500	-2.74163900	1.23193300
H	-5.61574300	-3.60584700	-0.60885300
H	-6.77491200	-1.18240500	-0.86767200
C	-5.66113700	-0.66723400	1.00683000
C	-4.76751600	-1.43840200	1.80738100
H	-4.04389700	-3.54904300	1.57776000
H	-5.88980700	0.37596000	1.16040000
H	-4.21861300	-1.05997600	2.65632600

TS5

Ni	1.26570600	-0.18278000	-1.12653500
H	1.02922600	0.79024100	-2.24819000
C	2.44597900	-1.14232500	0.02091700
C	2.02633600	-1.31103800	-2.60840400
P	0.39838100	1.41939900	0.11189600
N	3.74033000	-0.65073000	-0.21114700
N	2.47847500	-2.17808900	0.84631900
C	2.30739800	0.04227400	-2.94083800
H	1.20567800	-1.80153600	-3.12726200
H	2.81208300	-1.96201000	-2.24971700
C	-1.45293400	1.64276700	-0.25767500
C	0.43084700	1.36568200	1.93813500
C	1.22026000	2.99053300	-0.35808600
C	4.63033100	-1.41029800	0.53481200
C	4.01652900	0.57283800	-0.95649400
C	3.81498400	-2.37289400	1.19046900
C	3.66453000	0.58578900	-2.46572200
C	1.84201900	0.60800500	-4.27459700
C	-2.18372600	0.62629100	0.57471000
H	-1.55013100	1.37043900	-1.31262100
C	-1.97086100	3.06600200	-0.03979500
C	0.59558200	0.11977900	2.55900400
C	0.17262800	2.49955000	2.72713600
C	0.98032100	3.52626400	-1.63474900
C	2.19409000	3.58790600	0.45342200
C	6.01324700	-1.36735500	0.71031700
H	3.48683900	1.39693000	-0.47186900
H	5.08461400	0.78506000	-0.86483100

C	4.40363700	-3.31792200	2.03630500
H	3.76331200	1.62929900	-2.78356500
H	4.42351500	0.01588800	-3.01783000
H	0.86605300	0.20291000	-4.55321300
H	1.77989900	1.69993700	-4.25541100
H	2.56471900	0.32497800	-5.05118400
C	-2.25447900	-0.79936400	0.33780500
C	-2.85335300	0.88700800	1.80857400
H	-1.82397600	3.39887900	0.99033000
H	-3.04335700	3.09921500	-0.25251200
H	-1.46844400	3.77891500	-0.69497600
H	0.81385600	-0.75963100	1.96439900
C	0.49910800	0.01126700	3.94724100
C	0.08060900	2.38564200	4.11303500
H	0.05239400	3.47150000	2.26136700
H	0.25587200	3.05434300	-2.29187600
C	1.67825500	4.64743700	-2.07638800
C	2.90214200	4.70522900	0.00300700
H	2.41012400	3.17811500	1.43362800
C	6.58031300	-2.32127300	1.55869200
H	6.63141800	-0.62720900	0.21028300
C	5.78761400	-3.28247700	2.21094400
H	3.78834300	-4.05747100	2.54046000
P	-1.58158300	-1.59559100	-1.13594000
C	-2.98135200	-1.37975600	1.43386800
H	-2.99334000	1.86041800	2.25316900
C	-3.34324300	-0.34034800	2.33192300
H	0.63395300	-0.95826000	4.41699000
C	0.24006800	1.13966400	4.72499400
H	-0.11514200	3.26846800	4.71467300
H	1.47349500	5.05482600	-3.06205100
C	2.64436700	5.24039000	-1.25809300
H	3.65644000	5.15360400	0.64275400
H	7.65514700	-2.31980800	1.71609600
H	6.26430100	-4.00888100	2.86306800
O	-2.13177900	-1.08220300	-2.44734100
C	-1.60340600	-3.43800400	-0.94130000
H	-0.18194300	-1.34453600	-0.98077400
H	-3.24262300	-2.41945500	1.54689000
H	-3.93194100	-0.45758800	3.23087800
H	0.16871700	1.05251300	5.80526000
H	3.19366100	6.11017100	-1.60541800
C	-3.04804800	-3.96009000	-0.99762200
C	-0.87988500	-3.85139200	0.35060600

C	-0.81628400	-3.97576700	-2.15347900
H	-3.65149000	-3.61594100	-0.15443000
H	-3.04156200	-5.05604500	-0.97772600
H	-3.54451400	-3.64290900	-1.91968600
H	0.12605200	-3.42141700	0.41491800
H	-0.77425300	-4.94266500	0.36745300
H	-1.42672500	-3.55904600	1.24905600
H	-1.24907900	-3.63623100	-3.09856200
H	-0.83451500	-5.07134900	-2.13943900
H	0.23073600	-3.66027600	-2.11446000
Fe	-4.14167000	0.00089400	0.43970800
C	-6.20534600	0.03498300	0.60697700
C	-5.80163300	-0.98700400	-0.30653600
C	-5.72848800	1.28478200	0.10745000
H	-6.73983000	-0.11582600	1.53486000
H	-5.97878000	-2.04714700	-0.19061900
C	-5.07646100	-0.37046300	-1.36982600
C	-5.02960100	1.03214500	-1.11293300
H	-5.84316900	2.24594800	0.58957300
H	-4.55955400	-0.87300900	-2.17416100
H	-4.51434500	1.76576200	-1.71682700

TS5'

P	2.08175300	-0.21071000	0.43476000
C	0.37498000	-0.70149000	1.01245400
C	2.90950400	-1.73823900	-0.15990800
C	2.94792900	0.24891200	1.98326500
C	-0.54225900	-0.92008100	-0.17316600
H	0.04800500	0.23634500	1.47673000
C	0.34573100	-1.79183700	2.08913500
C	3.33541400	-1.79354400	-1.49403000
C	3.10405600	-2.86458700	0.65851400
C	2.36667500	1.24106500	2.79478100
C	4.20411500	-0.27022400	2.32699900
C	-1.97426800	-0.71535900	-0.16471700
C	-0.17501600	-1.25010800	-1.51450000
H	0.62359100	-2.76184800	1.67942400
H	-0.66600100	-1.86202800	2.49356300
H	1.02934000	-1.53915400	2.90547900
H	3.21038200	-0.91619200	-2.12185800
C	3.91033300	-2.95414200	-2.01290400
C	3.68383400	-4.02277700	0.14093900
H	2.82311800	-2.83378000	1.70377300
H	1.41899900	1.69598900	2.51814400

C	3.02343200	1.67038900	3.94665600
C	4.85775400	0.17223100	3.47811300
H	4.67516900	-1.01941900	1.70062200
P	-2.90857400	-0.32110500	1.33272500
C	-2.45151300	-0.91333200	-1.50531800
H	0.81494200	-1.51527600	-1.84861800
C	-1.34239400	-1.24020900	-2.33052200
H	4.23070900	-2.98047000	-3.05016000
C	4.07954100	-4.07362500	-1.19762100
H	3.83060400	-4.88402900	0.78586700
H	2.56302100	2.43178500	4.56928200
C	4.26686500	1.13716800	4.29395600
H	5.82898200	-0.24046400	3.73532800
O	-2.81451300	-1.35511000	2.43203200
C	-4.65284900	0.13296600	0.90598200
H	-2.35823500	0.93390200	1.68906000
H	-3.47841100	-0.87121700	-1.82995900
H	-1.38487900	-1.49169200	-3.38123300
H	4.52843300	-4.97758500	-1.59823400
H	4.77507800	1.47764100	5.19133000
C	-5.42031000	-1.11731200	0.44792100
C	-4.69693900	1.25671800	-0.13721100
C	-5.25734400	0.65054700	2.22725900
H	-5.02579700	-1.53004600	-0.48407600
H	-6.47303600	-0.86055700	0.28171700
H	-5.37991700	-1.90104300	1.20992900
H	-4.10226200	2.11586700	0.17824600
H	-5.73133900	1.60093300	-0.25582700
H	-4.33813400	0.94232400	-1.11838200
H	-5.19998600	-0.10288000	3.01709500
H	-6.31069200	0.90822800	2.06891500
H	-4.74077700	1.55254600	2.57284600
Fe	-1.55542600	-2.62894300	-0.81599700
C	-2.56049900	-4.30920500	-1.49555900
C	-2.94296900	-4.01561600	-0.15272800
C	-1.15105400	-4.53721200	-1.51153200
H	-3.21293500	-4.30826800	-2.35814100
H	-3.93375500	-3.74959400	0.18531100
C	-1.77372500	-4.06500300	0.66272300
C	-0.66625500	-4.38883500	-0.17656200
H	-0.54904500	-4.74171800	-2.38616500
H	-1.74071100	-3.81420500	1.71129400
H	0.36994500	-4.45393400	0.12406300
Ni	2.16332800	1.67222700	-0.65488900

H	3.04457200	1.27124800	-1.82266400
C	0.53269900	2.42720200	-0.03927600
C	2.67030800	3.53811200	-1.15060200
N	-0.20797800	2.73207900	-1.19548200
N	-0.10858100	2.83107300	1.04756500
C	2.72548200	2.78323100	-2.35357900
H	3.59765200	3.73966200	-0.61440200
H	1.87147800	4.24832700	-0.98463100
C	-1.37400400	3.37222200	-0.80280400
C	0.13506100	2.24601800	-2.53060900
C	-1.29116200	3.43004000	0.61511900
C	1.43003800	2.79451600	-3.18004300
C	4.00637400	2.74139200	-3.17250700
C	-2.44997400	3.91545000	-1.50508300
H	0.20126200	1.15581400	-2.48063600
H	-0.70114700	2.48352000	-3.19274000
C	-2.31263000	4.04712900	1.34512000
H	1.57807200	2.20968100	-4.09482000
H	1.26888300	3.83363700	-3.49379000
H	4.88531900	2.71079100	-2.52342800
H	4.03677200	1.87790500	-3.84405600
H	4.06787000	3.65036600	-3.78534300
C	-3.44993600	4.54288400	-0.75838300
H	-2.50817100	3.86845700	-2.58862700
C	-3.38303300	4.60728200	0.64540600
H	-2.25639100	4.09638800	2.42847000
H	-4.29832600	4.98474500	-1.27266000
H	-4.18199200	5.09905100	1.19258300

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Ni	1.56130400	0.29953700	-1.19241600
H	4.18371300	1.21924800	-1.96023500
C	1.95161900	-1.27552800	-0.34919800
C	2.72464500	-0.23007000	-2.58429700
P	0.55211900	1.56980500	0.39879100
N	3.18769300	-1.54505000	0.20805800
N	1.07724400	-2.24041800	-0.10308100
C	4.17888600	0.19618400	-2.36803300
H	2.22774900	0.43343300	-3.32543500
H	2.65495000	-1.25790900	-2.95578100
C	-1.31008700	1.78652100	0.52971800
C	1.07070500	1.28823000	2.12797000
C	1.21035200	3.20708100	-0.09368900
C	3.09384800	-2.76077900	0.87474700

C	4.36792700	-0.70773200	0.06199600
C	1.75310700	-3.18283600	0.66704700
C	4.93362700	-0.69440700	-1.36368700
C	4.94143100	0.23221300	-3.70380500
C	-1.88046200	0.42872200	0.82695200
H	-1.62467800	2.05228100	-0.48384200
C	-1.72261800	2.86813200	1.52711600
C	1.11806100	-0.04010100	2.58057700
C	1.35785100	2.33030400	3.02284800
C	0.48340500	4.03330300	-0.96611600
C	2.53010800	3.56262100	0.23534100
C	3.99887400	-3.50605300	1.62989400
H	4.11203800	0.31085100	0.37648100
H	5.11897400	-1.08281300	0.76137400
C	1.30463300	-4.37957500	1.23553300
H	5.97243700	-0.34452500	-1.30629300
H	4.96849100	-1.72691400	-1.73578400
H	4.45210100	0.90323000	-4.41790800
H	5.97411600	0.57745600	-3.56957800
H	4.97656900	-0.76640600	-4.15567100
C	-2.04713700	-0.64734900	-0.12644500
C	-2.30901100	-0.05497400	2.09895900
H	-1.37277200	2.64096200	2.53719900
H	-2.81244500	2.95059600	1.55777300
H	-1.31254000	3.84001500	1.24125900
H	0.87985400	-0.85024900	1.90232600
C	1.46258800	-0.31908700	3.90305000
C	1.70677300	2.04529100	4.34286600
H	1.31414400	3.36136200	2.68879900
H	-0.52607700	3.76641000	-1.26077800
C	1.05465800	5.20078100	-1.47357500
C	3.09580500	4.73073600	-0.27277900
H	3.11217300	2.92753600	0.89540500
C	3.53234300	-4.69945200	2.18477400
H	5.02270500	-3.17952300	1.78438400
C	2.20622000	-5.12887900	1.99132900
H	0.27980900	-4.70563600	1.08500400
P	-1.60525200	-0.46515500	-1.86555600
C	-2.58956600	-1.76828600	0.58342600
H	-2.33633200	0.52173100	3.01172100
C	-2.75381800	-1.39863300	1.94605100
H	1.50226100	-1.35161200	4.23629700
C	1.76288500	0.72103600	4.78403600
H	1.93267100	2.85808200	5.02696100

H	0.47719100	5.83227100	-2.14204800
C	2.35926000	5.55461800	-1.12704000
H	4.11334600	4.99666600	-0.00185200
H	4.20818700	-5.30822300	2.77835300
H	1.88127400	-6.06269800	2.44118700
O	-2.05337100	0.86289400	-2.44269400
C	-2.09405000	-1.95058600	-2.86351600
H	-0.18714800	-0.60329500	-1.85347600
H	-2.86273700	-2.71984100	0.15685200
H	-3.18249500	-2.01749500	2.72195400
H	2.03883600	0.50232600	5.81146200
H	2.80142800	6.46374700	-1.52295700
C	-3.61591200	-2.14780800	-2.84505400
C	-1.35809300	-3.20622900	-2.36911100
C	-1.62579300	-1.62014500	-4.29490200
H	-3.98394700	-2.37280200	-1.84179900
H	-3.88431600	-2.98466600	-3.50051000
H	-4.13758300	-1.25796800	-3.20883300
H	-0.27947000	-3.04556400	-2.30292300
H	-1.54490300	-4.02832000	-3.07043100
H	-1.69187400	-3.52812500	-1.38119100
H	-2.10424600	-0.71370100	-4.67399600
H	-1.87694700	-2.45296300	-4.96145700
H	-0.54001300	-1.47622100	-4.33467600
Fe	-3.85153500	-0.13472900	0.70707400
C	-5.85488500	-0.30292200	1.21022500
C	-5.66479400	-0.62800700	-0.16766100
C	-5.40565500	1.03696200	1.41318900
H	-6.23403800	-0.96815500	1.97377700
H	-5.87944800	-1.58102100	-0.62987900
C	-5.09523300	0.50998200	-0.81539300
C	-4.93700600	1.53766800	0.16031300
H	-5.38532400	1.56347000	2.35741200
H	-4.76650000	0.57091500	-1.84211600
H	-4.49932100	2.50967000	-0.01657700

TS6

Ni	1.29890800	0.15323800	-1.26487900
H	3.52816800	1.32659600	-2.17662200
C	2.21181400	-1.32309400	-0.68547200
C	2.65468700	-0.60901400	-2.47237300
P	0.53070600	1.53834000	0.22665600
N	3.34712600	-1.25871400	0.11155700
N	1.57029500	-2.48429800	-0.53335900

C	3.87754100	0.31743700	-2.43665600
H	1.89135100	-0.23429600	-3.19055000
H	2.90334900	-1.62063900	-2.79724800
C	-1.32665900	1.79017100	0.45114000
C	1.08320500	1.15900900	1.93056600
C	1.18460500	3.20267800	-0.17845200
C	3.40019400	-2.42074000	0.86152300
C	4.32405800	-0.18826900	0.03752300
C	2.26430600	-3.17139500	0.44885300
C	4.90987700	-0.09231900	-1.37301200
C	4.52921600	0.38907300	-3.82479200
C	-1.89551400	0.45613400	0.84485400
H	-1.69184000	2.02086800	-0.55405600
C	-1.68202400	2.91495000	1.42328500
C	1.17205100	-0.19673000	2.28389500
C	1.34984400	2.13698100	2.90099500
C	0.46415900	4.04444000	-1.04132200
C	2.47649900	3.58651000	0.21570500
C	4.26732700	-2.86701400	1.85725600
H	3.84266000	0.75527200	0.31935600
H	5.10695200	-0.39279900	0.77083900
C	1.99365500	-4.40363200	1.05629400
H	5.72626300	0.63997400	-1.36838700
H	5.34833500	-1.06427900	-1.63523900
H	3.81449000	0.73676300	-4.57828800
H	5.38263800	1.07707700	-3.82666000
H	4.89125700	-0.59787800	-4.13642200
C	-2.10853100	-0.67950900	-0.02948200
C	-2.28000700	0.05852100	2.16034800
H	-1.27282300	2.72963200	2.41957800
H	-2.76841600	3.00018400	1.51639100
H	-1.29121600	3.87362900	1.07490700
H	0.95323100	-0.95850400	1.54533700
C	1.53660000	-0.56829800	3.57755500
C	1.71963600	1.76235700	4.19316700
H	1.27700000	3.18903300	2.64725400
H	-0.52531300	3.75786400	-1.38377300
C	1.01375100	5.24960600	-1.47808700
C	3.02316200	4.79219300	-0.22263100
H	3.05514000	2.94255200	0.86973100
C	3.98032700	-4.10120000	2.44590100
H	5.12551600	-2.28168900	2.17319400
C	2.86019800	-4.85569300	2.05161500
H	1.12580800	-4.98220300	0.75439600

P	-1.75988600	-0.62107500	-1.79702500
C	-2.63769800	-1.74576000	0.77343600
H	-2.26628900	0.69057600	3.03565100
C	-2.74369700	-1.28600900	2.11422700
H	1.61209100	-1.62154400	3.82886400
C	1.81671800	0.41071400	4.53238300
H	1.93032700	2.52704900	4.93526200
H	0.44022500	5.89094000	-2.14078200
C	2.29314200	5.62930900	-1.06868800
H	4.02112100	5.07709800	0.09797500
H	4.63318000	-4.48225800	3.22567100
H	2.66744000	-5.80922700	2.53496700
O	-2.28413200	0.63040500	-2.46904100
C	-2.22251200	-2.20598300	-2.64149200
H	-0.32827400	-0.71473100	-1.82676000
H	-2.94697500	-2.71608100	0.42072600
H	-3.14818200	-1.84692400	2.94512300
H	2.10984700	0.12300100	5.53788600
H	2.71949500	6.56799000	-1.40925600
C	-3.74420400	-2.40747600	-2.62105300
C	-1.48184100	-3.39881100	-2.01389300
C	-1.73969200	-2.01436400	-4.09370800
H	-4.12349600	-2.52922900	-1.60369900
H	-4.00261900	-3.30980100	-3.18777500
H	-4.26441200	-1.56224500	-3.08120800
H	-0.42083800	-3.18919000	-1.84394100
H	-1.56188300	-4.26222300	-2.68525300
H	-1.91033200	-3.69245800	-1.05355000
H	-2.20900200	-1.14512600	-4.56167700
H	-1.99148400	-2.90468800	-4.68073500
H	-0.65247500	-1.88304400	-4.13708800
Fe	-3.87425600	-0.09488800	0.83349400
C	-5.86399000	-0.20187200	1.40439300
C	-5.71705300	-0.62129500	0.04659100
C	-5.39256200	1.14212700	1.50374700
H	-6.22898600	-0.80885200	2.22139900
H	-5.95525000	-1.60064900	-0.34357800
C	-5.15256400	0.46240900	-0.69229900
C	-4.95341300	1.55067400	0.20749700
H	-5.33888500	1.73051200	2.40937200
H	-4.83975100	0.44766900	-1.72578300
H	-4.50475500	2.50065000	-0.04532100

Ni	0.92866700	-0.65376200	-0.73138300
H	3.74059800	1.06036500	-1.11729300
C	2.76473100	-1.50070300	-1.11650500
C	3.43185900	-0.73889000	-2.22739600
P	0.75848900	1.21381400	0.28645300
N	3.54834100	-1.83823000	-0.00104300
N	1.71181700	-2.36771200	-1.26244100
C	4.36487000	0.34041800	-1.65651300
H	2.67051200	-0.29512500	-2.87392400
H	4.01879900	-1.43895200	-2.84348600
C	-1.02565400	1.80899600	0.51457300
C	1.40895400	1.16422100	2.00439200
C	1.54633800	2.64659900	-0.54858100
C	2.86286600	-2.81098600	0.70008600
C	4.58737300	-0.96055400	0.51435700
C	1.72981000	-3.14329800	-0.08990600
C	5.33186000	-0.29740800	-0.64658000
C	5.10214800	1.08840100	-2.76521700
C	-1.81925500	0.59445800	0.89150000
H	-1.32480000	2.09326100	-0.49766000
C	-1.20524100	3.00225900	1.44815800
C	1.56955100	-0.10943900	2.57246800
C	1.69329100	2.29354500	2.78980800
C	0.96959200	3.07203600	-1.75905200
C	2.75910500	3.21915200	-0.14005800
C	3.09776700	-3.40541100	1.93922300
H	4.13141500	-0.19797500	1.16178000
H	5.27016100	-1.55519300	1.12789100
C	0.83286200	-4.11694700	0.35352500
H	6.01052400	0.46027000	-0.23923500
H	5.94978800	-1.04677400	-1.15879200
H	4.39395700	1.55222800	-3.46003800
H	5.73174500	1.88437900	-2.35301900
H	5.74724700	0.41336000	-3.34090000
C	-2.19511400	-0.46964000	-0.01753900
C	-2.26013500	0.21971200	2.19391300
H	-0.90566900	2.77161000	2.47315100
H	-2.25471400	3.31143500	1.46542300
H	-0.60814100	3.85135700	1.10334700
H	1.35615800	-0.98593200	1.96907100
C	2.00536700	-0.25527800	3.88953300
C	2.13895600	2.14728200	4.10380500
H	1.57214500	3.28862500	2.37719000
H	0.05108600	2.61249100	-2.11635400

C	1.58096600	4.06456800	-2.52236500
C	3.37220100	4.20855500	-0.91192400
H	3.23789200	2.88403400	0.77301400
C	2.18387500	-4.37183900	2.37049600
H	3.95066400	-3.12595100	2.54947200
C	1.07167200	-4.72436200	1.58910900
H	-0.02958000	-4.38225800	-0.24817700
P	-1.83958500	-0.38031000	-1.78314200
C	-2.87352400	-1.47482200	0.75400000
H	-2.15993100	0.82071100	3.08563400
C	-2.91224600	-1.04426500	2.10874000
H	2.12350300	-1.25117600	4.30577400
C	2.29498000	0.87382800	4.65675000
H	2.36206400	3.02932000	4.69723900
H	1.12022400	4.38510400	-3.45221800
C	2.78425600	4.63736400	-2.10147700
H	4.31270900	4.64030400	-0.58161000
H	2.33912200	-4.85832700	3.32893700
H	0.38254600	-5.48002200	1.95422000
O	-2.16007700	0.96708700	-2.39431100
C	-2.53807600	-1.83904400	-2.69058000
H	-0.43061800	-0.70401300	-1.87414400
H	-3.31331100	-2.38437900	0.37634900
H	-3.39507600	-1.56651500	2.92300400
H	2.64210100	0.76481500	5.68018600
H	3.26223400	5.40624500	-2.70110500
C	-4.06850700	-1.88205200	-2.58135100
C	-1.89144400	-3.13123200	-2.16657400
C	-2.12472300	-1.62216700	-4.15915500
H	-4.40328500	-2.04754800	-1.55540900
H	-4.45521900	-2.70104700	-3.19909500
H	-4.51812400	-0.95200200	-2.94051100
H	-0.80061900	-3.08469500	-2.23196800
H	-2.23056800	-3.97835400	-2.77433500
H	-2.15846400	-3.33974600	-1.12838400
H	-2.53980700	-0.69342000	-4.55841500
H	-2.49039900	-2.45775600	-4.76664100
H	-1.03485300	-1.58292700	-4.26524200
Fe	-3.86180100	0.33136300	0.86854100
C	-5.84516000	0.48612500	1.44925300
C	-5.76076300	0.09196500	0.07846800
C	-5.19007900	1.74719800	1.58576300
H	-6.29007100	-0.08861200	2.24982100
H	-6.13243400	-0.83285000	-0.33938800

C	-5.05407600	1.10968000	-0.63126900
C	-4.70242200	2.13137300	0.29930500
H	-5.05033600	2.29243600	2.50894400
H	-4.75404700	1.08646800	-1.66822300
H	-4.13001000	3.01856000	0.06992400

TS7

Ni	1.43052200	0.33781000	1.39387800
Fe	-3.81787000	-0.60425500	-1.03484500
P	-1.69526500	-1.85862000	1.32165100
P	0.50124200	1.33786500	-0.33353000
O	-2.35655400	-3.20595200	1.13663400
C	-2.52589500	-0.44544900	0.55763200
C	-2.06586500	0.36973500	-0.54805500
C	-3.09273400	1.32865300	-0.81979900
H	-3.06589700	2.07508300	-1.59914000
C	-4.17459600	1.11342700	0.07811500
H	-5.11173900	1.65251400	0.08251500
C	-3.83529800	0.02083100	0.92202000
H	-4.47106000	-0.42235500	1.67426000
C	-0.75131500	0.29217300	-1.28230200
H	-0.34502700	-0.72166200	-1.20630700
C	-0.88710800	0.68008500	-2.75815900
H	-1.24114600	1.70648200	-2.87869700
H	-1.61239200	0.01979300	-3.23796000
H	0.06282600	0.59035800	-3.28604900
C	-5.35694200	-1.97354400	-1.24128300
H	-6.07501800	-2.18315600	-0.46056800
C	-4.09942300	-2.62311000	-1.41294000
H	-3.67013500	-3.36027200	-0.74896500
C	-3.43194700	-2.00032500	-2.50978400
H	-2.43954000	-2.24437300	-2.86297400
C	-4.27978000	-0.96937700	-3.02026300
H	-4.04726200	-0.29463100	-3.83252400
C	-5.47086500	-0.95118200	-2.23316700
H	-6.29272100	-0.25668800	-2.34146800
C	-0.34175700	2.94911600	-0.14472600
C	-0.89895600	3.25483100	1.10403900
H	-0.74919500	2.57183400	1.93244400
C	-1.64768700	4.41835600	1.28020600
H	-2.07958500	4.64067400	2.25141700
C	-1.83843200	5.29413700	0.21060500
H	-2.41867900	6.20183400	0.34703500
C	-1.27603500	5.00471200	-1.03490400

H	-1.41558700	5.68779400	-1.86755800
C	-0.53410100	3.83770000	-1.21434700
H	-0.09699600	3.62376100	-2.18363600
C	1.90699700	1.65381100	-1.46419500
C	2.43554200	0.60184700	-2.22921700
H	1.94725800	-0.36551200	-2.23739300
C	3.61225100	0.77639500	-2.95537100
H	4.01093600	-0.05388300	-3.52943800
C	4.28121800	2.00172100	-2.92527900
H	5.19960400	2.13585300	-3.48894800
C	3.76670900	3.05213600	-2.16339300
H	4.28160200	4.00797100	-2.13304900
C	2.58982800	2.88021200	-1.43293900
H	2.20462800	3.70168800	-0.83840100
C	-1.47124700	-1.43535400	3.12304400
C	-2.76250700	-1.78597600	3.87862900
H	-3.59294100	-1.13559600	3.58835100
H	-2.60474500	-1.65861100	4.95625100
H	-3.05778900	-2.82121000	3.69111700
C	-1.13152200	0.04687200	3.30680600
H	-0.24545400	0.33632800	2.72126400
H	-0.90659700	0.25154400	4.36030900
H	-1.95730800	0.69374100	3.00036500
C	-0.31760200	-2.31829200	3.63278800
H	-0.53712400	-3.37997600	3.48652800
H	-0.16312200	-2.14685800	4.70472800
H	0.61686600	-2.08802300	3.11271600
H	-0.39575700	-1.76244400	0.78887700
C	3.89048300	-1.97051300	-0.64360600
C	2.71439200	-2.70476500	-0.95301600
C	2.77396400	-3.76276600	-1.86615900
C	4.00339300	-4.05790300	-2.45404800
C	5.15862100	-3.31567000	-2.14454200
C	5.12114000	-2.25691700	-1.23570000
C	2.09585400	-1.14897400	0.43738700
H	1.87897400	-4.32933600	-2.10481100
H	4.07384400	-4.87483300	-3.16629100
H	6.09943300	-3.56990600	-2.62407100
H	6.01428400	-1.68295200	-1.00816900
H	2.01666500	-0.67996600	2.24977300
N	3.47789900	-1.00576500	0.26322700
N	1.62830800	-2.17060000	-0.26319300
C	4.27928500	0.09644700	0.78959400
H	5.31995200	-0.10804900	0.52985800

H	3.99560400	1.02423200	0.28138600
C	4.18797600	0.26458100	2.31739800
H	4.43644500	-0.69717100	2.77907100
H	4.97148600	0.97371500	2.61687100
C	2.60287400	0.32150500	4.33107200
H	1.60585700	0.61694900	4.66565200
H	2.70393700	-0.75988900	4.46062100
H	3.33639700	0.80555100	4.98899900
C	2.85490700	0.75250900	2.89761700
C	2.22121400	1.91801500	2.42203600
H	1.53108000	2.44702600	3.07328900
H	2.68423100	2.51995000	1.64420900

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Ni	1.38552400	0.34211000	1.31998800
Fe	-3.82201400	-0.60643500	-1.01813100
P	-1.62749100	-1.98987200	1.19102400
P	0.47121000	1.39997700	-0.29815400
O	-2.28363700	-3.32842600	0.93742800
C	-2.49408600	-0.53836900	0.55023900
C	-2.07675900	0.36691300	-0.50120000
C	-3.12840600	1.32127500	-0.67590100
H	-3.13271900	2.12502600	-1.39611000
C	-4.18318800	1.01713400	0.22863600
H	-5.12967000	1.53529900	0.29604600
C	-3.80136100	-0.12725100	0.98052300
H	-4.40743200	-0.63694200	1.71532500
C	-0.77915200	0.37366700	-1.26858800
H	-0.34261900	-0.62953000	-1.26846200
C	-0.95658300	0.85708200	-2.71264400
H	-1.33665200	1.88034200	-2.75655800
H	-1.67729500	0.21263100	-3.21995700
H	-0.01624200	0.82439000	-3.26417600
C	-5.31025800	-2.02134600	-1.27004700
H	-5.97602800	-2.33199100	-0.47678900
C	-4.03776800	-2.59495300	-1.56144300
H	-3.54664500	-3.36744900	-0.98653800
C	-3.45671200	-1.84900400	-2.62997900
H	-2.47656600	-2.01755300	-3.05380500
C	-4.37179900	-0.81631700	-3.00260700
H	-4.21050600	-0.06309400	-3.76154800
C	-5.51921300	-0.92282800	-2.15957000
H	-6.37478400	-0.26142400	-2.16608100
C	-0.40283200	2.97448700	0.00924800

C	-0.95518300	3.18557800	1.27920500
H	-0.77318700	2.45854600	2.06196500
C	-1.73574300	4.31318500	1.53138500
H	-2.16375800	4.46338100	2.51795400
C	-1.96293800	5.24600600	0.51840500
H	-2.56773400	6.12624000	0.71493500
C	-1.40552400	5.04991500	-0.74716400
H	-1.57309700	5.77800200	-1.53525900
C	-0.63184100	3.91838300	-1.00424100
H	-0.19994000	3.77581000	-1.98879400
C	1.85576800	1.79889500	-1.42447100
C	2.39377100	0.79551600	-2.24695200
H	1.92855800	-0.18234600	-2.29020700
C	3.55292200	1.03417300	-2.98252300
H	3.96106100	0.24349400	-3.60404100
C	4.19284500	2.27302800	-2.90369500
H	5.09801400	2.45612100	-3.47488200
C	3.66806200	3.27326000	-2.08381000
H	4.16192000	4.23803900	-2.01489400
C	2.50831500	3.03858200	-1.34358800
H	2.11513100	3.81871200	-0.70076600
C	-1.35932300	-1.68499100	3.01251000
C	-2.59596100	-2.18132400	3.77684800
H	-3.48168300	-1.58137800	3.54627100
H	-2.41736400	-2.10732800	4.85624100
H	-2.81841100	-3.22208700	3.53027700
C	-1.11275000	-0.20097100	3.30239200
H	-0.30043300	0.20875200	2.68477200
H	-0.82714400	-0.06625900	4.35275900
H	-2.00257000	0.40395400	3.11028800
C	-0.12865400	-2.51788700	3.41523700
H	-0.27170600	-3.57799400	3.18514200
H	0.04811000	-2.42543500	4.49346100
H	0.76995400	-2.17782900	2.89158900
H	-0.34627500	-1.84510900	0.62779200
C	3.93446500	-1.91372300	-0.70370600
C	2.78984200	-2.64780500	-1.11383900
C	2.92592000	-3.69769900	-2.02882300
C	4.19840600	-3.98484400	-2.52025300
C	5.32294300	-3.24294900	-2.11198200
C	5.20989200	-2.19558900	-1.19659400
C	2.05178200	-1.12041900	0.26330500
H	2.05460100	-4.26508900	-2.34204500
H	4.32788900	-4.79447300	-3.23268000

H	6.30003200	-3.49039800	-2.51689600
H	6.08302600	-1.62833700	-0.88799900
H	2.19352400	-0.43952600	2.54313200
N	3.44793300	-0.96405700	0.18286000
N	1.65298600	-2.12820400	-0.50142300
C	4.19726100	0.16692300	0.73325200
H	5.23584900	0.05615100	0.41510800
H	3.82357900	1.09072000	0.27881600
C	4.17247700	0.28038900	2.26923800
H	4.59838000	-0.63853100	2.68892500
H	4.83733500	1.10561100	2.55220300
C	2.78662200	0.23708600	4.42340800
H	1.78021000	0.34615500	4.83602400
H	3.14318900	-0.77378200	4.64630600
H	3.44225600	0.95263100	4.93033200
C	2.78982400	0.51430100	2.91387800
C	2.02076800	1.73440300	2.50153000
H	1.39095300	2.16790800	3.27749900
H	2.56637100	2.49435300	1.94084600

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Fe	3.59292000	-1.69234100	-0.41904400
P	0.55522800	-1.82744200	1.09550800
P	0.58725000	1.91022100	0.36633900
O	1.28448600	-1.69914300	2.41434400
C	1.57318600	-1.36009900	-0.32648400
C	2.28895200	-0.10373100	-0.35869800
C	3.03181300	-0.05972400	-1.57672600
H	3.69708700	0.73527100	-1.87995000
C	2.79561100	-1.26848500	-2.29394900
H	3.25491000	-1.55164100	-3.23083000
C	1.89808000	-2.06849500	-1.53295400
H	1.56260900	-3.05698000	-1.80388100
C	2.18646000	0.97298500	0.68431700
H	2.01987900	0.47472800	1.64498000
C	3.41599200	1.87862600	0.76921100
H	3.61444500	2.37578000	-0.18299000
H	4.29588100	1.28734000	1.03633300
H	3.28196100	2.65904100	1.52259800
C	4.48955500	-3.50708800	0.02764700
H	4.12448300	-4.46530100	-0.31485800
C	4.09669300	-2.84041100	1.22640100
H	3.35531500	-3.16914400	1.93877500
C	4.77014300	-1.58433400	1.27204200

H	4.64060000	-0.83291800	2.03734000
C	5.58246400	-1.47256500	0.10241900
H	6.18817800	-0.62053100	-0.17442900
C	5.40712300	-2.66148100	-0.66891000
H	5.85848400	-2.86736000	-1.62973200
C	1.09142600	3.28961300	-0.72385900
C	1.35487800	3.00344900	-2.07394800
H	1.23401800	1.99318500	-2.44721500
C	1.77598200	4.01375100	-2.93772400
H	1.97992200	3.78064300	-3.97865300
C	1.92613900	5.32034600	-2.46868100
H	2.24734000	6.10784800	-3.14377700
C	1.66067000	5.61133900	-1.12972800
H	1.77722900	6.62548500	-0.75912300
C	1.25001000	4.60174400	-0.25851700
H	1.05355600	4.83450600	0.78236900
C	0.12363800	2.67758200	1.96093600
C	0.84241700	2.51149700	3.15259200
H	1.77124800	1.95328800	3.16586100
C	0.36075300	3.05439400	4.34457400
H	0.92468100	2.91566800	5.26195500
C	-0.83903400	3.76622400	4.36117600
H	-1.21104100	4.18348400	5.29191900
C	-1.56580100	3.93157500	3.18017100
H	-2.50544000	4.47543000	3.18742600
C	-1.09301400	3.38432100	1.98951000
H	-1.66823300	3.49968500	1.07466500
C	-0.27496100	-3.45324800	0.80064600
C	0.76891300	-4.57851500	0.74103200
H	1.45626100	-4.46629500	-0.10128600
H	0.25808900	-5.54228200	0.63271800
H	1.36116100	-4.61575400	1.65996900
C	-1.12930400	-3.39025700	-0.47584600
H	-1.85106300	-2.57197500	-0.41918100
H	-1.69381900	-4.32480500	-0.57489200
H	-0.53178600	-3.26661300	-1.38131000
C	-1.20103500	-3.65206200	2.01773300
H	-0.63434400	-3.66518000	2.95269800
H	-1.72552800	-4.60947900	1.91783200
H	-1.94993500	-2.85537900	2.06832900
H	-0.54191500	-0.92554600	0.97065100
Ni	-1.32124400	0.73428500	-0.09472200
C	-5.17594800	-0.53634600	-0.36886900
C	-4.66992200	-1.23641000	0.75977100

C	-5.50660300	-2.10694600	1.46887400
C	-6.82116800	-2.25981600	1.03260800
C	-7.30688100	-1.55979800	-0.08920900
C	-6.49255300	-0.68539800	-0.80894200
C	-3.01997300	-0.02825400	-0.00058600
H	-5.13074000	-2.64470600	2.33426800
H	-7.48761800	-2.93183600	1.56573200
H	-8.33690000	-1.70540600	-0.40186200
H	-6.87049800	-0.15030600	-1.67503200
H	-2.32752000	-1.23140000	-2.29443300
N	-4.11215000	0.22749700	-0.81495300
N	-3.33361100	-0.90784800	0.95196200
C	-4.05659900	1.09189800	-1.97945400
H	-5.07153900	1.41626700	-2.22501400
H	-3.48675000	1.98101400	-1.69626600
C	-3.39336400	0.40943200	-3.17986500
H	-4.09029000	-0.30949400	-3.62761200
H	-3.20273800	1.18098000	-3.93881000
C	-1.37690000	-0.74171800	-4.14429500
H	-0.49173800	-1.35129700	-3.93387300
H	-2.04702800	-1.32956700	-4.78326300
H	-1.04965200	0.13373000	-4.71879400
C	-2.07775700	-0.31579000	-2.84246100
C	-1.12257000	0.51665300	-1.98952400
H	-0.12160400	0.06854200	-1.99717600
H	-1.04847600	1.54731300	-2.36092500

TS8

Ni	1.22125600	0.56920700	-0.03418600
Fe	-3.69771100	-1.59183700	0.21508400
P	-0.57087800	-1.60885800	-1.12891300
P	-0.54464800	1.91059900	-0.03632400
O	-1.14169200	-1.20280600	-2.46746700
C	-1.67052900	-1.28372100	0.25756100
C	-2.37676300	-0.02763900	0.40434400
C	-3.16651600	-0.11929100	1.58797500
H	-3.83070100	0.64752700	1.95821600
C	-2.98246300	-1.40970700	2.16093800
H	-3.48786300	-1.79387200	3.03598300
C	-2.06370500	-2.12976800	1.34969200
H	-1.75589200	-3.15006100	1.50871800
C	-2.21987200	1.17235700	-0.48406000
H	-2.08521700	0.80715300	-1.50672000
C	-3.39439400	2.14627200	-0.42270200

H	-3.53672600	2.54541300	0.58428200
H	-4.31738500	1.63747300	-0.71638000
H	-3.23777600	2.99014700	-1.09914500
C	-4.53254200	-3.31588800	-0.57178200
H	-4.13053100	-4.30786200	-0.42078500
C	-4.17574000	-2.41618900	-1.62162900
H	-3.43020600	-2.57908500	-2.38558300
C	-4.89680200	-1.20182000	-1.42365800
H	-4.81934100	-0.31618900	-2.03826100
C	-5.69942800	-1.34776700	-0.25126400
H	-6.33415100	-0.58847500	0.18427100
C	-5.47392100	-2.65533700	0.27572800
H	-5.90656000	-3.05855900	1.18092200
C	-0.83077000	2.61493200	1.62897500
C	-0.35476900	1.87627000	2.72332400
H	0.21002200	0.96469900	2.54481000
C	-0.59500300	2.31111400	4.02717300
H	-0.22197500	1.73017000	4.86526100
C	-1.30200500	3.49372000	4.24985100
H	-1.48332100	3.83659600	5.26433100
C	-1.76781300	4.24242700	3.16606700
H	-2.31149300	5.16716000	3.33658600
C	-1.53666300	3.80544800	1.86202500
H	-1.89484000	4.39540400	1.02496800
C	-0.34681700	3.34969000	-1.15027900
C	-0.77770400	3.28170200	-2.48471500
H	-1.32919600	2.41631200	-2.83831500
C	-0.49175500	4.31744900	-3.37400500
H	-0.83828900	4.25286500	-4.40127300
C	0.23792000	5.42925500	-2.94893500
H	0.46043100	6.23395000	-3.64318900
C	0.68469900	5.49787700	-1.62823500
H	1.25725800	6.35664200	-1.28993500
C	0.39844400	4.46525500	-0.73509000
H	0.75031200	4.52893600	0.28963100
C	0.13888900	-3.32002300	-1.05938500
C	-0.95849300	-4.36084100	-1.32307000
H	-1.73116200	-4.34095100	-0.55091300
H	-0.51508800	-5.36324800	-1.33250200
H	-1.43829600	-4.19575500	-2.29211000
C	0.84806300	-3.56517000	0.28284700
H	1.46261600	-2.71509400	0.58651200
H	1.51228600	-4.43114400	0.18786600
H	0.14830500	-3.77637500	1.09323600

C	1.18006800	-3.35014500	-2.19631700
H	0.72932300	-3.10619400	-3.16194500
H	1.61628500	-4.35307400	-2.25914900
H	1.99383300	-2.64461500	-2.00174700
H	0.63424900	-0.86795500	-0.80378900
C	4.28504200	-1.92667300	0.14240300
C	3.84382200	-1.82205800	1.49249300
C	4.32253900	-2.73009500	2.44566800
C	5.23508000	-3.70135600	2.03550400
C	5.66913300	-3.78205000	0.69914800
C	5.19722000	-2.89599600	-0.27176400
C	2.79501400	-0.26976900	0.39336900
H	3.98620100	-2.66782200	3.47621000
H	5.62036600	-4.41248100	2.76058700
H	6.38256600	-4.55028200	0.41578000
H	5.52659000	-2.96508500	-1.30418400
H	5.00127700	0.99217700	0.48645800
N	3.58891300	-0.94418000	-0.53736200
N	2.95183200	-0.77019700	1.62551400
C	3.87604800	-0.34078300	-1.82474800
H	4.42134300	-1.05696700	-2.44245300
H	2.91862300	-0.14418500	-2.31550400
C	4.66320100	0.97809400	-1.63522600
H	5.73467600	0.79987900	-1.77530400
H	4.35235000	1.68958100	-2.41036200
C	5.01849500	3.02104100	-0.19292700
H	4.92969700	3.44565600	0.81256200
H	6.07941400	3.02958000	-0.46863800
H	4.48504700	3.68185900	-0.88649800
C	4.44912700	1.59855900	-0.24182000
C	2.96626200	1.61903100	0.17267500
H	2.84590800	2.03929400	1.17311200
H	2.43594500	2.25333700	-0.55622900

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Ni	1.13373100	0.28597000	0.67871900
Fe	-4.10235900	-1.05976600	-0.41393600
P	-0.79094300	-1.75960300	-0.82618900
P	-0.32288800	1.74227000	0.38646800
O	-0.94392600	-1.41199900	-2.29390700
C	-2.15621500	-1.19148200	0.21034600
C	-2.57836300	0.19250500	0.20477100
C	-3.68122700	0.30740000	1.10201100
H	-4.24055100	1.21088300	1.29597600

C	-3.95440400	-0.97581700	1.65696100
H	-4.76101000	-1.21599200	2.33575300
C	-3.01773500	-1.90102400	1.11662200
H	-2.99572200	-2.95905700	1.32547100
C	-1.91590900	1.29872900	-0.55871700
H	-1.54733400	0.86938000	-1.49514400
C	-2.83847000	2.47664900	-0.86445300
H	-3.21667000	2.94225100	0.04840000
H	-3.69924400	2.13959500	-1.45002300
H	-2.31288100	3.24398700	-1.43846100
C	-5.03498100	-2.58603800	-1.45630900
H	-4.94273400	-3.63440400	-1.20859400
C	-4.17109800	-1.85068900	-2.32313700
H	-3.27900600	-2.21344600	-2.81186100
C	-4.61046200	-0.49398100	-2.33263300
H	-4.12800400	0.31704700	-2.85897700
C	-5.74642000	-0.38755500	-1.47273700
H	-6.28542200	0.52027900	-1.23857200
C	-6.00900400	-1.68209200	-0.92964400
H	-6.78319100	-1.92583500	-0.21516000
C	-1.00579800	2.68182300	1.81500200
C	-1.12760900	1.98496800	3.02647400
H	-0.75719700	0.96519400	3.08190700
C	-1.70665000	2.58973600	4.14217000
H	-1.79768300	2.03472600	5.07151400
C	-2.15609700	3.90941300	4.06644300
H	-2.59843900	4.38595700	4.93659500
C	-2.02789000	4.61793000	2.86979300
H	-2.37151500	5.64667400	2.80691600
C	-1.46292100	4.00699900	1.74964600
H	-1.37054000	4.56581100	0.82465200
C	0.43795100	3.01996400	-0.70158100
C	0.43360400	2.84931500	-2.09614100
H	-0.11565200	2.02626100	-2.54168800
C	1.14914000	3.71452000	-2.92418800
H	1.12983200	3.56500600	-4.00003600
C	1.88893900	4.76411400	-2.37541900
H	2.44479600	5.43847700	-3.02021700
C	1.90951500	4.93737500	-0.98896800
H	2.48511900	5.74761100	-0.54996100
C	1.19509400	4.07279900	-0.16051900
H	1.23081200	4.21098300	0.91543200
C	-0.43975700	-3.55223000	-0.50682300
C	-1.61666900	-4.42683800	-0.96368300

H	-2.52645400	-4.22806600	-0.39265100
H	-1.36295900	-5.48616900	-0.83577300
H	-1.83968800	-4.26037400	-2.02158700
C	-0.10221500	-3.76887700	0.97567000
H	0.70617200	-3.10565500	1.29762000
H	0.23626300	-4.80054000	1.12900100
H	-0.95771500	-3.59774800	1.63232100
C	0.80355300	-3.86883900	-1.36096200
H	0.61388000	-3.68456300	-2.42147200
H	1.07969600	-4.92192900	-1.23345000
H	1.65997100	-3.25757600	-1.05581400
H	0.34422100	-1.10444500	-0.19678000
C	4.70199500	-1.83358500	1.07977900
C	3.42103700	-1.48873700	1.56921200
C	2.91218200	-2.10147600	2.71673600
C	3.70766600	-3.05676900	3.34506500
C	4.98285300	-3.39284200	2.84901800
C	5.50595400	-2.78448000	1.70891400
C	3.76904800	-0.27555200	-0.20785600
H	1.93285000	-1.82657800	3.09442100
H	3.34123100	-3.55183200	4.23904400
H	5.57427400	-4.14018600	3.36893300
H	6.49110700	-3.04046700	1.33334300
H	5.54057200	1.66773900	-1.25286600
N	4.88759600	-1.05071600	-0.05182300
N	2.86621300	-0.51830900	0.73737400
C	6.09278600	-0.96273400	-0.87335500
H	6.86170900	-0.41909000	-0.31040700
H	6.46268100	-1.97684900	-1.05095300
C	5.78615400	-0.24907400	-2.19057200
H	6.73390000	-0.03353600	-2.69461600
H	5.21453000	-0.91744800	-2.84744800
C	4.78996900	1.83357900	-3.25877200
H	4.19363200	2.73367000	-3.07918000
H	5.75117700	2.13961700	-3.68532200
H	4.26419400	1.23122900	-4.00916600
C	4.98415600	1.04271600	-1.96598500
C	3.62606300	0.69042500	-1.33459400
H	3.10063600	1.57574700	-0.96419000
H	2.96884300	0.24810800	-2.09603000

TS7'

Fe	-4.30988600	-1.02104000	0.05327100
P	-2.85235400	2.05423000	0.02769800

P	0.45916200	-0.57647700	0.50635400
O	-4.10973700	2.60742100	0.65487700
C	-2.90799800	0.35419200	-0.56799100
C	-2.25393200	-0.80361800	0.00686400
C	-2.64024300	-1.93499400	-0.77740300
H	-2.33243200	-2.95415300	-0.60346800
C	-3.52224500	-1.50554800	-1.80620000
H	-4.01231100	-2.14406600	-2.52769600
C	-3.69936300	-0.10146400	-1.67819000
H	-4.35731000	0.51155700	-2.27500300
C	-1.29762800	-0.85619400	1.17106900
H	-1.48441100	-0.00379600	1.83106100
C	-1.44450400	-2.15578200	1.97173700
H	-1.22482200	-3.03112000	1.35781800
H	-2.47288700	-2.24846200	2.32681300
H	-0.77648700	-2.17901300	2.83314800
C	-6.35094000	-0.70225500	0.19794300
H	-6.93444100	-0.21760100	-0.57250500
C	-5.67907700	-0.04675300	1.27069100
H	-5.61145100	1.02173100	1.41714500
C	-4.97158100	-1.03827200	2.01445500
H	-4.34085700	-0.85159700	2.87251300
C	-5.20994000	-2.30799900	1.40376300
H	-4.79141700	-3.25532300	1.71442300
C	-6.06225900	-2.09928300	0.27792000
H	-6.39534000	-2.85947600	-0.41520300
C	0.56344700	-1.80289200	-0.84227100
C	0.45701600	-1.33332300	-2.15726300
H	0.42656700	-0.26560900	-2.33969400
C	0.41044500	-2.22999600	-3.22364400
H	0.32859900	-1.85443100	-4.23896700
C	0.48950800	-3.60282000	-2.98681600
H	0.46121900	-4.30087900	-3.81842300
C	0.62213900	-4.07881800	-1.68022100
H	0.70052500	-5.14579000	-1.49319900
C	0.65652700	-3.18377900	-0.61147300
H	0.76895500	-3.56039100	0.39945500
C	1.59974400	-1.18566100	1.80460300
C	1.39889000	-0.82888200	3.14846000
H	0.49801100	-0.29924000	3.44291300
C	2.35602200	-1.13799400	4.11443200
H	2.18301500	-0.86269100	5.15062000
C	3.53508600	-1.79172400	3.74854300
H	4.28320000	-2.02640700	4.49972500

C	3.74959100	-2.13548600	2.41295800
H	4.66979500	-2.62821700	2.11441300
C	2.79016500	-1.83563900	1.44567300
H	2.97965100	-2.08749200	0.40884400
C	-2.20546500	3.11672700	-1.34785100
C	-3.26818400	3.26319800	-2.44882000
H	-3.39912800	2.33642300	-3.01271400
H	-2.95132400	4.03605900	-3.15851000
H	-4.23511600	3.56172600	-2.03302400
C	-0.91685000	2.51499800	-1.92082900
H	-0.15194700	2.36416400	-1.14444300
H	-0.48925000	3.18753800	-2.67315800
H	-1.10073000	1.54830500	-2.39680800
C	-1.93997200	4.49396800	-0.71295400
H	-2.86746700	4.94322600	-0.34827700
H	-1.49818700	5.16762300	-1.45596700
H	-1.24813800	4.42326100	0.13197300
H	-1.74222300	2.00323000	0.89994300
Ni	1.34306000	1.38997500	0.09386600
C	5.03164700	0.09773300	-0.50252900
C	4.54156700	-0.28082500	-1.78228000
C	5.35527600	-1.02528600	-2.64455900
C	6.63142500	-1.37761300	-2.20928800
C	7.09958200	-1.00128200	-0.93571500
C	6.30638900	-0.25979900	-0.05940800
C	2.91333100	0.78779200	-0.82112600
H	4.98747800	-1.31953600	-3.62285000
H	7.27908200	-1.95669100	-2.86123800
H	8.09815000	-1.29657100	-0.62666700
H	6.67097200	0.01993300	0.92441700
N	3.99021100	0.79815300	0.08000600
N	3.23905600	0.17485200	-1.94781200
C	3.96724100	1.40482200	1.40680600
H	3.31939100	0.82154100	2.06645300
H	4.97961900	1.34767000	1.81215400
C	3.52677600	2.87837700	1.38447200
H	3.67832500	3.28932800	2.39073600
H	4.19852800	3.42240000	0.71135200
C	1.88477100	4.50513800	0.28897700
H	0.86654500	4.62810900	-0.08206100
H	2.07880400	5.30466500	1.01526100
H	2.57339200	4.64425600	-0.55046300
C	2.07696400	3.15479500	0.96102300
C	0.98852500	2.58790000	1.68107600

H	0.04383100	3.12428000	1.69627800
H	1.18763600	1.98228100	2.56254700
H	2.28727000	2.35635800	-0.48591900

14'

Fe	-4.08929400	-0.05292300	-0.57443400
P	-1.58665200	1.77651800	0.80900000
P	0.38567300	-1.48699200	0.20462500
O	-2.06508800	1.36942700	2.18356700
C	-2.20280000	0.74257700	-0.53148800
C	-2.13723400	-0.70417700	-0.51829800
C	-2.75534900	-1.16664000	-1.71961800
H	-2.88622700	-2.20061600	-1.99998100
C	-3.21042300	-0.04487400	-2.46406700
H	-3.75866800	-0.08059300	-3.39490000
C	-2.87497300	1.13083600	-1.74136800
H	-3.12439400	2.13639700	-2.03813900
C	-1.48144900	-1.58120500	0.51640900
H	-1.62247100	-1.12505400	1.50053900
C	-2.04117000	-3.00636500	0.50018300
H	-1.83346400	-3.50863800	-0.44727100
H	-3.12636300	-2.97177800	0.63016600
H	-1.61924900	-3.61690300	1.29877100
C	-5.78081100	1.04383500	-0.09165600
H	-5.95485400	2.06236100	-0.40936000
C	-5.09865800	0.64076000	1.09554300
H	-4.62807000	1.28588700	1.82284600
C	-5.04070400	-0.78415700	1.10608600
H	-4.55270800	-1.38686300	1.85879000
C	-5.68884200	-1.26463900	-0.07271000
H	-5.78172200	-2.29907300	-0.37345800
C	-6.14528000	-0.13339800	-0.81450600
H	-6.64210400	-0.16206400	-1.77445400
C	0.50961200	-1.94650100	-1.56020300
C	0.62558000	-0.92177300	-2.50893500
H	0.77084500	0.10232300	-2.18663800
C	0.59561400	-1.22440600	-3.87068800
H	0.69486900	-0.42354200	-4.59696600
C	0.45318000	-2.54582900	-4.29492400
H	0.43425500	-2.77842900	-5.35573000
C	0.34866700	-3.57275000	-3.35343700
H	0.25000100	-4.60425200	-3.67889700
C	0.37568100	-3.27637400	-1.99145100
H	0.30597900	-4.07931700	-1.26563300

C	1.17635400	-2.86583100	1.10930300
C	0.72474900	-3.25704000	2.37933000
H	-0.16015600	-2.79996100	2.80951600
C	1.41781600	-4.22182300	3.10961900
H	1.05131700	-4.52044000	4.08722400
C	2.57978100	-4.79601400	2.59018000
H	3.11916200	-5.54595100	3.16077300
C	3.04778200	-4.39709100	1.33730900
H	3.95498000	-4.83247400	0.92911100
C	2.35326500	-3.43692000	0.60062100
H	2.72615700	-3.13098400	-0.37134900
C	-1.79125600	3.57406600	0.40525100
C	-3.27925300	3.95131300	0.34713500
H	-3.80872700	3.42680300	-0.45091600
H	-3.37826300	5.02813100	0.16765300
H	-3.77982700	3.72156200	1.29240000
C	-1.05399400	3.91109500	-0.90177900
H	-0.01995700	3.55011700	-0.88915600
H	-1.02353400	4.99939500	-1.02833000
H	-1.53955100	3.49054000	-1.78393000
C	-1.11451000	4.32233800	1.57063700
H	-1.57429800	4.07295400	2.53026000
H	-1.21055200	5.40211500	1.41120700
H	-0.04587000	4.08972000	1.62761800
H	-0.17266000	1.65428200	0.63987900
Ni	1.24289300	0.36662200	0.84379000
C	4.77620100	1.27405200	-0.67698100
C	4.05946800	1.73136100	-1.81586200
C	4.75472500	2.30484400	-2.88646200
C	6.14241000	2.40942400	-2.79790800
C	6.83749300	1.95162200	-1.66313200
C	6.16508900	1.37603400	-0.58366800
C	2.54934300	0.92756900	-0.45776800
H	4.21545800	2.65681400	-3.76112200
H	6.70038300	2.85216800	-3.61819300
H	7.91879500	2.04886000	-1.62466500
H	6.70786900	1.02742700	0.29030000
N	3.80250800	0.76822400	0.16845300
N	2.69822900	1.50512800	-1.64313200
C	4.00513500	0.12704900	1.46600100
H	3.51519900	-0.85296500	1.44672600
H	5.07618900	-0.05347500	1.58658800
C	3.49825400	0.94640600	2.67233400
H	3.75945100	0.40131300	3.58757500

H	4.04324100	1.89744200	2.69320600
C	1.60729900	2.40601200	3.61496900
H	0.53584400	2.61133100	3.56035500
H	1.84665700	2.13262700	4.64802000
H	2.15557300	3.32123700	3.36738900
C	1.98467800	1.24893800	2.67845700
C	1.04594300	0.07957600	2.74484400
H	0.07770400	0.29119200	3.19721600
H	1.47891200	-0.86674700	3.06277900
H	1.83123200	1.76453600	1.63734900

15'

Ni	0.92700700	1.16147300	-0.33653700
Fe	-4.30997000	-0.75128900	0.11393700
P	-1.98709900	1.73906200	0.08256900
P	0.40388100	-0.99260300	0.25760000
O	-1.89065400	1.76618700	1.58538000
C	-2.66109500	0.22562800	-0.60076900
C	-2.29213700	-1.07685000	-0.08619800
C	-2.99913700	-2.04915300	-0.85196100
H	-2.96219700	-3.11692700	-0.69597500
C	-3.81054100	-1.37736700	-1.80959100
H	-4.49886400	-1.84646700	-2.49856000
C	-3.60899000	0.02160300	-1.66379500
H	-4.11365400	0.78921500	-2.22881900
C	-1.29596100	-1.33787600	1.00536200
H	-1.41913100	-0.55730900	1.76137700
C	-1.44193200	-2.71723900	1.64607400
H	-1.29717000	-3.51913700	0.91870300
H	-2.44447700	-2.82480900	2.07172800
H	-0.71285900	-2.85445500	2.44741200
C	-6.10096800	0.17842000	0.60116900
H	-6.57404400	0.95088300	0.01148900
C	-5.13872500	0.38257300	1.63560500
H	-4.73117800	1.32915700	1.95813200
C	-4.74209700	-0.89586800	2.12773500
H	-3.99645900	-1.07354000	2.88926400
C	-5.45921900	-1.89229300	1.39843400
H	-5.35225600	-2.96242500	1.50937000
C	-6.29829300	-1.22825000	0.45360000
H	-6.93984800	-1.70748300	-0.27295700
C	0.53026500	-2.25267400	-1.05377500
C	0.30307500	-1.83154900	-2.37114800
H	0.15642000	-0.77546700	-2.57344600

C	0.28304800	-2.75712600	-3.41290700
H	0.10909200	-2.42033700	-4.43036200
C	0.50535900	-4.11001000	-3.14945800
H	0.49867800	-4.83043200	-3.96219300
C	0.74841400	-4.53544600	-1.84188600
H	0.93209400	-5.58571900	-1.63518800
C	0.75826100	-3.61217100	-0.79629500
H	0.95565300	-3.94698800	0.21614800
C	1.58214000	-1.45959700	1.57467900
C	1.34633700	-1.01466000	2.88563300
H	0.42152600	-0.50110800	3.13155600
C	2.30531900	-1.20964700	3.87879100
H	2.10953900	-0.86485600	4.88992600
C	3.51618700	-1.83463600	3.57164800
H	4.26679200	-1.97628100	4.34358100
C	3.76170700	-2.26570500	2.26751800
H	4.70935200	-2.72985700	2.01289600
C	2.80072400	-2.08230200	1.27347100
H	3.01552100	-2.39050900	0.25756500
C	-2.72609100	3.24176000	-0.71078900
C	-4.24374000	3.27190500	-0.46675700
H	-4.75682300	2.42046700	-0.91716700
H	-4.65786000	4.18805700	-0.90241700
H	-4.47130400	3.27972300	0.60290900
C	-2.38801700	3.25873500	-2.21032000
H	-1.30706200	3.21468900	-2.37697600
H	-2.75197000	4.19422500	-2.64920600
H	-2.84804700	2.43395000	-2.75865600
C	-2.07050600	4.45228100	-0.01840800
H	-2.23072300	4.42985300	1.06218800
H	-2.51361900	5.37200700	-0.41612300
H	-0.99412800	4.48996300	-0.20517000
H	-0.69862700	1.78626000	-0.57807600
C	4.83120000	0.32176700	-0.01204200
C	4.50633000	-0.37378500	-1.20878700
C	5.47984500	-1.15239800	-1.84329000
C	6.75259200	-1.21119100	-1.27433100
C	7.05912300	-0.51201700	-0.09180600
C	6.10118300	0.26632500	0.56127200
C	2.68510500	0.62273800	-0.57535800
H	5.23994400	-1.69461200	-2.75314800
H	7.52450700	-1.80854200	-1.75129800
H	8.06120400	-0.57914600	0.32216600
H	6.33854400	0.80023200	1.47651000

N	3.65047600	0.93525500	0.36759100
N	3.16681700	-0.16284400	-1.52734200
C	3.43080500	1.88762700	1.43978700
H	2.43041500	1.69371000	1.83576400
H	4.14349000	1.68513200	2.24369900
C	3.53704100	3.33477800	0.93938000
H	3.06850500	3.98930700	1.68746100
H	4.59268600	3.62719300	0.88029700
C	2.91664200	5.06749300	-0.77011600
H	2.53903400	5.25301900	-1.78174300
H	2.29221200	5.63865000	-0.07141900
H	3.93527200	5.47163100	-0.71425100
C	2.88313400	3.56786900	-0.43673700
C	1.45770400	3.01783100	-0.52956200
H	1.01929800	3.31143500	-1.49487200
H	0.84374500	3.46450500	0.27217200
H	3.49969300	3.05503600	-1.18538500

TS8'

Ni	1.25278500	0.12516700	-1.31533500
Fe	-3.83222600	-0.10910700	0.90187000
P	-1.80032500	-0.56536700	-1.80367300
P	0.55813000	1.52594000	0.21480400
O	-2.34488700	0.70134300	-2.42824000
C	-2.09499000	-0.67195900	-0.02965400
C	-1.85381100	0.43940800	0.86827600
C	-2.19879300	0.00647700	2.18347600
H	-2.15931300	0.61588700	3.07393000
C	-2.66613900	-1.33602400	2.11438500
H	-3.04568200	-1.91969600	2.94140200
C	-2.60246300	-1.75904500	0.75885000
H	-2.92408500	-2.71920700	0.39008000
C	-1.29098800	1.78071800	0.49225600
H	-1.68133300	2.03588300	-0.49737400
C	-1.61580600	2.88473100	1.49799500
H	-1.18319000	2.67441300	2.47934000
H	-2.69914500	2.97503700	1.61884400
H	-1.22648800	3.84859400	1.16200200
C	-5.70266600	-0.61174100	0.16218700
H	-5.95625900	-1.58004100	-0.24555700
C	-5.16045200	0.48993200	-0.56645400
H	-4.88572200	0.50232500	-1.61083800
C	-4.92800500	1.55367600	0.35468000
H	-4.48605000	2.50959900	0.11248300

C	-5.32450300	1.11153900	1.65374900
H	-5.23915100	1.67538900	2.57231200
C	-5.80258100	-0.22842200	1.53475600
H	-6.14160500	-0.85610700	2.34738600
C	1.16080000	1.15860500	1.90509000
C	1.22797000	-0.19295400	2.27798000
H	0.96015700	-0.96044200	1.56234500
C	1.63437800	-0.55324900	3.56239800
H	1.69396900	-1.60392100	3.82789600
C	1.97624800	0.43289100	4.48917800
H	2.30208500	0.15344000	5.48690000
C	1.89771500	1.78109300	4.13190000
H	2.15467800	2.55194800	4.85273600
C	1.48755600	2.14460800	2.84887700
H	1.42822700	3.19402800	2.58178700
C	1.20455900	3.18733800	-0.21285100
C	0.45344500	4.04402100	-1.03374400
H	-0.55438600	3.77196100	-1.33102100
C	0.99531200	5.24668800	-1.48710200
H	0.39780100	5.89982600	-2.11621800
C	2.29708400	5.60892200	-1.13687000
H	2.71703100	6.54582400	-1.49006800
C	3.05767900	4.75651400	-0.33432800
H	4.07343400	5.02704400	-0.06075600
C	2.51901300	3.55330600	0.12031800
H	3.12223800	2.89782100	0.73977800
C	-2.27762000	-2.13026400	-2.67624700
C	-3.79729000	-2.34036400	-2.61733300
H	-4.14576300	-2.49268300	-1.59316400
H	-4.06804900	-3.22769000	-3.20159200
H	-4.33414900	-1.48512100	-3.03825200
C	-1.51419400	-3.33465300	-2.10075300
H	-0.44930300	-3.12711300	-1.95803700
H	-1.61228300	-4.18181700	-2.79006000
H	-1.90870100	-3.65278800	-1.13392900
C	-1.83735800	-1.89773300	-4.13593300
H	-2.32544500	-1.02006300	-4.56735200
H	-2.09972300	-2.77432200	-4.73875700
H	-0.75280400	-1.75652300	-4.20657500
H	-0.36736100	-0.66089700	-1.88229100
C	3.40516800	-2.37876400	0.84439900
C	2.24921700	-3.14221700	0.52640600
C	2.01271400	-4.34817400	1.19670000
C	2.93127200	-4.75793100	2.16366100

C	4.06938800	-3.98817400	2.46724300
C	4.32391400	-2.78029300	1.81267000
C	2.14012700	-1.34354000	-0.68054300
H	1.13082200	-4.93830800	0.96637400
H	2.76481300	-5.68924800	2.69745900
H	4.76050600	-4.33549200	3.22962100
H	5.19279400	-2.17855900	2.06047500
N	3.32337700	-1.25505400	0.04011500
N	1.50480800	-2.49139300	-0.44489400
C	4.29872900	-0.17869300	-0.03519500
H	4.11483400	0.55021300	0.76411100
H	5.27729000	-0.63163700	0.15389300
C	4.31091300	0.50856800	-1.41131400
H	3.59737400	1.34062100	-1.42653900
H	5.30709300	0.94179100	-1.55696300
C	4.43656900	0.11159600	-3.91085500
H	4.14451400	-0.54534200	-4.73718100
H	3.99207000	1.09745500	-4.09421600
H	5.52657200	0.22370700	-3.93784300
C	3.96846900	-0.45173900	-2.56388800
C	2.46014600	-0.73422600	-2.58841300
H	2.20326300	-1.68245400	-3.06177400
H	1.94219400	0.08227900	-3.15848900
H	4.49249400	-1.40055600	-2.38884500

16'

Ni	1.13958800	0.83672900	0.36779300
Fe	-3.77647900	-1.72139200	-0.02657300
P	-0.37766500	-1.95870000	-0.40487500
P	-0.60713300	1.86669700	-0.09086000
O	-0.62299100	-2.40661200	-1.83261100
C	-1.82558100	-1.36786200	0.50442800
C	-2.48344300	-0.12232100	0.17697800
C	-3.57995300	0.03244100	1.07712600
H	-4.28180100	0.85315000	1.07729600
C	-3.61979900	-1.09398600	1.94694600
H	-4.36436800	-1.28329400	2.70791500
C	-2.54458900	-1.95880400	1.60021200
H	-2.33525300	-2.91108400	2.06148700
C	-2.03899900	0.86733000	-0.85996100
H	-1.56289900	0.31537400	-1.67756900
C	-3.18766000	1.70507100	-1.42224300
H	-3.68011200	2.28684300	-0.63990500
H	-3.93968600	1.05382500	-1.87730900

H	-2.83275800	2.40264100	-2.18385900
C	-4.49543900	-3.59287400	-0.54394800
H	-4.25930000	-4.50043100	-0.00530900
C	-3.74249000	-3.03912600	-1.62235600
H	-2.80566200	-3.40816300	-2.01379600
C	-4.36242100	-1.81232000	-2.00475300
H	-4.00225200	-1.13813700	-2.76868200
C	-5.50033300	-1.60717300	-1.16538200
H	-6.15789900	-0.74888800	-1.18116000
C	-5.58167700	-2.70836200	-0.25988100
H	-6.31320700	-2.83079500	0.52716600
C	-1.50482000	2.79862000	1.21933000
C	-1.39033500	2.30630700	2.52814600
H	-0.73349900	1.46020800	2.71102700
C	-2.10718400	2.88702100	3.57427900
H	-2.01153900	2.49044000	4.58104100
C	-2.93974500	3.98021400	3.32742600
H	-3.49360100	4.43909900	4.14141000
C	-3.05247300	4.48730800	2.03106700
H	-3.69457200	5.34134400	1.83456000
C	-2.34410900	3.89836500	0.98273400
H	-2.43833100	4.30276500	-0.01932700
C	-0.24732300	3.11743500	-1.39527900
C	-0.18444300	2.72027200	-2.74164100
H	-0.44366700	1.70333100	-3.02060000
C	0.21885700	3.61488900	-3.73231700
H	0.25413900	3.28913100	-4.76818800
C	0.57651500	4.92206000	-3.39577800
H	0.89073200	5.61926600	-4.16687900
C	0.53118100	5.32399400	-2.05947900
H	0.81293700	6.33696800	-1.78571900
C	0.12679400	4.42996100	-1.06799600
H	0.10535000	4.75345800	-0.03237700
C	0.51953600	-3.21487900	0.62628500
C	-0.26103200	-4.53799100	0.64301100
H	-1.22836600	-4.44417100	1.14293900
H	0.31633300	-5.30448600	1.17379100
H	-0.44440600	-4.89399600	-0.37506500
C	0.77204400	-2.66994500	2.04026300
H	1.23094800	-1.67614500	2.00624300
H	1.45904400	-3.33734900	2.57476800
H	-0.14613900	-2.59428500	2.62618800
C	1.87021600	-3.42985800	-0.08520500
H	1.72803300	-3.73644600	-1.12523700

H	2.43837900	-4.21220600	0.43136600
H	2.46915600	-2.51554400	-0.06924500
H	0.48231300	-0.79362900	-0.29215500
C	4.98739700	-0.42122100	1.32669600
C	3.72839600	0.10725400	1.69202100
C	3.44812600	0.41756900	3.02461300
C	4.44910200	0.18489700	3.96433700
C	5.69989800	-0.34599000	3.59054100
C	5.99275700	-0.66004200	2.26445800
C	3.67576900	-0.22490400	-0.46173700
H	2.48023000	0.82556200	3.29676200
H	4.26450700	0.41610600	5.00887600
H	6.45360700	-0.51493300	4.35343200
H	6.95551400	-1.07151600	1.97985900
N	4.92399700	-0.61055200	-0.04732900
N	2.93308500	0.20881900	0.55187700
C	5.93807700	-1.23492000	-0.89480700
H	6.91250800	-0.80939700	-0.63745200
H	5.96887500	-2.30756800	-0.66686900
C	5.61102900	-1.00982800	-2.37120600
H	5.83581600	0.02899100	-2.64488000
H	6.26563900	-1.65092200	-2.97030500
C	3.83038300	-1.22321700	-4.17332200
H	2.77046200	-1.41704800	-4.36782000
H	4.06752500	-0.22766300	-4.56678600
H	4.41655200	-1.95655200	-4.73699200
C	4.13448300	-1.30359000	-2.67855800
C	3.25211900	-0.32286300	-1.88774500
H	2.19690300	-0.60988500	-1.91737600
H	3.30802100	0.67611200	-2.34250300
H	3.90911800	-2.32080900	-2.32879800

TS7s

Fe	-4.28612400	-0.40377700	0.42463300
P	-1.87125000	-1.88764500	-1.48088700
P	0.14538800	1.42762300	0.06990600
O	-2.94303800	-2.31289000	-2.45643900
C	-2.40797200	-1.16788000	0.08255100
C	-2.31975200	0.22116000	0.48255700
C	-2.89232500	0.31926300	1.78877300
H	-2.98754300	1.22632400	2.36515300
C	-3.34609700	-0.96631500	2.19187800
H	-3.86491000	-1.19513400	3.11224500
C	-3.06011100	-1.88400500	1.14511000

H	-3.33156000	-2.92853400	1.12721500
C	-1.71878600	1.37304800	-0.28121400
H	-1.78658200	1.16511500	-1.35321200
C	-2.43697700	2.69385900	0.02266300
H	-2.34864300	2.96642200	1.07593500
H	-3.49998600	2.58871900	-0.20474900
H	-2.03559900	3.51786800	-0.56750000
C	-6.06059500	-1.32364600	-0.11556700
H	-6.26297700	-2.37281100	0.04974900
C	-5.42896100	-0.76758800	-1.26675100
H	-5.01144900	-1.32748400	-2.09145800
C	-5.29336700	0.63727300	-1.05524600
H	-4.82275000	1.33489000	-1.73403400
C	-5.84243700	0.94999600	0.22644300
H	-5.86301300	1.92572700	0.69189500
C	-6.31648400	-0.26431000	0.80810900
H	-6.75552400	-0.36804400	1.79088100
C	0.19868100	1.41389700	1.89556600
C	0.55091400	0.21561000	2.52974300
H	0.87153100	-0.62901100	1.93299000
C	0.50559100	0.11272500	3.91937100
H	0.78209600	-0.82132800	4.39885800
C	0.12260700	1.21160300	4.68917800
H	0.09339400	1.13385600	5.77208000
C	-0.20838700	2.41746700	4.06662100
H	-0.49185300	3.27959900	4.66332300
C	-0.17245500	2.51948900	2.67626800
H	-0.41861800	3.46281600	2.20108300
C	0.71139200	3.10047800	-0.43639900
C	0.29085800	3.64870500	-1.66007500
H	-0.45721400	3.13674000	-2.25711500
C	0.83765300	4.84284300	-2.12657400
H	0.49571500	5.25892700	-3.06973200
C	1.82509900	5.49843100	-1.38658100
H	2.25269800	6.42738100	-1.75161200
C	2.26378100	4.94996900	-0.18071100
H	3.03935700	5.44684600	0.39452700
C	1.71571500	3.75720500	0.29258100
H	2.07851800	3.32629400	1.21936300
C	-0.66664300	-3.24053600	-1.07761700
C	0.34260500	-2.74023500	-0.03513400
H	0.81639400	-1.80023900	-0.33681500
H	1.13560900	-3.48271400	0.11081100
H	-0.13912700	-2.57068000	0.93126600

C	0.02760600	-3.59609900	-2.40536900
H	-0.69533000	-3.95714000	-3.14207200
H	0.76980100	-4.38482400	-2.23759400
H	0.54479000	-2.73533500	-2.84030600
C	-1.41932600	-4.47651100	-0.56050100
H	-1.83882100	-4.31058600	0.43474100
H	-0.72439200	-5.32088700	-0.48465000
H	-2.22921600	-4.76188700	-1.23804100
H	-1.01300900	-0.87386300	-1.96503400
Ni	1.77687000	0.55706100	-1.07838900
C	4.43169000	-1.88635800	0.59283100
C	4.37154800	-0.95642000	1.66646800
C	5.04507600	-1.23227300	2.86271900
C	5.75807600	-2.42517300	2.95907500
C	5.80619300	-3.33753200	1.88707600
C	5.14122100	-3.08535100	0.68730200
C	3.14829700	-0.10585000	0.08647800
H	5.00216000	-0.52721300	3.68728700
H	6.28790200	-2.66040900	3.87764100
H	6.37027500	-4.25910000	1.99744200
H	5.17859000	-3.79683600	-0.13215700
H	3.20694500	0.71012200	-1.36999400
N	3.67081700	-1.31417700	-0.41231800
N	3.58717200	0.13312500	1.31205400
C	3.41930000	-1.85860600	-1.74430300
H	4.08137100	-2.71680700	-1.87959400
H	2.39399300	-2.23093100	-1.80140000
C	3.68102700	-0.85393900	-2.88281600
H	4.73551200	-0.56050900	-2.83513800
H	3.53667000	-1.38222500	-3.83314300
C	3.53993200	1.66508100	-3.38891400
H	2.91450500	2.55323900	-3.27004700
H	4.48565200	1.84108500	-2.86620700
H	3.76483800	1.54266900	-4.45589000
C	2.82299700	0.42170300	-2.87463500
C	1.40396300	0.37554900	-3.03761400
H	0.91456500	1.22205900	-3.51147600
H	0.91152400	-0.58121400	-3.19302700

TS7s'

Fe	-3.81964000	0.28107400	-0.54984100
P	-1.60358200	-1.86103600	0.85317900
P	0.80869300	1.61377100	-0.13049100
O	-2.52476300	-2.99067100	0.46018400

C	-2.29586900	-0.19689400	0.74816700
C	-1.89937900	0.91244300	-0.09666600
C	-2.83177200	1.97097600	0.14251100
H	-2.83068500	2.93049200	-0.35032800
C	-3.79112000	1.54015500	1.09981700
H	-4.64457100	2.10821800	1.44284200
C	-3.47244000	0.20610100	1.47058500
H	-4.04596400	-0.42325600	2.13454300
C	-0.73561200	1.00303500	-1.04989300
H	-0.44153500	-0.00032500	-1.37403900
C	-1.06880300	1.84229800	-2.29078100
H	-1.30183600	2.87932900	-2.03819400
H	-1.94302800	1.41834400	-2.78743600
H	-0.24093000	1.84955900	-2.99959900
C	-5.49568000	-0.88189900	-0.89078200
H	-6.06505000	-1.34929000	-0.09943100
C	-4.36851900	-1.45123400	-1.55281500
H	-3.90328400	-2.39399100	-1.30264500
C	-3.86822200	-0.48504000	-2.47512500
H	-2.99611400	-0.60772300	-3.10188300
C	-4.68834600	0.68213200	-2.38681400
H	-4.54736300	1.60456800	-2.93305200
C	-5.69646000	0.43565900	-1.40605300
H	-6.45069800	1.13906400	-1.08069800
C	0.23552300	3.00284800	0.91137500
C	0.32679700	2.86108400	2.30195200
H	0.77394200	1.96304700	2.71382500
C	-0.14608100	3.86433700	3.14949100
H	-0.07474000	3.74000800	4.22591800
C	-0.70243500	5.02560300	2.61320700
H	-1.06795600	5.80848500	3.27108400
C	-0.77881300	5.18579900	1.22708200
H	-1.19911000	6.09445200	0.80612200
C	-0.31497300	4.18072300	0.38058700
H	-0.36447800	4.31890000	-0.69403400
C	1.89300200	2.37347900	-1.40821600
C	2.26232800	1.58654000	-2.51664200
H	1.84576400	0.59007200	-2.63609600
C	3.18096400	2.07086900	-3.44548900
H	3.45137800	1.45657500	-4.29936200
C	3.75891600	3.33180200	-3.27571200
H	4.47742400	3.70479900	-3.99959800
C	3.41312200	4.10672100	-2.16825800
H	3.86306900	5.08502100	-2.02517200

C	2.48661400	3.63219400	-1.23770800
H	2.23249600	4.24139200	-0.37766100
C	-0.93486100	-2.05398200	2.57410300
C	-2.08788500	-2.11433200	3.58715600
H	-2.58559700	-1.14699900	3.69271100
H	-1.69434300	-2.39114600	4.57250600
H	-2.83212000	-2.86233000	3.29856700
C	-0.00487900	-0.87743600	2.89141800
H	0.77027700	-0.74968000	2.12908500
H	0.48958800	-1.03685900	3.85767100
H	-0.56349800	0.06063000	2.95076200
C	-0.17466500	-3.39133900	2.58643100
H	-0.85307100	-4.22718400	2.39703600
H	0.29785700	-3.54323100	3.56422300
H	0.60174100	-3.42189600	1.82000200
H	-0.42895500	-1.74391800	0.08153900
Ni	2.42645200	0.25537600	0.38767400
C	1.96595900	-3.58496700	-0.49559200
C	1.34570700	-3.06835100	-1.66416300
C	0.71172100	-3.93945300	-2.55775900
C	0.71663600	-5.30125700	-2.26566800
C	1.33743200	-5.79849300	-1.10396300
C	1.96924000	-4.94872300	-0.19686900
C	2.11695700	-1.34021800	-0.58920200
H	0.22881000	-3.55180700	-3.44951400
H	0.22737300	-5.99557800	-2.94221800
H	1.31712400	-6.86582500	-0.90500100
H	2.43461400	-5.33703400	0.70375400
N	2.46609600	-2.47058900	0.16455200
N	1.47073200	-1.68262600	-1.69593500
C	3.16366400	-2.44734200	1.45168900
H	2.48873400	-2.07645400	2.22860900
H	3.40804400	-3.48080600	1.70675000
C	4.46271900	-1.62138600	1.44955200
H	4.94431200	-1.76318200	2.42531700
H	5.13365500	-2.04935500	0.69642900
C	5.51786500	0.50050300	0.45928600
H	5.32176200	1.54326600	0.19710400
H	6.39216700	0.47144300	1.12202500
H	5.77665000	-0.03882400	-0.45740100
C	4.32021700	-0.11754700	1.16914400
C	3.53382600	0.74239700	1.98784700
H	3.82302600	1.78629800	2.07380500
H	2.99548700	0.33814400	2.84365900

H	3.53887100	-0.45386900	-0.22701800
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TS9

Ni	0.45224200	0.52050600	1.23343300
Fe	-4.01376800	-1.52627000	-0.61103500
P	-0.65680700	-1.60310200	0.46757700
P	-0.68689900	1.77833400	-0.14517900
O	-0.06012500	-1.61622000	-0.92805900
C	-2.36498900	-1.01410800	0.54463900
C	-2.82585300	0.11996800	-0.22997600
C	-4.16838900	0.39337200	0.16594900
H	-4.80271000	1.16149600	-0.25199500
C	-4.55825100	-0.56430900	1.14674100
H	-5.53636900	-0.64967700	1.59966900
C	-3.45711600	-1.43353600	1.38079400
H	-3.46277000	-2.27877100	2.05050200
C	-1.98332200	0.89422000	-1.19738500
H	-1.37649000	0.17300900	-1.75018200
C	-2.76992200	1.76508100	-2.17218100
H	-3.38988200	2.50353800	-1.65809300
H	-3.42953700	1.14129400	-2.78447800
H	-2.09261400	2.29922800	-2.84416800
C	-4.58713500	-3.46647000	-1.08851900
H	-4.55003000	-4.30341600	-0.40550900
C	-3.53563800	-3.03936000	-1.95481300
H	-2.55624400	-3.48606000	-2.04054400
C	-3.98231400	-1.88056800	-2.65484400
H	-3.39901500	-1.30665100	-3.36100400
C	-5.31206000	-1.58978800	-2.22327800
H	-5.91373800	-0.74972900	-2.54194300
C	-5.68589800	-2.56992800	-1.25526300
H	-6.62191200	-2.60250400	-0.71470400
C	-1.60494600	3.17989500	0.59895700
C	-1.90255700	3.08397000	1.96708000
H	-1.53191200	2.22924600	2.52614600
C	-2.65922800	4.06969300	2.60190900
H	-2.88398600	3.98045000	3.66077400
C	-3.11845800	5.17052500	1.87738700
H	-3.70201300	5.94242900	2.37066200
C	-2.82201500	5.28098800	0.51667800
H	-3.17495900	6.13820900	-0.04937400
C	-2.07397400	4.29119500	-0.12103400
H	-1.84863600	4.38821900	-1.17738200
C	0.46752100	2.47614600	-1.38786600

C	1.02286300	1.58522000	-2.32490900
H	0.70779900	0.54565000	-2.33869800
C	2.00803400	2.01642300	-3.21175400
H	2.42652400	1.31712000	-3.92982000
C	2.46554400	3.33607100	-3.16911700
H	3.23621400	3.66890700	-3.85799000
C	1.93627300	4.21929000	-2.22797100
H	2.29457600	5.24369600	-2.17963700
C	0.94556300	3.79345100	-1.34001000
H	0.55206600	4.48896500	-0.60663000
C	-0.50763800	-3.26334400	1.32589900
C	-1.45969500	-4.29471500	0.70475500
H	-2.50761800	-4.02115400	0.83835400
H	-1.29865700	-5.26974800	1.17956000
H	-1.26933800	-4.41222400	-0.36533100
C	-0.75209200	-3.11732700	2.83617800
H	-0.08978400	-2.36705900	3.28039900
H	-0.54620700	-4.07286200	3.33191800
H	-1.78002100	-2.83720600	3.07527700
C	0.94829300	-3.70522000	1.08892000
H	1.16516100	-3.79798700	0.02242500
H	1.11609800	-4.67840800	1.56380800
H	1.66094000	-2.99721100	1.52397400
H	0.18243000	-0.97314300	1.58119200
C	5.73348100	-0.70361600	-0.27390900
C	6.36562200	-1.77833700	-0.95043300
C	7.76076800	-1.79483500	-1.07790400
C	8.48097900	-0.73848400	-0.52839800
C	7.83559200	0.32427300	0.13722200
C	6.45048800	0.36174500	0.27748100
C	4.26419700	-2.17326400	-1.01716400
H	8.25397600	-2.61272300	-1.59386400
H	9.56373400	-0.72779300	-0.61285500
H	8.43264400	1.13172800	0.55088100
H	5.95594600	1.18121500	0.78925300
H	3.28793000	-2.60249000	-1.20259500
N	4.37891000	-0.98801800	-0.33230700
N	5.41232500	-2.68150400	-1.40423900
C	3.29184600	-0.20029900	0.23819200
H	3.43517500	0.83982400	-0.06559800
H	2.35972700	-0.54404500	-0.21997000
C	3.21418600	-0.32753200	1.76653400
H	3.07977800	-1.38730000	2.01398800
H	4.18393600	-0.04121900	2.20150100

C	1.83033400	0.12494500	3.86138600
H	0.98118200	0.68589000	4.26390600
H	1.61668800	-0.94310000	3.98366700
H	2.70466100	0.34829500	4.49227500
C	2.10059900	0.48750500	2.41310400
C	1.79398400	1.78361800	1.95499900
H	1.31269800	2.49412800	2.62587400
H	2.33966800	2.24142800	1.13302200

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Ni	0.23672200	0.30124600	1.47323200
Fe	-4.11910000	-1.11697800	-0.82060600
P	-0.97541200	-1.37154000	0.73733000
P	-0.41315000	1.63476400	-0.19431900
O	-0.40604500	-1.79495200	-0.62635900
C	-2.65555100	-0.65985700	0.56386300
C	-2.87020800	0.43808800	-0.35114900
C	-4.22613300	0.86556500	-0.22535900
H	-4.70044000	1.64392800	-0.80528100
C	-4.86610300	0.03361100	0.73915600
H	-5.90914600	0.07432800	1.02157800
C	-3.90611800	-0.90062500	1.22601800
H	-4.11116200	-1.67805000	1.94503000
C	-1.81105900	0.98236400	-1.26372200
H	-1.33979600	0.12795400	-1.75497900
C	-2.32256000	1.96305400	-2.31404500
H	-2.78260700	2.84506400	-1.86175400
H	-3.07432200	1.47382800	-2.94145200
H	-1.50744900	2.29666100	-2.96230700
C	-4.57622300	-3.08597100	-1.27578100
H	-4.63923000	-3.88337400	-0.54956400
C	-3.39748000	-2.67434200	-1.96964600
H	-2.39609400	-3.05192500	-1.82279000
C	-3.74384700	-1.56532300	-2.79727900
H	-3.05893200	-1.00178000	-3.41538400
C	-5.13439500	-1.29109100	-2.61784300
H	-5.68973000	-0.48682500	-3.08065500
C	-5.64899400	-2.23231600	-1.67621000
H	-6.66274300	-2.26652300	-1.30142400
C	-0.94802800	3.30564900	0.30704900
C	-1.43745400	3.44372400	1.61524000
H	-1.42320000	2.58276500	2.27780600
C	-1.93478500	4.66843700	2.06001100
H	-2.31361000	4.76191400	3.07332600

C	-1.93765700	5.77124200	1.20435800
H	-2.31711500	6.72773100	1.55123200
C	-1.45177100	5.64405200	-0.09877000
H	-1.45496000	6.50006600	-0.76699600
C	-0.96578000	4.41702200	-0.54984100
H	-0.59903300	4.32594000	-1.56620000
C	0.98578000	1.79251600	-1.36304200
C	1.32157800	0.65378900	-2.11860200
H	0.71251400	-0.24344400	-2.04687500
C	2.48606000	0.63889900	-2.88412700
H	2.74278700	-0.25107300	-3.45058900
C	3.33721700	1.74672900	-2.89676500
H	4.25285500	1.72352600	-3.47943400
C	3.01604000	2.87394800	-2.13986300
H	3.67708500	3.73571900	-2.13757600
C	1.84709100	2.89912400	-1.37530500
H	1.61648600	3.77575200	-0.77995500
C	-1.12403600	-2.88198500	1.84634100
C	-2.10331000	-3.89022000	1.22551200
H	-3.12099300	-3.50113800	1.17610000
H	-2.11946500	-4.80900100	1.82439000
H	-1.79246300	-4.15430400	0.21135900
C	-1.55007300	-2.49510400	3.26754700
H	-0.86139100	-1.76110300	3.69892600
H	-1.54362100	-3.38219700	3.91249500
H	-2.55438300	-2.06712900	3.30377000
C	0.27568200	-3.51792200	1.88312600
H	0.60023900	-3.80007700	0.87827400
H	0.25859300	-4.41896500	2.50735800
H	1.01793300	-2.83153700	2.30450900
H	0.45434500	-0.80763400	2.38031200
C	5.30045600	-0.93904800	-0.33264100
C	5.89350400	-2.09103500	-0.90926700
C	7.23309600	-2.05030500	-1.31641900
C	7.93509000	-0.86149700	-1.13897700
C	7.32562200	0.27631000	-0.57097500
C	5.99582900	0.25908100	-0.15666400
C	3.86066200	-2.60964200	-0.47435300
H	7.69831800	-2.92513000	-1.75954100
H	8.97495500	-0.80399500	-1.44665500
H	7.90638900	1.18651700	-0.45463800
H	5.52417800	1.13696400	0.27323800
H	2.90990500	-3.11824600	-0.38081800
N	3.99364200	-1.30565400	-0.05965800

N	4.96022400	-3.11919100	-0.98224200
C	2.96629500	-0.46562400	0.53312800
H	3.03260300	0.51429900	0.05886500
H	1.99444300	-0.89048700	0.26550500
C	3.08671700	-0.35526400	2.05794900
H	3.00343100	-1.35699900	2.49138500
H	4.08553400	0.01730400	2.32428300
C	1.83309300	0.35812200	4.17829900
H	0.97879700	0.93607200	4.53985100
H	1.67390600	-0.69288500	4.43288600
H	2.72592800	0.69914100	4.72025900
C	2.04613800	0.55484000	2.69372500
C	1.65722400	1.73505600	2.08380500
H	1.12106700	2.48768000	2.65522100
H	2.12804600	2.07806800	1.17030500

TS10

Ni	0.22679500	0.31395800	1.44482400
Fe	-4.12531900	-1.10265100	-0.84769600
P	-0.98815900	-1.37190600	0.71318600
P	-0.42046900	1.65233500	-0.17414600
O	-0.44356200	-1.83224200	-0.65137900
C	-2.67040800	-0.65849500	0.54590200
C	-2.87937000	0.45075700	-0.35683800
C	-4.23655700	0.87659000	-0.23688200
H	-4.70717300	1.66096900	-0.81179000
C	-4.88220300	0.03597700	0.71626400
H	-5.92676100	0.07461700	0.99345600
C	-3.92460900	-0.90279200	1.19983400
H	-4.13360700	-1.68694300	1.91028300
C	-1.81352800	1.00567300	-1.25503000
H	-1.33798800	0.15628200	-1.75121100
C	-2.31671100	1.99501700	-2.30127600
H	-2.78010300	2.87354800	-1.84562700
H	-3.06383000	1.51016000	-2.93739700
H	-1.49688600	2.33316100	-2.94121900
C	-3.37565000	-2.63964200	-2.00560400
H	-2.36439800	-2.99081000	-1.85790900
C	-3.74908200	-1.53499400	-2.82765800
H	-3.07864700	-0.95495300	-3.44652800
C	-5.14440200	-1.28998000	-2.64184300
H	-5.71826500	-0.49639200	-3.10051800
C	-5.63525200	-2.24486600	-1.70116700
H	-6.64647400	-2.30156500	-1.32220100

C	-4.54282100	-3.07725200	-1.30807100
H	-4.58531600	-3.87695700	-0.58280300
C	-0.92916300	3.33175900	0.32104300
C	-1.40313200	3.49225700	1.63194800
H	-1.39683400	2.63929800	2.30441000
C	-1.87524700	4.73035900	2.06708200
H	-2.24277400	4.84174600	3.08271300
C	-1.86726800	5.82339800	1.19910600
H	-2.22719300	6.79001000	1.53864800
C	-1.39516200	5.67378400	-0.10675000
H	-1.38888800	6.52249600	-0.78416100
C	-0.93447000	4.43380200	-0.54824300
H	-0.57608800	4.32536500	-1.56582700
C	0.99692700	1.78179900	-1.32318600
C	1.32416300	0.63579400	-2.07123000
H	0.70265800	-0.25365800	-2.00348100
C	2.49800400	0.60185300	-2.82221100
H	2.74905200	-0.29376700	-3.38224400
C	3.36540500	1.69677900	-2.82678600
H	4.28838000	1.65808200	-3.39682200
C	3.05170500	2.83084000	-2.07643400
H	3.72590200	3.68230900	-2.06792700
C	1.87432300	2.87551200	-1.32626800
H	1.64929500	3.75625000	-0.73482600
C	-1.13320600	-2.84825900	1.86774500
C	-2.12448800	-3.87345100	1.29642300
H	-3.14339500	-3.48631300	1.25918900
H	-2.12813400	-4.77675500	1.91899500
H	-1.83585400	-4.16400700	0.28255600
C	-1.53652400	-2.40152000	3.27826600
H	-0.83803100	-1.65237400	3.66643900
H	-1.52305200	-3.25920100	3.96202300
H	-2.53876200	-1.96783400	3.31130400
C	0.26308500	-3.49016600	1.91175200
H	0.58054900	-3.79967800	0.91253000
H	0.24782400	-4.37426000	2.55996400
H	1.01150600	-2.79677900	2.31024200
C	5.28747100	-0.93572700	-0.34524100
C	5.91215200	-2.05611100	-0.95002400
C	7.24326700	-1.96153900	-1.37543800
C	7.90570700	-0.75187400	-1.18742400
C	7.26536800	0.35371100	-0.59041300
C	5.94339500	0.28272100	-0.15726100
C	3.90439900	-2.65259000	-0.49941800

H	7.73195900	-2.81184500	-1.84046400
H	8.93813000	-0.65234200	-1.50910700
H	7.81583400	1.28150300	-0.46592300
H	5.44844600	1.13555600	0.29600100
H	2.97303400	-3.19557400	-0.40379700
N	3.99751800	-1.35226900	-0.06291300
N	5.01422100	-3.11480600	-1.02950800
C	2.94673700	-0.55655400	0.54929800
H	2.99042400	0.43748700	0.10340400
H	1.98599400	-0.99547300	0.26450300
C	3.05576400	-0.48058300	2.07683800
H	3.01501000	-1.49498000	2.48732100
H	4.03047500	-0.06336500	2.36139100
C	1.78362200	0.16987800	4.20951300
H	0.91287400	0.71631900	4.58090700
H	1.66822300	-0.88603000	4.47039000
H	2.67089900	0.54917000	4.73229300
C	1.96161900	0.37065200	2.71587200
C	1.62663100	1.61594900	2.14814800
H	1.13511100	2.36109500	2.76862300
H	2.17991600	2.00627700	1.30063100
H	0.68779500	-0.73153900	2.36493700

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Ni	0.19912000	0.29817500	1.43528800
Fe	-4.16990500	-0.99042500	-0.89768500
P	-1.05531200	-1.39017400	0.67584600
P	-0.36350200	1.63345800	-0.14135200
O	-0.55277100	-1.91177300	-0.68708800
C	-2.71584400	-0.62606900	0.51454900
C	-2.86867700	0.50678500	-0.36969800
C	-4.20992300	0.98459500	-0.26139600
H	-4.64254500	1.79544200	-0.82950900
C	-4.89968200	0.15646900	0.67190100
H	-5.94507400	0.23332600	0.93800000
C	-3.98569600	-0.82753000	1.15198700
H	-4.23376400	-1.61389500	1.84748900
C	-1.76607900	1.03125600	-1.24139300
H	-1.30966900	0.17017600	-1.73596300
C	-2.21191400	2.04497200	-2.29086600
H	-2.65837300	2.93424600	-1.83945100
H	-2.95854900	1.58666500	-2.94686900
H	-1.36750800	2.36110500	-2.90978400
C	-3.46010000	-2.55384700	-2.04401700

H	-2.46493700	-2.93941400	-1.87250800
C	-3.77385400	-1.43375400	-2.87083000
H	-3.06918800	-0.88091200	-3.47639300
C	-5.16169100	-1.13339700	-2.71151100
H	-5.69549100	-0.31842200	-3.18101600
C	-5.70811700	-2.06856200	-1.78165900
H	-6.72803100	-2.08568900	-1.42259500
C	-4.65680300	-2.94403100	-1.36916500
H	-4.74423400	-3.74007200	-0.64367200
C	-0.81265100	3.32759800	0.35315500
C	-1.29517900	3.51441900	1.65686400
H	-1.32687800	2.66788500	2.33597000
C	-1.72551600	4.77262800	2.07668600
H	-2.10025600	4.90540300	3.08704500
C	-1.66623800	5.85817400	1.20117700
H	-1.99359400	6.84005400	1.52965800
C	-1.18421500	5.68162400	-0.09753600
H	-1.13702200	6.52439100	-0.78063200
C	-0.76552100	4.42195200	-0.52462800
H	-0.39856800	4.29203700	-1.53647900
C	1.07780000	1.69463400	-1.26112600
C	1.36692300	0.53074600	-1.99688300
H	0.70877400	-0.33294000	-1.93112600
C	2.54934700	0.44516100	-2.73067100
H	2.77410000	-0.46462900	-3.27871700
C	3.45894200	1.50485300	-2.72991100
H	4.38935900	1.42392200	-3.28265800
C	3.17977500	2.65703000	-1.99284200
H	3.88810200	3.48020100	-1.98040000
C	1.99642200	2.75371500	-1.25815500
H	1.79921600	3.64498700	-0.67262700
C	-1.23609400	-2.82289900	1.88184600
C	-2.25556900	-3.84608500	1.36048200
H	-3.26686000	-3.43822300	1.32032700
H	-2.27339800	-4.72865700	2.01262100
H	-1.98541500	-4.17619200	0.35332100
C	-1.61543900	-2.29924000	3.27305400
H	-0.89454500	-1.55024700	3.62175200
H	-1.61799200	-3.12090600	4.00010000
H	-2.60522700	-1.83698300	3.29166500
C	0.14569800	-3.49543100	1.94760900
H	0.45479800	-3.84754900	0.95978500
H	0.11353000	-4.35533600	2.62730700
H	0.91351000	-2.80841100	2.32060800

C	5.23229600	-0.95166700	-0.38026500
C	5.90926900	-2.02979300	-1.00487700
C	7.20333000	-1.83886500	-1.50584100
C	7.77733200	-0.57807400	-1.37080700
C	7.08604000	0.48365800	-0.75111900
C	5.79995900	0.31673400	-0.24295100
C	3.98045000	-2.77158100	-0.44021600
H	7.73098500	-2.65603500	-1.98736800
H	8.77924800	-0.40351900	-1.75158200
H	7.56791100	1.45333900	-0.66843100
H	5.26480800	1.13573200	0.22585900
H	3.10136800	-3.38442300	-0.28869700
N	3.99445300	-1.46088600	-0.02568700
N	5.09358200	-3.15569900	-1.02294700
C	2.91807600	-0.73124900	0.62318000
H	2.88756700	0.26243200	0.17714900
H	1.97544000	-1.22302500	0.36275000
C	3.06883000	-0.63725500	2.14590500
H	3.14492700	-1.64788800	2.56311700
H	3.99677300	-0.11317700	2.40123300
C	1.89521200	0.02061500	4.32723500
H	1.01204300	0.51060800	4.74703500
H	1.91514900	-1.01679500	4.67757000
H	2.78338800	0.52981400	4.71538600
C	1.88487500	0.09962100	2.79694700
C	1.56608900	1.43353300	2.22316900
H	1.16098400	2.16523200	2.92263600
H	2.28360600	1.86743100	1.53029500
H	0.97064400	-0.64658800	2.55501000

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Fe	-3.21006300	-1.71503300	1.09824200
P	-1.86554100	0.14601900	-1.55871600
P	0.02615800	1.63917700	0.53112900
O	-3.02889700	1.12833700	-1.29950500
C	-1.75232100	-1.07361700	-0.20074200
C	-1.52650200	-0.54478600	1.12452000
C	-1.35107800	-1.64105500	2.02175200
H	-1.20450200	-1.57124400	3.08994400
C	-1.47459400	-2.84633500	1.27074500
H	-1.42987900	-3.85027300	1.66973700
C	-1.71476800	-2.50175000	-0.09173000
H	-1.87370700	-3.20921900	-0.89128600
C	-1.48561900	0.92655200	1.40838300

H	-2.32226700	1.38085300	0.87341800
C	-1.54337300	1.29993000	2.88673300
H	-0.71611500	0.86695900	3.45356800
H	-2.48022600	0.92945100	3.31457400
H	-1.51721000	2.38566600	3.01826800
C	-5.03571800	-2.31732200	0.34012400
H	-5.14982900	-2.90404900	-0.56039000
C	-4.97289900	-0.89179500	0.40782700
H	-4.95411300	-0.20387400	-0.42552200
C	-4.75887500	-0.53062300	1.77155200
H	-4.62406100	0.47631000	2.14106100
C	-4.69050300	-1.72862100	2.54750700
H	-4.50318400	-1.78907600	3.61086500
C	-4.86134900	-2.83502900	1.66088000
H	-4.82625500	-3.88052000	1.93487300
C	1.36094600	1.29153200	1.71857600
C	1.96618100	0.02692400	1.63948400
H	1.66798900	-0.67059100	0.86430400
C	2.94403200	-0.34400000	2.56272600
H	3.41008200	-1.31968700	2.48132000
C	3.32217100	0.54046600	3.57325900
H	4.09108900	0.25504400	4.28502700
C	2.70208500	1.78715400	3.67689600
H	2.97738800	2.46953900	4.47554400
C	1.71872200	2.16022200	2.76138100
H	1.22713800	3.11948000	2.87083200
C	-0.29576400	3.42985400	0.39830900
C	-1.55014100	3.80259000	-0.11967400
H	-2.27718300	3.04022500	-0.39585900
C	-1.83638700	5.14874600	-0.34199400
H	-2.80747300	5.42765100	-0.74024600
C	-0.88180900	6.13083400	-0.06957300
H	-1.11070900	7.17794400	-0.24429300
C	0.37479800	5.76022200	0.41067200
H	1.13011000	6.51567800	0.60605800
C	0.67176900	4.41601300	0.63714200
H	1.66022000	4.14481000	0.98617200
C	-2.21383400	-0.80009700	-3.14616200
C	-3.51922400	-1.59612900	-3.01897000
H	-3.43949900	-2.39823400	-2.28212000
H	-3.78387100	-2.04759300	-3.98410300
H	-4.33888700	-0.93884700	-2.71623100
C	-1.03605700	-1.71131700	-3.50622900
H	-0.12708300	-1.12077900	-3.67599500

H	-1.24325900	-2.25313100	-4.43763900
H	-0.82426200	-2.45228000	-2.73181200
C	-2.37598000	0.27718400	-4.23209800
H	-3.20067400	0.95213900	-3.99039200
H	-2.57769900	-0.19035200	-5.20376700
H	-1.46619800	0.88307400	-4.33206400
H	1.36167200	-1.71793600	-2.27614900
Ni	0.26689500	0.95776300	-1.46563100
C	4.12984200	-2.23997900	-0.68563500
C	3.16064300	-2.98402100	0.03832500
C	3.53875800	-3.70280400	1.17925700
C	4.87409900	-3.65338700	1.56858700
C	5.82435200	-2.90658600	0.84111400
C	5.47157600	-2.18843600	-0.29857500
C	2.12166300	-2.05551700	-1.58770900
H	2.80148400	-4.27259700	1.73558600
H	5.19532800	-4.19958300	2.45030600
H	6.85663800	-2.89247200	1.17725900
H	6.20772400	-1.61845300	-0.85516400
H	3.14165100	0.45183900	-0.39816000
N	3.42987500	-1.65998800	-1.73353000
N	1.91138600	-2.83974300	-0.55405300
C	3.93177100	-0.71478300	-2.72685800
H	4.76593100	-1.17688100	-3.26484500
H	3.12495800	-0.56858800	-3.44916300
C	4.36579400	0.62450100	-2.11447400
H	5.30928200	0.47898400	-1.57580700
H	4.57611800	1.31855100	-2.93820800
C	3.96114300	2.40691200	-0.38103200
H	3.25769300	2.80508500	0.35356500
H	4.86198000	2.09810400	0.16080200
H	4.23370300	3.22004100	-1.06499700
C	3.34062700	1.23133000	-1.13921500
C	2.01850000	1.62967900	-1.79303700
H	1.96658100	2.70891800	-1.98681100
H	1.85897500	1.11096000	-2.77803600

TS11

Fe	-3.95592900	-1.34924600	0.06570500
P	-0.49028700	-1.59383900	-0.37280100
P	-0.45897700	1.74775700	-0.05430200
O	-0.64350300	-1.26195200	-1.85545700
C	-1.96517200	-1.14110500	0.58870900
C	-2.59804300	0.14558300	0.39970300

C	-3.66208100	0.25538200	1.34325600
H	-4.34842400	1.08554400	1.42585200
C	-3.72058600	-0.95465700	2.09337700
H	-4.45439800	-1.19903900	2.84887600
C	-2.68331300	-1.81453100	1.63465800
H	-2.50149200	-2.81333600	1.99745300
C	-2.15162200	1.15975200	-0.60708600
H	-1.92943300	0.62969600	-1.53606100
C	-3.15766500	2.27564300	-0.87320700
H	-3.39982700	2.83594400	0.03243600
H	-4.08618000	1.84711600	-1.26242100
H	-2.77002300	2.97782200	-1.61648200
C	-4.71739500	-3.07915600	-0.79007000
H	-4.44261500	-4.08257700	-0.49930700
C	-4.06485300	-2.28010300	-1.77785900
H	-3.18069300	-2.54206600	-2.33938000
C	-4.72150400	-1.01532400	-1.82284400
H	-4.43288900	-0.17758300	-2.44152400
C	-5.77776000	-1.02841900	-0.86138600
H	-6.43315200	-0.20180900	-0.62422900
C	-5.77510100	-2.30534000	-0.22355000
H	-6.43185100	-2.61637800	0.57715800
C	-0.81088900	2.92093100	1.29546200
C	-0.59957600	2.46398300	2.60514000
H	-0.17200900	1.47811700	2.76009300
C	-0.92620400	3.26969900	3.69506100
H	-0.75818300	2.90529300	4.70385500
C	-1.45961500	4.54274800	3.48708300
H	-1.70727200	5.17370200	4.33547600
C	-1.67419700	5.00521100	2.18713900
H	-2.09034200	5.99456500	2.02232900
C	-1.35828700	4.19768500	1.09478600
H	-1.53822900	4.56298400	0.09008700
C	0.18760700	2.65092200	-1.50402400
C	0.26271800	1.92337600	-2.70569400
H	-0.11065500	0.90268700	-2.74550000
C	0.85881100	2.49236300	-3.82955300
H	0.91366700	1.92306000	-4.75271600
C	1.39395800	3.78178400	-3.76729600
H	1.86136600	4.22041100	-4.64380500
C	1.33477000	4.50013800	-2.57291000
H	1.75846300	5.49828900	-2.51461100
C	0.73717300	3.93806400	-1.44294000
H	0.71366000	4.49968800	-0.51628500

C	-0.13450700	-3.41824800	-0.10304800
C	-1.34718100	-4.25270100	-0.53960800
H	-2.22539700	-4.05437900	0.07536100
H	-1.10069500	-5.31732500	-0.44777700
H	-1.60693000	-4.05813900	-1.58330200
C	0.23672800	-3.71045200	1.35932600
H	1.11020400	-3.14036000	1.68622200
H	0.48454900	-4.77459600	1.45531600
H	-0.58313700	-3.50396900	2.05011800
C	1.05601400	-3.75555600	-1.02130400
H	0.83151400	-3.50935400	-2.06231300
H	1.26460700	-4.82949200	-0.95581000
H	1.96692700	-3.22615500	-0.73297300
H	1.15665200	-1.30902900	0.29561300
Ni	1.02894700	0.20850600	0.44312000
C	4.56059100	-1.66385100	-0.11369500
C	4.29593500	-2.16355400	1.19038400
C	5.25773800	-2.94383700	1.84476300
C	6.46150300	-3.18707400	1.18870200
C	6.71506400	-2.66975400	-0.09781500
C	5.76960200	-1.89876200	-0.77160600
C	2.55359200	-1.02175600	0.61415100
H	5.06240300	-3.33596300	2.83812200
H	7.22546900	-3.78493500	1.67694400
H	7.66886100	-2.87627000	-0.57430400
H	5.96764700	-1.50106600	-1.76199200
H	4.28356500	0.91445100	0.89755900
N	3.41563600	-0.97676800	-0.47161700
N	3.03543300	-1.75618100	1.60568600
C	3.25144700	0.00492300	-1.53476700
H	3.73230800	-0.36908900	-2.44265400
H	2.17873800	0.06347800	-1.73638400
C	3.80152500	1.38589300	-1.12854000
H	4.85835500	1.45063500	-1.41426800
H	3.26808900	2.15064100	-1.70548800
C	4.36174500	3.03543600	0.68110000
H	4.33608500	3.25425300	1.75405400
H	5.41063300	3.04926000	0.36004700
H	3.84144600	3.84958200	0.16179700
C	3.69740400	1.68255800	0.38013800
C	2.27202700	1.66233000	0.95017300
H	2.30929800	1.53935100	2.03976100
H	1.81003100	2.63470200	0.75523100

TS9'

Ni	0.32141800	1.01510500	-1.11184100
Fe	-2.66070900	-2.58919600	1.07649000
P	-0.95574800	-1.06086800	-1.60170800
P	-1.24478800	1.80545500	0.19557800
O	-2.20519500	-0.49113100	-2.24524100
C	-1.16117800	-1.51288400	0.13562400
C	-1.90389600	-0.67401000	1.05170000
C	-1.75854400	-1.22770400	2.35724000
H	-2.22139700	-0.84507100	3.25508500
C	-0.96787100	-2.41004000	2.26422100
H	-0.72677700	-3.07981200	3.07798200
C	-0.59884700	-2.59149400	0.90163700
H	-0.03149700	-3.42219100	0.51253300
C	-2.61053200	0.58890800	0.66302300
H	-3.10064800	0.40873000	-0.29648200
C	-3.63405700	1.08432400	1.67943800
H	-3.18208000	1.29541000	2.65151800
H	-4.41275300	0.32890100	1.82687400
H	-4.11530900	1.99951400	1.32326000
C	-3.42045200	-4.40064300	0.40230400
H	-2.82657400	-5.19377700	-0.02893700
C	-4.02340000	-3.31922100	-0.30869800
H	-3.96000500	-3.13670200	-1.37069800
C	-4.68232500	-2.48079400	0.63688800
H	-5.20383500	-1.56244700	0.40742800
C	-4.48699200	-3.04134100	1.93553800
H	-4.83498100	-2.61969900	2.86843600
C	-3.70711500	-4.22822400	1.79038200
H	-3.35961900	-4.86122600	2.59524000
C	-0.68502300	2.44478700	1.82090100
C	0.53089400	1.94997500	2.31555100
H	1.10911300	1.26851900	1.70120000
C	0.99568300	2.32514900	3.57633400
H	1.93813100	1.93033900	3.94449900
C	0.25245200	3.21143500	4.35679500
H	0.61463500	3.51144900	5.33570000
C	-0.95850800	3.71385300	3.87482100
H	-1.54055700	4.40359300	4.47909200
C	-1.42829500	3.32992800	2.61890800
H	-2.37133300	3.72499500	2.25814800
C	-2.14005400	3.16626300	-0.64091600
C	-2.98051100	2.82040600	-1.71447700
H	-3.10796700	1.77593800	-1.98565200

C	-3.61081300	3.81418800	-2.46125500
H	-4.26168600	3.53376500	-3.28442400
C	-3.39742300	5.16275000	-2.16460900
H	-3.88802700	5.93491300	-2.74985800
C	-2.53815800	5.51249000	-1.12287100
H	-2.35325500	6.55862500	-0.89601100
C	-1.90914200	4.52168400	-0.36631900
H	-1.23645300	4.80834600	0.43444500
C	-0.28205200	-2.51144100	-2.57157300
C	-1.20441700	-3.72965000	-2.43880900
H	-1.25831500	-4.09014700	-1.41018900
H	-0.82763600	-4.54402400	-3.06869100
H	-2.21744900	-3.49157200	-2.77302800
C	1.15084600	-2.85437200	-2.13796400
H	1.81016100	-1.98426200	-2.21054500
H	1.55681200	-3.62730500	-2.80019600
H	1.20654000	-3.23911300	-1.11730200
C	-0.26488400	-2.03091000	-4.03481600
H	-1.26919700	-1.77626400	-4.37997700
H	0.13716100	-2.82503500	-4.67404800
H	0.36901300	-1.14621500	-4.16050600
H	0.39791600	-0.34785900	-1.82221800
C	5.64026500	-0.33523500	0.42021400
C	6.23582200	-1.56766700	0.79259000
C	7.62002600	-1.63718500	0.99637200
C	8.36549000	-0.47519500	0.82312100
C	7.75598900	0.74232300	0.45544200
C	6.38237500	0.83563700	0.24641300
C	4.13694800	-1.94142300	0.60883600
H	8.08549400	-2.57531900	1.28155900
H	9.44053800	-0.50191000	0.97396700
H	8.37257400	1.62746400	0.33092600
H	5.91604000	1.77354500	-0.03742700
H	3.15509500	-2.39690700	0.59405600
N	4.28617200	-0.60834300	0.30957600
N	5.26135500	-2.55314800	0.90154700
C	3.23263600	0.32155200	-0.07382600
H	2.27409800	-0.13216400	0.19789100
H	3.34485500	1.22894100	0.52634000
C	1.92438700	1.59227600	-3.53649400
H	1.88882500	0.59939800	-3.99819500
H	2.77895800	2.12287000	-3.98376700
C	3.23559400	0.64370300	-1.57128300
H	3.21855700	-0.30520900	-2.12003300

H	4.18851800	1.12495500	-1.83853100
C	2.06990300	1.50804200	-2.02895800
C	1.56807400	2.55286600	-1.23039100
H	1.98685700	2.78326900	-0.25326800
H	1.04170100	3.38127700	-1.70217700
H	1.01402100	2.12767100	-3.82142400

17'

Ni	0.34394300	0.70098700	-1.16237900
Fe	-3.19906200	-2.22821200	1.07400900
P	-1.11748900	-0.91370800	-1.45347200
P	-0.99641300	1.79258300	0.24418400
O	-2.39057100	-0.36345000	-2.11141300
C	-1.46141000	-1.44493700	0.26715500
C	-2.08684800	-0.50922600	1.17432000
C	-2.14654300	-1.11086100	2.46693000
H	-2.59279300	-0.67356300	3.34858800
C	-1.59061400	-2.41990700	2.37254600
H	-1.53701200	-3.14701300	3.17133400
C	-1.16787800	-2.62696800	1.02634900
H	-0.73685200	-3.54095100	0.64867100
C	-2.54194000	0.85948300	0.76466500
H	-3.08253500	0.75492400	-0.17907200
C	-3.41074900	1.57914000	1.78962200
H	-2.89223100	1.72067400	2.74088500
H	-4.31529400	0.99380500	1.98274400
H	-3.71709000	2.56092600	1.41724200
C	-4.23401600	-3.74705000	0.11633600
H	-3.76719400	-4.58622800	-0.37883700
C	-4.54096500	-2.48507700	-0.47853300
H	-4.30402400	-2.16850200	-1.48353600
C	-5.10630500	-1.65254700	0.53156300
H	-5.40655100	-0.62202300	0.40245900
C	-5.14830600	-2.39565200	1.75089500
H	-5.49028100	-2.02850000	2.70884300
C	-4.60908000	-3.69219900	1.49333600
H	-4.46902300	-4.47845100	2.22241900
C	-0.25205800	2.30050200	1.83321900
C	0.81067100	1.51460300	2.30624100
H	1.17533700	0.69636400	1.69432000
C	1.38761400	1.76963300	3.54979500
H	2.20648600	1.14990400	3.90269500
C	0.91199900	2.82109400	4.33478200
H	1.36408500	3.02743900	5.30023800

C	-0.15093600	3.60353800	3.87902400
H	-0.53020400	4.41606900	4.49152500
C	-0.73749400	3.34119300	2.64059900
H	-1.57546100	3.94349700	2.30936900
C	-1.63388500	3.25934100	-0.63726500
C	-2.44924300	2.99150000	-1.75303700
H	-2.69254500	1.96131100	-2.00827400
C	-2.90068400	4.03960400	-2.55276300
H	-3.53265200	3.82485900	-3.40953600
C	-2.53335400	5.35689100	-2.26493600
H	-2.88607500	6.17047900	-2.89182400
C	-1.69943400	5.62200700	-1.17869000
H	-1.39678200	6.64176500	-0.95924500
C	-1.24635000	4.57854600	-0.36826900
H	-0.58491800	4.79711300	0.46226400
C	-0.53208000	-2.43220600	-2.39443500
C	-1.60635200	-3.52777600	-2.32981800
H	-1.75596600	-3.89463100	-1.31349500
H	-1.30950500	-4.37628600	-2.95833500
H	-2.56356100	-3.15254600	-2.69978500
C	0.80994900	-2.95128500	-1.86278900
H	1.58096700	-2.17878600	-1.93434800
H	1.14092500	-3.80806700	-2.46184300
H	0.75223100	-3.27911400	-0.82180200
C	-0.36243300	-1.98484200	-3.85562500
H	-1.30523300	-1.61008700	-4.26195200
H	-0.02945100	-2.83206300	-4.46686400
H	0.38430600	-1.18822900	-3.94479000
H	0.93152300	-0.22390000	-2.11007000
C	5.65628000	-0.76198900	0.38727800
C	6.27541800	-2.02852800	0.54021000
C	7.63801400	-2.10141300	0.85578800
C	8.33833200	-0.90855400	1.00842300
C	7.70539500	0.34200800	0.85379300
C	6.35193200	0.43935900	0.53978200
C	4.21991600	-2.41360900	0.07788800
H	8.12213300	-3.06530400	0.97586200
H	9.39611900	-0.93698000	1.25195500
H	8.28698600	1.25006100	0.98134000
H	5.86702000	1.40308200	0.42025600
H	3.26794500	-2.88203200	-0.13602700
N	4.33156500	-1.04240300	0.09290200
N	5.34332300	-3.04050500	0.33903800
C	3.28394700	-0.07582700	-0.19281800

H	2.31725300	-0.57200400	-0.06073000
H	3.34988800	0.72234900	0.55145700
C	3.37278600	0.48177600	-1.61625000
H	4.32841600	1.00853900	-1.74521400
H	3.38634600	-0.35893300	-2.31719900
C	2.09155300	1.69094400	-3.47211600
H	1.18490600	2.26330300	-3.68324500
H	2.95219300	2.27253100	-3.83042300
H	2.05590100	0.76301500	-4.04877000
C	2.24460100	1.42652600	-1.99013000
C	1.69885600	2.30960600	-1.07482200
H	1.13492100	3.16792000	-1.42850800
H	2.05159100	2.36393500	-0.05079600

TS10'

C	5.66691000	-0.71450500	0.39975500
C	6.31262500	-1.96284800	0.58818100
C	7.67835300	-1.99843500	0.89649500
C	8.35529800	-0.78754500	1.00633600
C	7.69604400	0.44450200	0.81701200
C	6.33883700	0.50484500	0.50976600
C	4.26284400	-2.40404100	0.15084200
H	8.18255400	-2.94823200	1.04323700
H	9.41499900	-0.78706900	1.24305300
H	8.25991200	1.36759400	0.91182900
H	5.83428200	1.45477500	0.36431000
H	3.31992400	-2.89824000	-0.04351700
N	4.34655400	-1.03079200	0.12249500
N	5.40026100	-2.99927200	0.42446700
C	3.27940400	-0.09427000	-0.18898400
H	3.33130000	0.72777900	0.52991800
H	2.32375200	-0.60489800	-0.03574100
C	3.35563900	0.42340100	-1.62838800
H	3.41725600	-0.43659100	-2.30357400
H	4.28118800	0.99694400	-1.76710300
C	2.08611000	1.58534300	-3.52284100
H	1.15700100	2.10609900	-3.76665900
H	2.13291200	0.66772400	-4.11622300
H	2.92604200	2.22449300	-3.82359400
C	2.17893900	1.30151900	-2.03410100
C	1.66168100	2.25747100	-1.13586800
H	1.15615900	3.13282500	-1.53511400
H	2.07438600	2.37150900	-0.13921400
H	1.10326200	-0.01301400	-2.10864300

Ni	0.31068200	0.74032600	-1.13030400
Fe	-3.16767200	-2.26991500	1.08378900
P	-1.10124600	-0.92946900	-1.43233400
P	-1.03735400	1.79698900	0.24573700
O	-2.39969500	-0.45257700	-2.10562100
C	-1.44011000	-1.46242600	0.29015900
C	-2.08606300	-0.53019700	1.18656500
C	-2.15101100	-1.12523700	2.48231900
H	-2.61376500	-0.68985600	3.35641900
C	-1.57189200	-2.42529600	2.40189000
H	-1.51419900	-3.14646800	3.20581400
C	-1.13248900	-2.63337100	1.06072900
H	-0.68486900	-3.54334100	0.69256300
C	-2.56206700	0.82756100	0.76278400
H	-3.08957400	0.70544200	-0.18677900
C	-3.45904200	1.53453400	1.77221400
H	-2.95605400	1.69222900	2.72926800
H	-4.35196800	0.92918300	1.95717300
H	-3.78327600	2.50691900	1.39033400
C	-4.47271600	-2.55047200	-0.49433300
H	-4.21366400	-2.22009900	-1.48971000
C	-5.07577400	-1.73456000	0.50790400
H	-5.39668900	-0.71047600	0.37624100
C	-5.12576900	-2.48282600	1.72389900
H	-5.49432600	-2.12643100	2.67610200
C	-4.55234800	-3.76593900	1.47277100
H	-4.40906600	-4.55166300	2.20182400
C	-4.14928300	-3.80718100	0.10290700
H	-3.65241200	-4.63287600	-0.38577200
C	-0.30564100	2.35964200	1.82002600
C	0.81525700	1.65667100	2.28803800
H	1.23150400	0.86080400	1.68002900
C	1.38574400	1.96641300	3.52211900
H	2.25038100	1.41057600	3.87225000
C	0.84501700	2.99029400	4.30132100
H	1.29128600	3.23848600	5.25959500
C	-0.27415300	3.69214300	3.84885500
H	-0.70198500	4.48425600	4.45600100
C	-0.85313600	3.37532500	2.61992000
H	-1.73129400	3.91639200	2.28717000
C	-1.70236300	3.22945700	-0.67027500
C	-2.48969500	2.92135400	-1.79551000
H	-2.69775700	1.88065600	-2.04082300
C	-2.96030600	3.94543400	-2.61523100

H	-3.57087200	3.70111300	-3.47955600
C	-2.63969400	5.27691800	-2.33690400
H	-3.00708100	6.07159400	-2.97944400
C	-1.83412800	5.58155200	-1.23954200
H	-1.56863500	6.61311000	-1.02719900
C	-1.36208400	4.56278000	-0.40901600
H	-0.72312900	4.81064500	0.43092000
C	-0.42940100	-2.42499000	-2.35120200
C	-1.45026600	-3.57151800	-2.30257000
H	-1.59149200	-3.95264400	-1.28987500
H	-1.10997600	-4.40185800	-2.93370900
H	-2.42109600	-3.23810700	-2.67761200
C	0.92563300	-2.86955600	-1.78798900
H	1.66071300	-2.06367500	-1.86631900
H	1.30769600	-3.72353000	-2.36032100
H	0.86602200	-3.17365200	-0.73983000
C	-0.25143600	-1.97586000	-3.81065800
H	-1.20408500	-1.65579500	-4.24028100
H	0.14283100	-2.80432600	-4.41131100
H	0.45034700	-1.13788300	-3.88730100

18'

C	5.54572700	-0.77775600	0.32778100
C	6.26634600	-1.98839400	0.48751400
C	7.58978900	-1.95292100	0.94445800
C	8.15096300	-0.71100700	1.22613100
C	7.41876000	0.48272400	1.06072900
C	6.10194200	0.47250100	0.60723100
C	4.31437900	-2.53506900	-0.20460800
H	8.15049000	-2.87329000	1.07228500
H	9.17556700	-0.65551800	1.58125400
H	7.89326700	1.43193200	1.29076900
H	5.54175400	1.39325700	0.47830000
H	3.43758200	-3.07864200	-0.53246600
N	4.29063900	-1.16239700	-0.11605800
N	5.46184000	-3.06916900	0.14366000
C	3.18736100	-0.27733500	-0.44926600
H	3.14476600	0.50160700	0.31507200
H	2.25721100	-0.84991300	-0.37876600
C	3.31760200	0.33619900	-1.84743100
H	3.48853000	-0.47089200	-2.56883200
H	4.19422300	0.99195800	-1.88779400
C	2.12033200	1.59491200	-3.72560200
H	1.19019900	2.10033300	-3.99899000

H	2.26761300	0.75078000	-4.40758200
H	2.94754900	2.29827500	-3.86775100
C	2.07516700	1.13697600	-2.26447700
C	1.59817400	2.15410800	-1.29620400
H	1.21385600	3.07976500	-1.72455500
H	2.18433300	2.31708900	-0.39488000
H	1.25110000	0.25086100	-2.34154800
Ni	0.21459600	0.79385900	-1.19458500
Fe	-3.04467100	-2.28355500	1.21656800
P	-1.26829600	-0.86416100	-1.47569700
P	-0.97304500	1.80681600	0.27761700
O	-2.64649600	-0.38761500	-1.98188400
C	-1.41281100	-1.48039200	0.24705600
C	-1.92204600	-0.56858000	1.24724100
C	-1.84324900	-1.20923200	2.52132300
H	-2.18412900	-0.79819500	3.46067400
C	-1.30698200	-2.51601000	2.32631700
H	-1.17014600	-3.26702700	3.09248100
C	-1.03845800	-2.68291600	0.93437700
H	-0.66337000	-3.58796500	0.48127300
C	-2.42825800	0.80738200	0.92484200
H	-3.06199300	0.71905200	0.03833100
C	-3.19856600	1.48652600	2.05227900
H	-2.58854000	1.61415500	2.94977000
H	-4.06789400	0.87778500	2.31925300
H	-3.55913000	2.47078700	1.73962400
C	-4.52420900	-2.44229000	-0.21241900
H	-4.35568600	-2.04141700	-1.20184700
C	-4.99559200	-1.69140100	0.90554200
H	-5.30683700	-0.65653200	0.88145400
C	-4.91969900	-2.52032200	2.06679600
H	-5.17460900	-2.22788400	3.07628500
C	-4.40172800	-3.78897900	1.66632400
H	-4.19277000	-4.62530100	2.31926300
C	-4.15769700	-3.73988000	0.25960500
H	-3.72952500	-4.53337500	-0.33606600
C	-0.10002900	2.34856700	1.78407300
C	1.01978500	1.59998600	2.17571800
H	1.35481700	0.78442000	1.54514300
C	1.69033000	1.89096400	3.36273100
H	2.55410100	1.30067500	3.65351400
C	1.25128400	2.94173700	4.16995500
H	1.77616200	3.17652300	5.09103600
C	0.13208200	3.68710900	3.79409400

H	-0.21764200	4.49949200	4.42401900
C	-0.54833000	3.38838400	2.61326500
H	-1.42612300	3.96393200	2.34298100
C	-1.72544500	3.23949800	-0.56225400
C	-2.66213700	2.94344800	-1.56971600
H	-2.91914300	1.90684000	-1.78474500
C	-3.21820000	3.97563300	-2.32342900
H	-3.94302800	3.74142000	-3.09750500
C	-2.83832200	5.30082000	-2.09597600
H	-3.27415000	6.10148200	-2.68615800
C	-1.88565000	5.59191900	-1.11899900
H	-1.57391200	6.61839000	-0.94950700
C	-1.32502700	4.56602900	-0.35580200
H	-0.57274200	4.80191700	0.38816300
C	-0.68538100	-2.30685100	-2.53413100
C	-1.69499700	-3.46079200	-2.45840300
H	-1.72297700	-3.91662300	-1.46684000
H	-1.43055800	-4.24242600	-3.18206200
H	-2.70079200	-3.10461000	-2.69641600
C	0.71816600	-2.77061100	-2.12487600
H	1.45256400	-1.97233000	-2.26813900
H	1.03134300	-3.61733300	-2.74815700
H	0.76591200	-3.09196800	-1.08135800
C	-0.64346800	-1.76744100	-3.97367600
H	-1.63491800	-1.43935500	-4.29597600
H	-0.29275500	-2.54756700	-4.66028300
H	0.03645200	-0.91158800	-4.06073500

19'

H	-4.19343100	-2.96769700	0.25460400
C	-6.35617800	-0.73085700	-0.63665800
C	-6.99572300	-1.43741700	0.41448000
C	-8.28860400	-1.07600900	0.81294900
C	-8.90733100	-0.02238500	0.14784200
C	-8.26189500	0.66415500	-0.90077900
C	-6.97625200	0.32330400	-1.31335300
C	-5.07476400	-2.34722000	0.16012900
H	-8.78313700	-1.61205400	1.61659500
H	-9.90955700	0.27874300	0.43735300
H	-8.77972100	1.47762400	-1.39995700
H	-6.48922300	0.85101300	-2.12648500
H	-1.98589800	-0.29360500	-0.12797200
N	-5.11494300	-1.33414500	-0.77111300
N	-6.16160500	-2.44296900	0.88936900

C	-4.05446900	-0.96831000	-1.69970000
H	-4.44986000	-1.03642700	-2.71952600
H	-3.27431600	-1.72751700	-1.60628100
C	-3.46582300	0.43229800	-1.49286400
H	-4.26400400	1.18008600	-1.54529800
H	-2.80544700	0.61972000	-2.34689100
C	-3.46647700	0.64962300	1.10543800
H	-2.82371400	0.93829400	1.94191700
H	-3.87344600	-0.33921000	1.31996300
H	-4.30073500	1.35665400	1.05362100
C	-2.66773600	0.69791800	-0.20337500
C	-1.77798800	1.88460200	-0.30631900
H	-1.82264000	2.59480000	0.51796100
H	-1.71145900	2.36623800	-1.28088700
Ni	-0.50111300	0.45224400	-0.02503700
Fe	4.06679900	-1.85799200	-0.35995600
P	0.68788400	-1.37455000	0.51383400
P	1.16815900	1.78358400	0.16223800
O	1.20087700	-1.32353100	1.96831700
C	2.10305300	-1.29700400	-0.65733200
C	2.96836000	-0.14188700	-0.60090600
C	3.92792600	-0.24373600	-1.65377200
H	4.73398200	0.44945400	-1.84786700
C	3.68207200	-1.45880500	-2.35752800
H	4.26820400	-1.84674300	-3.17946500
C	2.56328900	-2.10414700	-1.75078700
H	2.17164500	-3.06459400	-2.04678200
C	2.82833700	0.94102200	0.42666600
H	2.68069400	0.45252100	1.39408000
C	4.01243100	1.89937400	0.50460900
H	4.18817500	2.41227400	-0.44401400
H	4.91787400	1.33851400	0.75629700
H	3.85618300	2.65396900	1.28082800
C	4.12717800	-2.73202100	1.51034700
H	3.24286100	-2.73227600	2.13210300
C	5.07181400	-1.66563600	1.43011000
H	5.05996500	-0.76747200	2.03163600
C	5.99780300	-1.96416400	0.38376700
H	6.81351400	-1.33439200	0.05582500
C	5.62436800	-3.21849200	-0.18682300
H	6.10758900	-3.70505900	-1.02302200
C	4.46922400	-3.69132600	0.50883200
H	3.92369700	-4.59782800	0.28812600
C	1.43141600	2.92339000	-1.23501200

C	0.92245600	2.54071800	-2.48534800
H	0.34050500	1.62757400	-2.56335000
C	1.16136400	3.32086100	-3.61592100
H	0.76538200	3.01145900	-4.57842900
C	1.90236400	4.49877400	-3.50741500
H	2.08217400	5.11136000	-4.38574700
C	2.41453900	4.88723200	-2.26814300
H	2.99478500	5.80078700	-2.18022100
C	2.18974800	4.10091000	-1.13830900
H	2.60471000	4.40543100	-0.18479500
C	0.91243800	2.72281300	1.70547800
C	0.91579700	1.96335600	2.89022100
H	1.09774600	0.89006400	2.84735500
C	0.64188700	2.58019300	4.10949900
H	0.64781600	1.98954600	5.02079700
C	0.34890400	3.94564200	4.16023400
H	0.13413700	4.42145100	5.11247500
C	0.31802100	4.69332900	2.98287000
H	0.07527100	5.75143300	3.01461900
C	0.59412500	4.08560000	1.75628800
H	0.54899100	4.67236100	0.84581100
C	-0.16837900	-3.01834600	0.19662000
C	0.77822700	-4.18797800	0.49728800
H	1.62806100	-4.21315200	-0.18787300
H	0.24383200	-5.14282400	0.41039700
H	1.16912500	-4.10907800	1.51550100
C	-0.69656900	-3.07448500	-1.24238600
H	-1.19740800	-2.13832900	-1.51383200
H	-1.42045400	-3.89158100	-1.35498100
H	0.09757400	-3.23788300	-1.97322800
C	-1.34703100	-3.06247300	1.18386400
H	-0.99577300	-2.98887400	2.21653900
H	-1.89690900	-4.00538000	1.07333200
H	-2.04632300	-2.23640100	1.01486000

TS11'

H	-1.27865400	-1.17213800	0.39812700
C	-4.51481100	-1.58778400	-0.73341900
C	-4.55151400	-1.82460700	0.66648100
C	-5.66442600	-2.45564500	1.23685500
C	-6.71659200	-2.81184800	0.39748200
C	-6.67278700	-2.55215200	-0.98734300
C	-5.57114900	-1.93513000	-1.57773500
C	-2.67398900	-0.82624500	0.27158300

H	-5.69775200	-2.64838200	2.30460800
H	-7.59362300	-3.29698300	0.81559600
H	-7.51692100	-2.83818100	-1.60785700
H	-5.54110300	-1.73411200	-2.64409500
H	-4.30795000	1.13004700	-0.10425400
N	-3.28723100	-0.99225800	-0.96310600
N	-3.38772400	-1.35228000	1.25567600
C	-2.89304100	-0.21134400	-2.12387500
H	-3.17174900	-0.75141500	-3.03327600
H	-1.80073500	-0.15588600	-2.09478500
C	-3.51161500	1.19738900	-2.08814900
H	-4.51193700	1.16086900	-2.53577400
H	-2.90669600	1.86069900	-2.72013100
C	-4.31076300	3.16382200	-0.74517800
H	-4.45604000	3.58191600	0.25645900
H	-5.29281900	3.10550700	-1.23092100
H	-3.69575100	3.87120600	-1.31553400
C	-3.63537900	1.78504300	-0.66947600
C	-2.30784700	1.89446500	0.08877000
H	-2.50181700	2.11886700	1.14525600
H	-1.75105300	2.73922100	-0.33056600
Ni	-1.09187000	0.34443800	0.29442000
Fe	3.67760500	-1.60035500	-0.61881600
P	0.45947400	-1.55074600	0.79164800
P	0.58888500	1.77767100	0.33387500
O	1.04476100	-1.18281200	2.15189500
C	1.63945200	-1.24622200	-0.55895500
C	2.38884300	-0.01021000	-0.60601500
C	3.14234000	0.00158500	-1.81726500
H	3.82832200	0.77652300	-2.12661500
C	2.89661500	-1.22078400	-2.50798700
H	3.36440100	-1.53360100	-3.43127700
C	1.97504600	-1.98917800	-1.74083300
H	1.62577900	-2.97675500	-1.99742200
C	2.31487800	1.05093800	0.44839700
H	2.30285500	0.54928100	1.41865900
C	3.44209900	2.07771100	0.40175800
H	3.47769700	2.60866800	-0.55199900
H	4.40325100	1.57476900	0.54242400
H	3.32584600	2.81578600	1.20027200
C	4.24558400	-2.49905300	1.15582900
H	3.54607700	-2.67121700	1.95997000
C	4.98177800	-1.29542800	0.95350000
H	4.95452500	-0.42650600	1.59531100

C	5.71007400	-1.41977800	-0.26869000
H	6.33294200	-0.65908100	-0.71874000
C	5.42398500	-2.70430700	-0.82147000
H	5.79567200	-3.08815400	-1.76156200
C	4.51945200	-3.37163800	0.05877700
H	4.09450800	-4.35265800	-0.09551300
C	0.70444000	2.89349700	-1.10789700
C	0.18261700	2.43258300	-2.32556300
H	-0.33470300	1.47999400	-2.35289700
C	0.31369200	3.19152100	-3.48729400
H	-0.09587700	2.82175500	-4.42243500
C	0.96247300	4.42687600	-3.44362800
H	1.05812300	5.02381800	-4.34560500
C	1.48798500	4.89372900	-2.23768800
H	1.99626600	5.85250000	-2.19942000
C	1.36766100	4.12962700	-1.07656500
H	1.79055000	4.49727900	-0.14904500
C	0.40537600	2.76900700	1.85311400
C	0.60276500	2.08314300	3.06519800
H	0.88599900	1.03312000	3.05424800
C	0.38724100	2.73578900	4.27702200
H	0.54265800	2.19984100	5.20857700
C	-0.04260300	4.06496300	4.29502500
H	-0.21345100	4.56902100	5.24161000
C	-0.26793800	4.73790300	3.09415100
H	-0.61937600	5.76542200	3.10191000
C	-0.04949700	4.09360600	1.87503800
H	-0.24588800	4.62082600	0.94876200
C	-0.06449700	-3.35553700	0.73616100
C	1.17402100	-4.26234400	0.77819900
H	1.78171500	-4.17601200	-0.12277300
H	0.84748100	-5.30521500	0.87005900
H	1.80281800	-4.03355700	1.64163400
C	-0.91059100	-3.66319700	-0.51012000
H	-1.87449100	-3.15236500	-0.49191300
H	-1.11538900	-4.73964400	-0.54462500
H	-0.40637600	-3.39582700	-1.44252600
C	-0.89643500	-3.58719600	2.01158600
H	-0.29492400	-3.40242900	2.90497200
H	-1.23538600	-4.63009300	2.03106000
H	-1.77884600	-2.94280800	2.05282000

15"

Ni	-1.31499800	0.56510900	0.32086100
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Fe	3.63600000	-1.68485100	-0.54637200
P	0.60967100	-1.84353000	0.96507900
P	0.59729600	1.83286300	0.34865100
O	1.27705200	-1.60813800	2.29615500
C	1.61809600	-1.35787200	-0.44284700
C	2.33445400	-0.10022000	-0.45071900
C	3.06431600	-0.03187900	-1.67374500
H	3.72064200	0.77291000	-1.96969600
C	2.82842700	-1.22717500	-2.41128100
H	3.28395900	-1.49061700	-3.35567300
C	1.93849200	-2.04599400	-1.66325700
H	1.60161300	-3.02928800	-1.95137400
C	2.24442100	0.95527000	0.61272900
H	2.13461400	0.44642300	1.57482300
C	3.44934600	1.89380300	0.65649600
H	3.58487300	2.42500600	-0.28823000
H	4.35800900	1.31751600	0.85202900
H	3.33747200	2.63651700	1.44972800
C	4.53054400	-3.49964100	-0.09128000
H	4.14893900	-4.46185900	-0.40273600
C	4.17981300	-2.80605200	1.10577500
H	3.46581300	-3.12246300	1.85128300
C	4.86534600	-1.55584100	1.10780700
H	4.76691500	-0.78824100	1.86167600
C	5.64151900	-1.47357100	-0.08812200
H	6.24584100	-0.63236500	-0.39887600
C	5.43331000	-2.67531800	-0.83063700
H	5.85335400	-2.90298800	-1.80064700
C	0.86986300	2.70069100	-1.23816800
C	0.38293000	2.07408500	-2.39534300
H	-0.18783400	1.15573200	-2.29708500
C	0.62516700	2.62226200	-3.65402400
H	0.24343200	2.12668800	-4.54157200
C	1.35117500	3.80917900	-3.76872700
H	1.53501100	4.24211700	-4.74750700
C	1.83725000	4.44198400	-2.62267400
H	2.40093000	5.36616700	-2.70870400
C	1.60246300	3.89029900	-1.36286200
H	1.98271500	4.38875500	-0.47812500
C	0.54449100	3.11179600	1.65204300
C	0.93774400	2.77059900	2.95629000
H	1.34562000	1.78682000	3.16625900
C	0.79679700	3.68648000	3.99751700
H	1.10975300	3.41068300	4.99998200

C	0.25031000	4.94815900	3.75456100
H	0.13978600	5.65967400	4.56722300
C	-0.16061800	5.28751300	2.46517000
H	-0.59519900	6.26339300	2.26993800
C	-0.01889700	4.37537400	1.41896100
H	-0.34882200	4.64748500	0.42271900
C	-0.14920700	-3.51281400	0.72849400
C	0.95709500	-4.57807800	0.65894000
H	1.60956100	-4.44636100	-0.20715400
H	0.49277800	-5.56791800	0.58504400
H	1.57720900	-4.56767800	1.55967000
C	-1.02915500	-3.53364900	-0.53188700
H	-1.79538800	-2.75714100	-0.49971200
H	-1.54223900	-4.49998600	-0.58859500
H	-0.45252600	-3.41068400	-1.45150700
C	-1.02261900	-3.73916400	1.97902600
H	-0.41875600	-3.72739800	2.89013500
H	-1.50886200	-4.71806500	1.89813200
H	-1.80205800	-2.97538500	2.06184100
H	-0.56215300	-1.01885700	0.79409200
C	-4.63824400	-1.55458800	-0.63672100
C	-4.43498000	-1.95519600	0.71119300
C	-5.29822200	-2.89107600	1.29354000
C	-6.34812400	-3.38903000	0.52360100
C	-6.54276100	-2.97228400	-0.80762100
C	-5.68914800	-2.04840500	-1.41137700
C	-2.84814300	-0.52625900	0.26039100
H	-5.14859700	-3.20872600	2.32122900
H	-7.03378700	-4.11170900	0.95688200
H	-7.37504300	-3.37761700	-1.37591400
H	-5.84255500	-1.72925500	-2.43806500
N	-3.60617900	-0.67088100	-0.89796900
N	-3.32488100	-1.30102900	1.23294800
C	-3.44679800	0.18857600	-2.05575000
H	-2.37229100	0.30621600	-2.21934000
H	-3.86230300	-0.31356800	-2.93409300
C	-4.09564400	1.56129200	-1.83858700
H	-3.70292300	2.24951800	-2.59993300
H	-5.17700800	1.48800900	-2.00592500
C	-4.41696800	3.57279600	-0.36766500
H	-4.33502400	3.98164000	0.64491000
H	-3.87240300	4.24286300	-1.04473900
H	-5.47533400	3.59617600	-0.65467000
C	-3.85263200	2.14352200	-0.43428500

C	-2.38283200	2.15167400	-0.01723300
H	-2.28055000	2.62242300	0.96896200
H	-1.80050700	2.73320000	-0.74431600
H	-4.41645300	1.53633500	0.28282300

TS8''

Ni	-1.30368200	0.86771500	0.16679800
Fe	3.32499000	-2.15584700	-0.24136700
P	0.08316900	-1.90331400	0.67711400
P	0.72452400	1.76010700	0.37684200
O	0.53120100	-1.96211400	2.11694600
C	1.40516500	-1.48308100	-0.47270600
C	2.29628600	-0.37232700	-0.21621700
C	3.26207800	-0.34798800	-1.26575500
H	4.08361000	0.34787800	-1.34475300
C	2.99174600	-1.42398200	-2.15897800
H	3.57953500	-1.69286100	-3.02568800
C	1.84982800	-2.12471000	-1.67999000
H	1.42305800	-3.00653400	-2.13131500
C	2.14611000	0.62407300	0.89659500
H	1.76322300	0.09171300	1.77235200
C	3.44174800	1.35235500	1.24955300
H	3.83412000	1.91672800	0.40009400
H	4.20390600	0.62915600	1.55498200
H	3.28544800	2.05311500	2.07249000
C	3.78072000	-4.13181100	0.19023800
H	3.29841800	-4.98193500	-0.27147600
C	3.34113500	-3.45660800	1.36845200
H	2.45114700	-3.66685400	1.94266000
C	4.22584100	-2.36338200	1.60494200
H	4.12888800	-1.63786700	2.40002600
C	5.21411300	-2.36088400	0.57350700
H	6.00622300	-1.63504300	0.45130100
C	4.93803000	-3.45411200	-0.30246100
H	5.48445900	-3.70079000	-1.20236600
C	1.48201900	2.64381100	-1.04222700
C	1.26783500	2.11125200	-2.32261400
H	0.62973900	1.24139700	-2.43675800
C	1.87086800	2.68348300	-3.44194100
H	1.69625700	2.25774100	-4.42557400
C	2.69022800	3.80419200	-3.29653200
H	3.15347200	4.25760400	-4.16781100
C	2.91150000	4.34191600	-2.02706700
H	3.55058700	5.21193700	-1.90810000

C	2.31741500	3.76248400	-0.90550000
H	2.50002300	4.18370700	0.07675900
C	0.59938200	2.99946600	1.71983500
C	0.75426000	2.60064400	3.05703300
H	1.05621800	1.58552300	3.29384900
C	0.50664800	3.49655500	4.09624300
H	0.63556900	3.17244600	5.12461200
C	0.08879900	4.79937500	3.81847800
H	-0.10555100	5.49475600	4.62937100
C	-0.08629100	5.19966800	2.49313500
H	-0.41838400	6.20881800	2.26715600
C	0.16171100	4.30648300	1.45057800
H	0.01646500	4.62961400	0.42526900
C	-0.88593500	-3.36481300	0.08640300
C	0.00584500	-4.61369500	0.01066900
H	0.79334700	-4.52195300	-0.74021000
H	-0.61031300	-5.48168100	-0.25096000
H	0.47857500	-4.81960300	0.97524000
C	-1.53344900	-3.04091500	-1.26936300
H	-2.16975100	-2.15497400	-1.19881200
H	-2.16997500	-3.87820900	-1.57641400
H	-0.79641300	-2.87298900	-2.05880500
C	-1.98252900	-3.57117600	1.14887400
H	-1.54826200	-3.82012600	2.12023900
H	-2.63950700	-4.39115800	0.83813300
H	-2.59861400	-2.67734400	1.27176600
H	-0.88055400	-0.85552200	0.42601000
C	-4.70581900	-1.01666700	-0.53983900
C	-4.60250800	-1.00424200	0.87828900
C	-5.43819500	-1.83797300	1.63437200
C	-6.34828700	-2.65027900	0.95873000
C	-6.43854500	-2.64506500	-0.44555900
C	-5.61363800	-1.82596000	-1.22081400
C	-3.07261100	0.35841100	0.15013900
H	-5.36433600	-1.84800600	2.71747500
H	-7.00272700	-3.30474900	1.52744800
H	-7.15977500	-3.29183200	-0.93642300
H	-5.67646300	-1.82834600	-2.30484500
N	-3.73679000	-0.13389700	-0.97990800
N	-3.61086000	-0.12889300	1.27568400
C	-3.53677900	0.27537400	-2.36079200
H	-3.17212200	-0.57675500	-2.94944500
H	-4.51366900	0.55983500	-2.77247700
C	-2.57294900	1.45122900	-2.47348800

H	-1.55670000	1.12050900	-2.21750700
H	-2.55926000	1.77290700	-3.52136700
C	-2.06752600	3.84998300	-1.88095600
H	-2.34003700	4.70518200	-1.25366300
H	-1.01076100	3.62444700	-1.71013000
H	-2.17778100	4.15241700	-2.92868700
C	-2.93802200	2.63175200	-1.55587100
C	-2.82414700	2.25249200	-0.06510300
H	-3.77126600	2.35938700	0.46077900
H	-2.11546100	2.88356800	0.48545700
H	-3.98523200	2.89334200	-1.76376100

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Fe	-3.77211200	-0.19029200	-0.59641500
P	-0.97647700	1.49459200	0.71324400
P	0.70543900	-1.22278800	0.27258600
O	-1.49463900	1.01142200	2.08415700
C	-1.87973800	0.63277400	-0.63408100
C	-1.81993200	-0.80960200	-0.67591600
C	-2.50771300	-1.25713800	-1.84470800
H	-2.66717300	-2.28621400	-2.13250700
C	-3.01318700	-0.11054300	-2.52414300
H	-3.62031100	-0.11824500	-3.41907800
C	-2.62709600	1.04792800	-1.78628100
H	-2.89989000	2.05992000	-2.04168000
C	-1.12511700	-1.63640500	0.36374700
H	-1.40677200	-1.23705900	1.34261100
C	-1.43508100	-3.12786400	0.29595000
H	-1.15484900	-3.55998300	-0.66761800
H	-2.50979000	-3.28260500	0.43200600
H	-0.91005200	-3.67346000	1.08484900
C	-4.56591000	0.29560700	1.24796000
H	-3.95133400	0.79971400	1.98057500
C	-4.60614600	-1.11654300	1.04695000
H	-4.08441300	-1.85177200	1.64353000
C	-5.39578700	-1.38190200	-0.11429300
H	-5.58523400	-2.35456900	-0.54735800
C	-5.84504200	-0.13014400	-0.63403400
H	-6.43704800	0.01167500	-1.52786300
C	-5.33204200	0.90460500	0.20762900
H	-5.46616300	1.96643100	0.05833500
C	1.27388000	-2.02275800	-1.26288400
C	1.51632300	-1.18529800	-2.36243500

H	1.42494900	-0.11076500	-2.23829600
C	1.87964600	-1.72427700	-3.59529200
H	2.06380600	-1.06549700	-4.43838800
C	2.01474300	-3.10602200	-3.74012700
H	2.30438300	-3.52686200	-4.69838300
C	1.77797800	-3.94759400	-2.65141200
H	1.88063400	-5.02301900	-2.76139000
C	1.40376900	-3.41190500	-1.41899200
H	1.21364800	-4.07632600	-0.58389800
C	1.41158300	-2.07943600	1.72001300
C	0.87414700	-1.71172600	2.96769900
H	0.06106500	-0.99030000	3.01517100
C	1.40500800	-2.24418000	4.14013900
H	0.98148100	-1.95871000	5.09847300
C	2.48348200	-3.13181100	4.08516700
H	2.89737100	-3.54284500	5.00108000
C	3.03388500	-3.47928000	2.85177900
H	3.87992200	-4.15856500	2.80395300
C	2.50299100	-2.95513500	1.67093900
H	2.94535500	-3.22522700	0.71903800
C	-1.34095800	3.33073500	0.50272400
C	-2.84910800	3.59565300	0.60919800
H	-3.40412400	3.15360600	-0.21969500
H	-3.04452600	4.67585100	0.60819900
H	-3.24485200	3.18085900	1.54045000
C	-0.77100700	3.84068600	-0.82616800
H	0.29398600	3.60146400	-0.91543400
H	-0.87407200	4.93132700	-0.89042900
H	-1.27701800	3.40875000	-1.69240900
C	-0.63379100	4.03766400	1.67105600
H	-0.99336700	3.65943900	2.63174200
H	-0.82499900	5.11687000	1.62793900
H	0.45143300	3.89081200	1.63790900
H	4.82596000	4.23517900	-1.43721900
H	6.69477200	1.16053400	-1.73256200
C	5.67274700	1.50325000	-1.52479900
H	5.17454500	-0.58967000	-1.86326200
H	3.20729000	0.35337300	1.63669500
C	4.86521500	0.25950900	-1.25309800
H	5.34300300	1.97260600	-2.46627400
C	3.89852600	-0.01741200	-0.35656700
C	3.13843700	0.76970100	0.62732000
H	3.62421600	-1.07031400	-0.32214000
H	5.66584400	2.07127100	0.56138500

C	5.72650500	2.56577000	-0.41488500
H	6.70188100	3.06504900	-0.44499700
C	2.84900100	2.22312600	0.59834300
Ni	1.16827600	0.88105900	0.44431100
H	3.10806000	2.72916300	1.53542800
C	4.63725500	3.63279300	-0.53926200
C	3.22054400	3.06319000	-0.62488900
H	3.10389000	2.45502100	-1.52788100
H	4.69643100	4.32111800	0.31438900
H	2.51259100	3.89420200	-0.71663000
H	1.65727900	2.40120500	0.68293200

TS12

Fe	-3.75845900	-0.16389500	-0.39119500
P	-0.91935400	1.54241500	0.75567100
P	0.71064500	-1.25221600	0.30410900
O	-1.42520100	1.17133200	2.15675700
C	-1.84142400	0.59245000	-0.51891000
C	-1.83363800	-0.85057000	-0.45141200
C	-2.55041300	-1.35727500	-1.57762900
H	-2.74239600	-2.39880600	-1.79008300
C	-3.02823900	-0.24827900	-2.33297100
H	-3.64851900	-0.30084000	-3.21730100
C	-2.59314900	0.94699200	-1.68867500
H	-2.83363700	1.94594200	-2.01636200
C	-1.10522600	-1.63465200	0.59991600
H	-1.31339500	-1.17063200	1.56924900
C	-1.45283400	-3.11964700	0.62536500
H	-1.22674800	-3.60531600	-0.32735400
H	-2.52313600	-3.24354200	0.81821700
H	-0.90136400	-3.64035000	1.41198400
C	-4.52756200	0.50030500	1.40828000
H	-3.90074100	1.06053600	2.08717800
C	-4.58611500	-0.92319000	1.33940000
H	-4.07015500	-1.60571800	2.00001700
C	-5.39167700	-1.28460000	0.21609000
H	-5.59875300	-2.29079400	-0.12195800
C	-5.83243400	-0.08077900	-0.41240800
H	-6.43453600	-0.01548900	-1.30832900
C	-5.29851300	1.02075500	0.32450500
H	-5.42374600	2.06592300	0.08027100
C	0.99997800	-1.95779200	-1.35481600
C	0.95046700	-1.06679900	-2.43805700
H	0.81834800	-0.00668800	-2.24437200

C	1.06453300	-1.53742800	-3.74490000
H	1.02149800	-0.83918900	-4.57527200
C	1.23884200	-2.90234400	-3.98240500
H	1.33358700	-3.26949600	-5.00003900
C	1.29237100	-3.79546000	-2.91052200
H	1.42707700	-4.85757300	-3.09259800
C	1.16810500	-3.32812700	-1.60170700
H	1.20724000	-4.02881800	-0.77484100
C	1.62127100	-2.27740700	1.51147900
C	1.16991500	-2.29376100	2.84191500
H	0.25538300	-1.77560500	3.11317400
C	1.89670500	-2.96210700	3.82571500
H	1.53247000	-2.97087400	4.84860900
C	3.08903300	-3.61198900	3.49938100
H	3.65471700	-4.13107600	4.26717700
C	3.55297200	-3.58567600	2.18385900
H	4.48248100	-4.08299700	1.92281600
C	2.82652400	-2.92110000	1.19474500
H	3.20128100	-2.90549200	0.17766800
C	-1.26357300	3.35965100	0.40625400
C	-2.77211900	3.64024900	0.48205000
H	-3.33195900	3.12130000	-0.29669300
H	-2.95805100	4.71608100	0.37223200
H	-3.17191000	3.32735200	1.45052800
C	-0.68166200	3.77272600	-0.95148800
H	0.38383400	3.52799900	-1.01403600
H	-0.78363900	4.85626900	-1.09096700
H	-1.18310600	3.28345800	-1.78983200
C	-0.56924600	4.15160000	1.52649600
H	-0.93794600	3.84335500	2.50855400
H	-0.76354100	5.22347400	1.40033300
H	0.51628900	4.00494800	1.51371400
H	4.87740600	4.42405600	-0.84756800
H	6.57549400	1.36861100	-1.94548700
C	5.59265500	1.74782700	-1.63354500
H	4.82676300	-0.09224400	-2.50450900
H	3.35337000	0.02888500	1.38419500
C	4.67285100	0.55270500	-1.63816500
H	5.29772600	2.43877100	-2.43954800
C	3.76700300	0.10227900	-0.75161400
H	1.28919400	2.32793300	0.71331600
C	3.25813600	0.67614600	0.51288300
H	3.35481100	-0.87427000	-0.98987400
H	5.75424800	1.82674300	0.51983800

C	5.76394200	2.52791300	-0.32158100
H	6.75581500	2.99482100	-0.31892400
C	2.96528100	2.03325400	0.75673100
Ni	1.18853300	0.89788100	0.48505900
H	2.97813300	2.34337700	1.80123500
C	4.71800600	3.62702300	-0.10987400
C	3.26777100	3.14045300	-0.23192000
H	3.07477300	2.78440700	-1.24857200
H	4.86506200	4.08372600	0.87758800
H	2.59231300	3.98474900	-0.05947100

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Fe	-3.74703900	-0.21171900	-0.40230700
P	-0.94851700	1.56012800	0.74080500
P	0.73561700	-1.21739700	0.30890700
O	-1.40090600	1.15496900	2.14724600
C	-1.84377900	0.58180500	-0.52833600
C	-1.81027900	-0.86087900	-0.45811800
C	-2.51400700	-1.38022400	-1.58636500
H	-2.68677800	-2.42517900	-1.79821800
C	-3.01140500	-0.28095900	-2.34314400
H	-3.62881100	-0.34554500	-3.22862200
C	-2.60077200	0.92246300	-1.69923700
H	-2.85987200	1.91639200	-2.02753800
C	-1.07505400	-1.63157200	0.59713800
H	-1.29334300	-1.16936700	1.56482000
C	-1.40223800	-3.12092400	0.62423300
H	-1.16784600	-3.60503800	-0.32708400
H	-2.47099300	-3.26021200	0.81549100
H	-0.84445000	-3.63191100	1.41274700
C	-4.54286900	0.42921000	1.39366600
H	-3.94146900	1.00830700	2.07926500
C	-4.55909700	-0.99516500	1.32500700
H	-4.02538700	-1.66214800	1.98721900
C	-5.34859100	-1.37950400	0.19793700
H	-5.52266300	-2.39111600	-0.14238900
C	-5.82259100	-0.18909400	-0.43188100
H	-6.42221700	-0.14141200	-1.33054600
C	-5.32512800	0.92746200	0.30741400
H	-5.48292600	1.96835300	0.06444700
C	1.03491700	-1.92221700	-1.35026500
C	1.00206100	-1.02426200	-2.42841900
H	0.87844100	0.03571600	-2.22731400
C	1.12331100	-1.48670000	-3.73756900

H	1.09294600	-0.78255200	-4.56355500
C	1.28900800	-2.85131700	-3.98293500
H	1.38944900	-3.21252200	-5.00216900
C	1.32679800	-3.75171600	-2.91648000
H	1.45510700	-4.81363100	-3.10445700
C	1.19471000	-3.29213200	-1.60559000
H	1.22110600	-3.99923300	-0.78377400
C	1.64326500	-2.24148700	1.52119700
C	1.20267200	-2.22162900	2.85564800
H	0.30295300	-1.67567600	3.12286000
C	1.92108700	-2.88787400	3.84671300
H	1.56499200	-2.86831100	4.87235100
C	3.09578000	-3.57142800	3.52419400
H	3.65552500	-4.08845300	4.29772600
C	3.54972600	-3.58072200	2.20521600
H	4.46579100	-4.10383600	1.94694500
C	2.83064800	-2.91877700	1.20853400
H	3.19802700	-2.93180900	0.18882500
C	-1.38218000	3.36318400	0.41860400
C	-2.90227600	3.56894500	0.49828200
H	-3.43656400	3.04014500	-0.29121700
H	-3.13695100	4.63685800	0.40851300
H	-3.28864900	3.22077000	1.45984300
C	-0.82473500	3.83060500	-0.93235500
H	0.25478300	3.65733800	-0.99430300
H	-0.99737900	4.90691200	-1.05535900
H	-1.29072400	3.32211500	-1.77966200
C	-0.72579200	4.17170200	1.55070200
H	-1.08019300	3.83407400	2.52814800
H	-0.97173700	5.23415600	1.43671700
H	0.36561500	4.07749700	1.53651700
H	4.84854700	4.40752900	-0.91041700
H	6.60656600	1.34307800	-1.92241400
C	5.61885700	1.72264200	-1.62617600
H	4.86532100	-0.13647800	-2.46417300
H	3.33554300	0.01113500	1.41023200
C	4.70910900	0.51956900	-1.60657800
H	5.32143300	2.38511800	-2.45473100
C	3.80880300	0.07483900	-0.71214100
H	0.95821600	2.38025500	0.62214000
C	3.30572600	0.66920900	0.54320200
H	3.39836800	-0.90600400	-0.93230700
H	5.78957900	1.86807800	0.52265100
C	5.77943300	2.54458200	-0.33861000

H	6.76203000	3.03044800	-0.35678700
C	3.01465900	2.00722200	0.76540300
Ni	1.16942600	0.96466900	0.47761800
H	2.91871100	2.32719500	1.80152500
C	4.71332800	3.62868500	-0.14861500
C	3.27116400	3.10509100	-0.23836000
H	3.07461100	2.73132300	-1.24828100
H	4.86280800	4.11575600	0.82381800
H	2.57671700	3.93331900	-0.06593800

TS13

Ni	1.27899100	0.96316000	0.10649800
Fe	-3.73610400	-0.25897700	-0.24035300
P	-0.88660500	1.66765400	0.41691700
P	0.82834500	-1.18452600	0.19805500
O	-1.00391400	1.32634200	1.89956700
C	-1.87037100	0.55177700	-0.63029300
C	-1.79306200	-0.88130000	-0.45786500
C	-2.60268700	-1.48597000	-1.46518700
H	-2.77647500	-2.54579500	-1.57763200
C	-3.20880800	-0.45571500	-2.23952500
H	-3.91613600	-0.59484600	-3.04120600
C	-2.76324600	0.79991000	-1.72772700
H	-3.08060100	1.76175200	-2.09170500
C	-0.97843000	-1.56702800	0.59199900
H	-1.13647000	-1.03490800	1.53469100
C	-1.30053900	-3.04970700	0.76104100
H	-1.12889800	-3.61097400	-0.15957800
H	-2.34872700	-3.17461500	1.04202100
H	-0.68308800	-3.49375300	1.54848600
C	-4.41366800	0.47950300	1.56760900
H	-3.82033800	1.15192300	2.17066000
C	-4.34676000	-0.94351000	1.60846900
H	-3.71690100	-1.52505300	2.26535800
C	-5.20580400	-1.45817100	0.58979000
H	-5.34276000	-2.50322900	0.34155300
C	-5.80536400	-0.35310000	-0.08159700
H	-6.47806800	-0.40839300	-0.92776400
C	-5.31903300	0.84692900	0.52297700
H	-5.56733200	1.85489400	0.21967000
C	1.07698600	-2.19310700	-1.31061200
C	0.91052800	-1.52077300	-2.53169800
H	0.73238800	-0.44959300	-2.51848700
C	0.96370100	-2.21213400	-3.74016600

H	0.82993100	-1.67674100	-4.67554400
C	1.19687600	-3.58939100	-3.74794500
H	1.24966600	-4.12772200	-4.68811600
C	1.35626900	-4.27047200	-2.53923400
H	1.52475800	-5.34391400	-2.53937700
C	1.28405300	-3.58202800	-1.32885400
H	1.38133600	-4.12838600	-0.39797400
C	1.70523700	-1.99763200	1.58745300
C	1.31233500	-1.61137800	2.88483700
H	0.48724500	-0.91763100	3.01279300
C	1.99516200	-2.08595500	4.00168000
H	1.67782800	-1.78333900	4.99322900
C	3.09632900	-2.93457100	3.84721600
H	3.63177700	-3.29761800	4.71928400
C	3.51031700	-3.29656400	2.56438000
H	4.37403000	-3.94105800	2.43434200
C	2.82322100	-2.82900100	1.44214200
H	3.16777900	-3.11204100	0.45550100
C	-1.48257400	3.42499200	0.11893400
C	-2.96670200	3.56950200	0.48209100
H	-3.60693700	2.98014700	-0.17608700
H	-3.26450000	4.62071500	0.39489900
H	-3.14935300	3.25205300	1.51115500
C	-1.23037700	3.87387300	-1.32787400
H	-0.18088900	3.75186900	-1.61004400
H	-1.47656100	4.93630400	-1.43258500
H	-1.82901000	3.32166700	-2.05518400
C	-0.64156800	4.29795700	1.06877700
H	-0.79438000	4.00422100	2.10866600
H	-0.93021100	5.35037900	0.95452700
H	0.42831600	4.21843500	0.84676500
H	0.54183600	2.22639400	-0.20159600
H	4.61654300	4.30319400	-1.48786200
H	6.61425100	1.24994200	-1.70402100
C	5.58425100	1.59169400	-1.52913300
H	5.03289200	-0.47433300	-1.92940200
H	3.27335600	0.44022600	1.73416800
C	4.77519900	0.34538700	-1.26016400
H	5.27627700	2.02727500	-2.49314700
C	3.86586400	0.05113400	-0.31118500
C	3.22746400	0.87366700	0.73219100
H	3.54096100	-0.99046400	-0.29554700
H	5.60618100	2.22982600	0.53717600
C	5.61503400	2.69455700	-0.45567400

H	6.56824500	3.23059500	-0.53469500
C	2.81178100	2.21978800	0.62441300
H	2.67893500	2.76498700	1.56099300
C	4.48015100	3.71574100	-0.57165700
C	3.07988800	3.07695900	-0.58979200
H	2.97120500	2.47253700	-1.49881000
H	4.54234700	4.42240900	0.26853200
H	2.33079000	3.87373300	-0.65287700

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Ni	-1.48761700	0.78167000	-0.55659100
Fe	3.70212700	-0.28033500	0.52052400
P	1.24571200	1.65144900	-0.82199700
P	-0.84429700	-1.27070900	-0.29356600
O	1.52957300	1.09579600	-2.19607800
C	1.85898700	0.62430900	0.52115800
C	1.71674200	-0.81777800	0.52529800
C	2.33839700	-1.30144100	1.71433800
H	2.42680400	-2.33995700	1.99605400
C	2.88095500	-0.19758300	2.43095400
H	3.45564700	-0.25422100	3.34482100
C	2.59174700	0.98911700	1.70393200
H	2.90812700	1.98195600	1.98035500
C	0.99869500	-1.63764300	-0.50597000
H	1.22462300	-1.20764300	-1.48624600
C	1.38193100	-3.11568500	-0.48503700
H	1.15310200	-3.58117700	0.47623200
H	2.45592200	-3.22751100	-0.66326800
H	0.84658000	-3.66621500	-1.26210200
C	4.68109300	0.28058700	-1.21171200
H	4.21903000	0.92324800	-1.94605700
C	4.54244400	-1.13787500	-1.16040400
H	3.98871300	-1.74112700	-1.86548400
C	5.20846800	-1.60614100	0.01315900
H	5.25086600	-2.63096400	0.35510900
C	5.76044300	-0.47503900	0.68707200
H	6.29467700	-0.49440000	1.62696200
C	5.43530800	0.69116700	-0.07087800
H	5.68719600	1.70870400	0.19204900
C	-1.22331100	-2.01020000	1.34135600
C	-1.43001400	-1.11987700	2.40566400
H	-1.42113400	-0.05242900	2.20540200
C	-1.65798700	-1.59613400	3.69678200
H	-1.81624400	-0.89492300	4.51082500

C	-1.69404500	-2.97050300	3.93692200
H	-1.87759700	-3.34362700	4.94029100
C	-1.50322900	-3.86650000	2.88232100
H	-1.53893000	-4.93677200	3.06416700
C	-1.26705400	-3.39086700	1.59255600
H	-1.13138200	-4.09466800	0.77874400
C	-1.64554300	-2.36427800	-1.52824000
C	-1.14309600	-2.39253900	-2.84002500
H	-0.24153400	-1.84120300	-3.08939200
C	-1.80109900	-3.11211100	-3.83595900
H	-1.39503600	-3.12863500	-4.84318900
C	-2.97985800	-3.80211400	-3.54354500
H	-3.49332100	-4.35970400	-4.32110300
C	-3.49684000	-3.76405200	-2.24823600
H	-4.41668300	-4.29147600	-2.01231700
C	-2.83629900	-3.05030200	-1.24721200
H	-3.24905600	-3.03048000	-0.24441600
C	1.72243200	3.43253400	-0.59350000
C	3.24526200	3.60821600	-0.66880700
H	3.75918700	3.09229700	0.14470900
H	3.49342700	4.67409100	-0.60489000
H	3.64003700	3.23011500	-1.61589700
C	1.15476000	3.97489300	0.72734400
H	0.08234600	3.77541500	0.81653400
H	1.29232500	5.06167400	0.76016700
H	1.64819800	3.55369200	1.60483200
C	1.05055600	4.16180700	-1.77349600
H	1.41387300	3.78564400	-2.73281400
H	1.27083600	5.23328600	-1.71179500
H	-0.03788100	4.03913000	-1.75127000
H	-0.16891400	1.87554700	-0.53147000
H	-4.15968000	4.78175100	1.12384700
H	-6.50255100	2.09352300	1.92795100
C	-5.46128100	2.25635600	1.61643600
H	-5.16170000	0.18988400	2.23409800
H	-3.65355200	0.39531800	-1.64715300
C	-4.86347900	0.88054600	1.44376600
H	-4.99300200	2.75521200	2.48085200
C	-4.10196100	0.34442000	0.47134500
C	-3.45872800	0.93693700	-0.71839300
H	-3.92619800	-0.72753200	0.56108700
H	-5.61172700	2.63432900	-0.50645600
C	-5.45953900	3.21180700	0.41134000
H	-6.32165300	3.88431600	0.49770800

C	-2.85913400	2.21282800	-0.82456400
H	-2.74842000	2.61701800	-1.83327300
C	-4.19469500	4.06782800	0.28901800
C	-2.89599800	3.24469800	0.27955800
H	-2.77681400	2.75034200	1.25089600
H	-4.25160300	4.66543000	-0.63068800
H	-2.04695300	3.93090400	0.17256400

TS14

Ni	1.26296500	1.20612000	0.23371600
Fe	-3.50523000	-0.78347700	-0.24430300
P	-1.00693200	1.54675900	0.59792300
P	1.15085700	-0.98546100	0.23133300
O	-1.04939600	1.10152100	2.05533600
C	-1.78599500	0.34497600	-0.52230000
C	-1.48058700	-1.06410400	-0.41971900
C	-2.15059800	-1.73561200	-1.48551600
H	-2.14277400	-2.80133900	-1.66058800
C	-2.89496000	-0.77331300	-2.22675300
H	-3.54903000	-0.98134600	-3.06226200
C	-2.67739900	0.50468200	-1.63701700
H	-3.14017000	1.42310000	-1.96029700
C	-0.57200200	-1.66267800	0.60798600
H	-0.81162900	-1.20087900	1.56896300
C	-0.66017100	-3.18171300	0.71357800
H	-0.40699000	-3.67165000	-0.22990000
H	-1.67749300	-3.48171800	0.98559300
H	0.01989500	-3.55617500	1.48316800
C	-4.37632400	-0.26404500	1.56040400
H	-3.94477400	0.46772800	2.22645100
C	-4.05731700	-1.65346600	1.54492300
H	-3.36213300	-2.14744600	2.20900600
C	-4.76764400	-2.25988800	0.46438100
H	-4.70582400	-3.29718200	0.16519800
C	-5.52681000	-1.24255800	-0.18891700
H	-6.14210400	-1.37525900	-1.06812100
C	-5.28540500	-0.00897200	0.48888300
H	-5.69567300	0.95311700	0.21786400
C	1.53906800	-1.89574900	-1.31221500
C	1.24123900	-1.22669100	-2.50986000
H	0.89036800	-0.20134100	-2.46464800
C	1.38659500	-1.86757400	-3.74002800
H	1.14826200	-1.33551200	-4.65635700
C	1.84159900	-3.18622200	-3.79098600

H	1.96527500	-3.68413300	-4.74819100
C	2.12969600	-3.86585900	-2.60597700
H	2.47196300	-4.89615000	-2.63827900
C	1.96843900	-3.23046400	-1.37388300
H	2.17003800	-3.77993500	-0.46183300
C	2.15573700	-1.69833800	1.58788800
C	1.71431800	-1.43348100	2.89745700
H	0.78872300	-0.88693200	3.05434000
C	2.47488200	-1.83084100	3.99477000
H	2.11701100	-1.62265300	4.99886800
C	3.69753900	-2.48121500	3.80620700
H	4.29122500	-2.78679000	4.66258600
C	4.15637900	-2.72222500	2.51205000
H	5.11233200	-3.21341200	2.35447800
C	3.39268800	-2.33235000	1.40907000
H	3.77207200	-2.51664200	0.41081900
C	-1.89125200	3.19366700	0.41054900
C	-3.37156500	3.05954100	0.78813500
H	-3.90664500	2.40042400	0.10245200
H	-3.85062800	4.04575100	0.75608600
H	-3.48288700	2.66546000	1.80128600
C	-1.74239200	3.76869700	-1.00457400
H	-0.69311800	3.83358800	-1.30535100
H	-2.15408200	4.78451500	-1.03147900
H	-2.26655600	3.18246900	-1.76072200
C	-1.19157500	4.13347400	1.41035700
H	-1.27479100	3.75347500	2.43129800
H	-1.65353000	5.12660200	1.36665900
H	-0.12754000	4.24740900	1.17691400
H	0.29142000	2.33258400	0.01164700
H	2.73376400	4.56788500	-2.12499300
C	2.28092600	3.78249400	-1.50035100
H	1.46041800	2.29986900	-2.90138000
H	4.88578300	2.55344400	-1.26334600
C	2.30990700	2.46704000	-2.23913200
H	1.23093300	4.06865000	-1.39528300
C	3.25750100	1.52042600	-2.20963100
H	5.29558700	0.97885800	-1.90292800
C	4.50965200	1.53558600	-1.37904000
H	3.10032100	0.62797700	-2.81015700
H	4.00237800	3.95037500	-0.17828200
C	2.91732000	3.83547700	-0.09519700
H	2.56630400	4.76216700	0.37317600
C	4.31521200	0.88129500	0.00359600

H	5.26690400	0.94406900	0.55342900
C	2.59966200	2.68288600	0.84996000
C	3.21219400	1.42958800	0.88514100
H	4.13708000	-0.19027000	-0.14261100
H	2.12604100	2.98827300	1.78185100
H	3.14218800	0.90153400	1.83572100

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Ni	1.23448100	1.20078800	0.26965300
Fe	-3.53422200	-0.65348400	-0.40396400
P	-0.91551400	1.46601800	0.68013900
P	1.06435600	-1.04753800	0.28068700
O	-1.19628400	0.93685300	2.09570400
C	-1.75845500	0.40632300	-0.56406100
C	-1.52585900	-1.01823700	-0.53297700
C	-2.18868500	-1.60765700	-1.65162200
H	-2.22487200	-2.66256600	-1.88175600
C	-2.85902100	-0.57084700	-2.36377800
H	-3.49211800	-0.70127300	-3.23090600
C	-2.59603900	0.66417900	-1.69994900
H	-3.00089300	1.62002800	-1.99325100
C	-0.69013200	-1.69213200	0.51086700
H	-0.97616500	-1.27286800	1.47799800
C	-0.80697300	-3.21196000	0.53841800
H	-0.51194400	-3.66553900	-0.41096100
H	-1.84411100	-3.49869200	0.73948400
H	-0.17976700	-3.63548500	1.32772300
C	-4.36040900	-0.19076200	1.43100500
H	-3.84113300	0.45298300	2.12533100
C	-4.16523900	-1.59877800	1.31570400
H	-3.51453200	-2.19688200	1.93813200
C	-4.92356300	-2.06493000	0.19834100
H	-4.95297600	-3.08056100	-0.17174800
C	-5.59034900	-0.94196900	-0.37831500
H	-6.21654900	-0.95840700	-1.25986500
C	-5.24302800	0.21504200	0.38336000
H	-5.56420600	1.22603000	0.17889000
C	1.58751200	-1.99503000	-1.19518500
C	1.32735100	-1.38094100	-2.43067500
H	0.91928100	-0.37666600	-2.44344800
C	1.57904500	-2.05186100	-3.62655500
H	1.36880300	-1.56290900	-4.57317800
C	2.10216700	-3.34577600	-3.60381800
H	2.30924800	-3.86693800	-4.53377000

C	2.34633000	-3.97321400	-2.38093600
H	2.73536000	-4.98690400	-2.35717700
C	2.07862200	-3.30945700	-1.18282600
H	2.23954000	-3.82428000	-0.24333900
C	1.91967200	-1.68888300	1.76489500
C	1.34437400	-1.33080300	2.99883400
H	0.42450200	-0.75067500	3.01748000
C	1.97847200	-1.66893200	4.19248700
H	1.52210500	-1.39084800	5.13795000
C	3.19998300	-2.34762700	4.17574300
H	3.69251900	-2.60805400	5.10785200
C	3.79280600	-2.67206500	2.95597900
H	4.75204500	-3.18105600	2.93343200
C	3.16035800	-2.34089500	1.75532000
H	3.64805900	-2.57771500	0.81698700
C	-1.66155900	3.18716900	0.50526200
C	-3.17738300	3.12537900	0.73729100
H	-3.68447600	2.53664200	-0.02789100
H	-3.59757300	4.13885000	0.72120900
H	-3.40126400	2.68288700	1.71113600
C	-1.33915700	3.79847200	-0.86230900
H	-0.26439000	3.77701600	-1.05302800
H	-1.66665300	4.84520100	-0.89158300
H	-1.83278100	3.27558200	-1.68398400
C	-1.02890100	4.04422900	1.61413100
H	-1.21930200	3.61011800	2.59921100
H	-1.45487300	5.05455300	1.58963600
H	0.05525700	4.13092000	1.48693800
H	0.92422800	2.60724700	0.39825000
H	3.15249400	4.69183600	-1.76927800
C	2.61010600	3.92854100	-1.19151000
H	1.24568300	2.91720300	-2.58864900
H	4.88428600	2.22654200	-1.72244800
C	2.21449400	2.79730400	-2.10670600
H	1.69285400	4.41605300	-0.84956800
C	2.92199800	1.70384100	-2.41888200
H	4.81003900	0.74116700	-2.64131800
C	4.27950500	1.33224400	-1.88624500
H	2.47930900	0.99806100	-3.11570700
H	4.50735600	3.49228300	-0.22328000
C	3.45299400	3.57686500	0.05408800
H	3.39540300	4.43318500	0.73428000
C	4.22409600	0.49013700	-0.59476200
H	5.25396700	0.32440000	-0.24346100

C	3.06401900	2.33601600	0.84197800
C	3.42204000	1.03456400	0.56717400
H	3.83849900	-0.50356100	-0.84670100
H	2.73683100	2.52403700	1.86159000
H	3.36771500	0.35024700	1.40893000

TS15

Ni	1.26577900	1.12274100	0.30543100
Fe	-3.54244700	-0.62828900	-0.43801700
P	-0.90201500	1.43338700	0.69586600
P	1.04964800	-1.08507900	0.27063900
O	-1.22867900	0.88450600	2.09877600
C	-1.75974700	0.41800500	-0.57638800
C	-1.53667600	-1.00876900	-0.57858200
C	-2.20680500	-1.56935800	-1.70820400
H	-2.25197300	-2.61875200	-1.96126200
C	-2.86959100	-0.51178700	-2.39666900
H	-3.50413100	-0.61796800	-3.26611300
C	-2.59563000	0.70643400	-1.70582100
H	-2.99431600	1.67146300	-1.97691600
C	-0.71385600	-1.71439800	0.45599300
H	-1.00701600	-1.31673200	1.43031000
C	-0.84237300	-3.23372800	0.44500500
H	-0.53868200	-3.66590000	-0.51164700
H	-1.88448500	-3.51594000	0.62565900
H	-0.22929600	-3.68253600	1.23152200
C	-4.34358400	-0.18421600	1.41151600
H	-3.79878700	0.43633500	2.10778700
C	-4.17752000	-1.59369800	1.26844900
H	-3.53282800	-2.21570600	1.87363500
C	-4.95445600	-2.02505700	0.14982900
H	-5.00803300	-3.03336400	-0.23729600
C	-5.60363500	-0.87892800	-0.40077500
H	-6.23822800	-0.86720300	-1.27641100
C	-5.22706300	0.25701900	0.37887700
H	-5.52918600	1.27782500	0.19452100
C	1.61327900	-2.00538300	-1.20372700
C	1.40618400	-1.36358200	-2.43468400
H	1.01366600	-0.35313200	-2.44027700
C	1.69332300	-2.01491600	-3.63335300
H	1.52493300	-1.50573000	-4.57765200
C	2.19808800	-3.31619200	-3.61608100
H	2.43188500	-3.82272300	-4.54777000
C	2.39068800	-3.96999500	-2.39762500

H	2.76680900	-4.98862000	-2.37991700
C	2.08855500	-3.32558800	-1.19733000
H	2.21110400	-3.85806000	-0.26176300
C	1.87638000	-1.73116300	1.76693400
C	1.27885100	-1.38155900	2.99238400
H	0.35933700	-0.80001900	2.99839900
C	1.89355500	-1.72775700	4.19394800
H	1.42141900	-1.45668800	5.13370200
C	3.11568300	-2.40554400	4.19259700
H	3.59269800	-2.67229300	5.13099100
C	3.72940300	-2.72151900	2.98080000
H	4.68897600	-3.23028000	2.97121900
C	3.11700300	-2.38262600	1.77201800
H	3.61858400	-2.61374600	0.83955600
C	-1.59596300	3.17775400	0.54144800
C	-3.11032900	3.16229700	0.78851300
H	-3.64106200	2.59352700	0.02355900
H	-3.50199500	4.18751900	0.78392700
H	-3.33672800	2.71764400	1.76101200
C	-1.26345700	3.78506700	-0.82498700
H	-0.19915600	3.68303900	-1.04379000
H	-1.51035900	4.85422900	-0.83449300
H	-1.81555400	3.31316800	-1.64006400
C	-0.92240100	4.00455300	1.64885500
H	-1.10134100	3.56059300	2.63193700
H	-1.32495900	5.02487600	1.64885800
H	0.16057000	4.07033700	1.49971900
H	1.27184100	2.56779000	0.55943100
H	3.17279100	4.74180900	-1.71440700
C	2.59437900	3.98277300	-1.16759800
H	1.25918100	2.99573000	-2.61252600
H	4.85905100	2.30414700	-1.65475100
C	2.21581700	2.86683300	-2.10935300
H	1.67236100	4.48667700	-0.86237800
C	2.92667700	1.77368000	-2.41138000
H	4.82804500	0.83014600	-2.59334000
C	4.26967000	1.40461700	-1.84540800
H	2.50206100	1.07443300	-3.12614300
H	4.43942500	3.51030400	-0.10656300
C	3.37325700	3.61161700	0.11191000
H	3.29022600	4.46160800	0.79733300
C	4.19202700	0.54592300	-0.56586900
H	5.21559200	0.41888600	-0.18082900
C	2.92535600	2.36118200	0.86723400

C	3.31906900	1.03895900	0.57314800
H	3.85953700	-0.45927700	-0.84664800
H	2.73464200	2.53958900	1.92349900
H	3.36519200	0.38541200	1.44121300

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Fe	-3.60776500	-0.60858700	-0.11263000
P	-0.78891600	1.58848600	0.28044800
P	1.02296700	-1.03238200	0.27136000
O	-0.90254700	1.34155800	1.80464500
C	-1.82774200	0.35228400	-0.61415200
C	-1.62115200	-1.04626600	-0.32028400
C	-2.38215300	-1.82483700	-1.24504000
H	-2.45940300	-2.90254800	-1.25496700
C	-3.09034300	-0.92584100	-2.09493500
H	-3.79623700	-1.20225900	-2.86631900
C	-2.74963700	0.40646600	-1.71182500
H	-3.15751300	1.29928500	-2.16106500
C	-0.71913400	-1.52130200	0.77495100
H	-0.90600700	-0.88990500	1.64673500
C	-0.87326100	-2.99457200	1.13840200
H	-0.69615500	-3.65202500	0.28409100
H	-1.89170300	-3.17695500	1.49486600
H	-0.18080600	-3.27560400	1.93683800
C	-4.27880100	0.19807600	1.66868300
H	-3.70220300	0.93781000	2.20316500
C	-4.11552800	-1.21267000	1.79434200
H	-3.42693700	-1.70727400	2.46427500
C	-4.96752900	-1.84743300	0.83996200
H	-5.04190000	-2.91148200	0.66163600
C	-5.66124400	-0.82563500	0.12344500
H	-6.35768000	-0.98042400	-0.68930400
C	-5.23539400	0.43780200	0.63527700
H	-5.55604800	1.40566500	0.27787100
C	1.40726400	-2.27654700	-1.00862200
C	1.20271800	-1.87936400	-2.33946500
H	0.91010700	-0.85454700	-2.54632800
C	1.36743800	-2.78761100	-3.38442000
H	1.20316000	-2.46652200	-4.40862300
C	1.74681300	-4.10306100	-3.11226400
H	1.88368700	-4.80985200	-3.92520800
C	1.94358000	-4.50996300	-1.79156200
H	2.22889600	-5.53496800	-1.57415100
C	1.76516600	-3.60653800	-0.74314500

H	1.89587400	-3.94374400	0.27818700
C	1.99200700	-1.32096000	1.79026300
C	1.57748900	-0.57881300	2.91181600
H	0.71410600	0.08107300	2.83064100
C	2.30041800	-0.65550000	4.10086700
H	1.97464100	-0.08079600	4.96295300
C	3.44352000	-1.45516300	4.18243100
H	4.00526300	-1.50998900	5.11027100
C	3.86883600	-2.17283400	3.06450100
H	4.76525000	-2.78381400	3.11654500
C	3.14936600	-2.10508900	1.86982400
H	3.50355200	-2.64961600	1.00258900
C	-1.61567400	3.27059600	-0.07443900
C	-3.12126100	3.18678100	0.21899400
H	-3.64423800	2.51981100	-0.46461300
H	-3.56819200	4.18569600	0.12859300
H	-3.29525300	2.83359100	1.23727500
C	-1.39181700	3.72864300	-1.52315600
H	-0.34948000	3.98672500	-1.72423800
H	-1.98864900	4.62668300	-1.72809300
H	-1.68931700	2.96612400	-2.24890000
C	-1.02906600	4.28582700	0.92380600
H	-1.18791300	3.93999700	1.94787000
H	-1.52796700	5.25511500	0.79971400
H	0.04355500	4.45535100	0.79959200
H	3.74199800	0.84731400	1.40627200
H	3.43301000	4.44826500	0.20094900
C	3.16777500	3.38570500	0.31526300
H	1.13120700	3.59588200	-0.39066800
H	4.10201900	2.69814300	-2.51712100
C	2.05090700	3.09579800	-0.65378100
H	2.73988300	3.30272300	1.32373400
C	2.06868100	2.49665100	-1.88594800
H	3.05575700	1.93037500	-3.69186300
C	3.28457700	1.97935300	-2.62243300
H	1.13858500	2.53598600	-2.45082900
H	4.97380000	2.71460100	-0.68458700
C	4.43211500	2.52756600	0.24728000
H	5.10116800	2.85871900	1.05094600
C	3.70183800	0.58834600	-2.10191600
Ni	1.40364300	1.02032300	-0.40852500
H	4.78617800	0.44167500	-2.24172600
C	4.17293600	1.02679100	0.41259600
C	3.29303100	0.35310000	-0.64753200

H	3.21256100	-0.17277800	-2.71733600
H	5.15343600	0.52146300	0.42130800
H	3.39498600	-0.72150200	-0.47485500

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Fe	3.81768900	0.27751800	0.13810700
P	0.83723600	-1.58472500	-0.01938000
P	-0.78375800	1.21012500	0.09277000
O	0.94899000	-1.63601500	1.52016300
C	2.04765000	-0.37748600	-0.70108500
C	1.94099500	0.99989800	-0.28098300
C	2.91600000	1.76659100	-0.98855900
H	3.10889500	2.82199300	-0.86087200
C	3.64149900	0.88004200	-1.83761800
H	4.47778900	1.14713700	-2.46926400
C	3.11022200	-0.43303300	-1.66467400
H	3.48864200	-1.31938200	-2.14928500
C	0.96112500	1.46965100	0.75167800
H	0.98887700	0.74932000	1.57489800
C	1.23159100	2.87130100	1.28900100
H	1.20525300	3.62652300	0.49979200
H	2.22492400	2.89969600	1.74748900
H	0.49884400	3.14519300	2.05336500
C	4.08306100	-0.84518000	1.85154600
H	3.31298100	-1.53479700	2.16670800
C	4.11068400	0.54714000	2.16161000
H	3.40872000	1.06243600	2.80228500
C	5.18171200	1.14842700	1.43123100
H	5.43990000	2.19864800	1.42768300
C	5.81853200	0.12488300	0.66592500
H	6.64299400	0.26391000	-0.01990400
C	5.13926800	-1.10522200	0.92598500
H	5.35996600	-2.05921500	0.46878700
C	-1.10117900	2.63689500	-0.99951900
C	-1.10003000	2.39533100	-2.38186800
H	-0.97169100	1.37837000	-2.73863200
C	-1.25895100	3.44491800	-3.28625600
H	-1.25226500	3.24328100	-4.35316200
C	-1.43062900	4.74863100	-2.81896400
H	-1.56200700	5.56610600	-3.52158400
C	-1.42914300	5.00114400	-1.44573200
H	-1.55626900	6.01487200	-1.07774400
C	-1.25695800	3.95504500	-0.53971100
H	-1.24110700	4.16827600	0.52238400

C	-1.79104100	1.34322800	1.61100900
C	-1.53390400	0.35951400	2.58488700
H	-0.74473900	-0.37511800	2.42064000
C	-2.31052000	0.30807000	3.74103600
H	-2.10700000	-0.45374700	4.48783500
C	-3.35074600	1.22076400	3.93463000
H	-3.95615200	1.17421500	4.83511000
C	-3.61615100	2.18602700	2.96312700
H	-4.43079100	2.89078700	3.10233000
C	-2.84271600	2.24668800	1.80244500
H	-3.07875000	2.98244100	1.04280300
C	1.31963000	-3.26021400	-0.73396400
C	2.73872100	-3.63902500	-0.28773300
H	3.49246500	-2.97066000	-0.70739700
H	2.97659800	-4.66167600	-0.60788800
H	2.81953500	-3.59688700	0.80184600
C	1.19389100	-3.26585000	-2.26277200
H	0.18736000	-2.97344800	-2.58118300
H	1.38351600	-4.27410100	-2.65246300
H	1.89979900	-2.58671700	-2.74506000
C	0.32529100	-4.27084800	-0.13931900
H	0.34994500	-4.24827900	0.95353100
H	0.57351200	-5.28606000	-0.47271000
H	-0.69987100	-4.05652700	-0.45787000
H	-3.62526900	-0.30181600	0.60001300
H	-6.50350100	-2.46733600	0.29201800
C	-5.63352300	-1.84958900	0.55923200
H	-4.39296200	-2.95800600	2.00648800
H	-4.41993100	-3.02017300	-1.79534200
C	-4.47015200	-2.73446800	0.94327000
H	-5.93132200	-1.30616400	1.46437600
C	-3.51898800	-3.23540000	0.14890800
H	-2.96001500	-3.98818100	-1.75879200
C	-3.42611300	-3.08595800	-1.34581800
H	-2.72230100	-3.81342800	0.61341100
H	-5.47135400	-1.25944600	-1.54389800
C	-5.37364600	-0.80844900	-0.55231000
H	-6.17134500	-0.05890800	-0.49185000
C	-2.60011800	-1.87492800	-1.83008200
Ni	-1.12121700	-0.74874400	-0.75357200
H	-2.41429200	-1.95294100	-2.90564000
C	-3.99443300	-0.11325700	-0.41077000
C	-2.93898900	-0.47915300	-1.44548400
H	-1.50916900	-2.17727400	-1.42306800

H	-4.12805000	0.97074800	-0.47581900
H	-2.94191400	0.19608400	-2.30108100

TS16

Fe	3.75047900	0.47661300	0.15973100
P	0.91087000	-1.58605900	-0.08051000
P	-0.88720800	1.09647500	0.09717100
O	0.95403800	-1.63971100	1.45764400
C	2.03003300	-0.27164100	-0.70964500
C	1.83493900	1.08327200	-0.24949000
C	2.75859800	1.92945900	-0.93415400
H	2.88283100	2.99101300	-0.77561700
C	3.54288900	1.11476600	-1.80265600
H	4.36199200	1.45217300	-2.42299800
C	3.09759600	-0.23382400	-1.66790100
H	3.53285600	-1.08052300	-2.17463700
C	0.82467600	1.46088300	0.79130100
H	0.89888500	0.72154300	1.59400000
C	1.00189100	2.86293100	1.36329600
H	0.91246000	3.63475800	0.59497500
H	1.99570000	2.95047900	1.81362000
H	0.25914000	3.06439300	2.14054100
C	4.09599200	-0.66142500	1.84748800
H	3.38885900	-1.42248700	2.14407300
C	4.00251000	0.71922600	2.19289200
H	3.25335900	1.15656500	2.83796400
C	5.02519500	1.42677400	1.48955900
H	5.19220800	2.49504300	1.51319700
C	5.75417300	0.48068400	0.70707700
H	6.57126200	0.70635600	0.03558000
C	5.18036400	-0.80849800	0.92945100
H	5.49017700	-1.72913700	0.45627300
C	-1.27350800	2.55318900	-0.93667100
C	-1.16677700	2.38733300	-2.32640600
H	-0.91678900	1.40897500	-2.72414200
C	-1.36891600	3.46416200	-3.18940600
H	-1.28036100	3.31943500	-4.26193400
C	-1.68773600	4.72111400	-2.67391800
H	-1.85404700	5.55885400	-3.34454900
C	-1.78641000	4.90077200	-1.29275200
H	-2.02454400	5.87919300	-0.88615400
C	-1.57131900	3.82800400	-0.42784900
H	-1.63082100	3.98724400	0.64220300
C	-1.92053900	1.11437500	1.60892000

C	-1.59663800	0.13286200	2.56487600
H	-0.75841300	-0.54094000	2.38682700
C	-2.36959800	0.00139000	3.71711400
H	-2.11060200	-0.75732300	4.44991300
C	-3.47789300	0.82684400	3.92393300
H	-4.08036000	0.71697500	4.82087000
C	-3.81382400	1.78621900	2.96858300
H	-4.68141900	2.42292200	3.11544000
C	-3.04104700	1.92983300	1.81445000
H	-3.33089000	2.66085700	1.06908000
C	1.56363600	-3.21472500	-0.76593500
C	2.99979600	-3.44958500	-0.27469000
H	3.69771300	-2.71298300	-0.67567700
H	3.34327600	-4.44496900	-0.58363800
H	3.04521300	-3.39986500	0.81637900
C	1.48761100	-3.25856200	-2.29688400
H	0.47092700	-3.05341400	-2.64869800
H	1.76866500	-4.25647600	-2.65600400
H	2.15352200	-2.53654800	-2.77414700
C	0.65763200	-4.31124500	-0.18138600
H	0.65879400	-4.28021300	0.91133700
H	1.01268500	-5.29818900	-0.50188500
H	-0.37609500	-4.20085900	-0.52444900
H	-3.68595400	0.06574600	0.18700400
H	-6.13371900	-2.58221000	0.55584500
C	-5.35378700	-1.80937800	0.61951400
H	-3.86891700	-2.34590600	2.16170200
H	-4.13800600	-3.35314600	-1.50589300
C	-4.05275000	-2.41748500	1.09149900
H	-5.68721600	-1.12197200	1.40622900
C	-3.09628000	-2.97961600	0.34689500
H	-2.53779300	-4.05940500	-1.40402100
C	-3.11956200	-3.16743600	-1.14874100
H	-2.18774900	-3.31343600	0.84393300
H	-5.37910400	-1.68306000	-1.57034000
C	-5.30257700	-1.01752900	-0.70607700
H	-6.19637700	-0.38381400	-0.74249200
C	-2.53691200	-1.98500100	-1.91595400
Ni	-1.05358900	-0.89729200	-0.85384500
H	-2.16257800	-2.23600700	-2.90745800
C	-4.04338500	-0.12675000	-0.82422900
C	-2.92488800	-0.64457000	-1.72381100
H	-0.95268300	-2.26195000	-1.34238000
H	-4.32896500	0.85044500	-1.22736900

H	-2.70542200	0.00461800	-2.56869000
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Fe	3.71613900	0.53636800	0.16965300
P	0.93961300	-1.60264500	-0.08105200
P	-0.92875500	1.04547400	0.09655400
O	0.94061200	-1.64336200	1.45434200
C	2.01391500	-0.25087700	-0.70356700
C	1.78792100	1.09726800	-0.23700100
C	2.68956100	1.96620900	-0.92180000
H	2.78851900	3.02988800	-0.76007100
C	3.49262600	1.17310900	-1.79284000
H	4.30309800	1.53167300	-2.41258000
C	3.08046500	-0.18587400	-1.66195600
H	3.53406300	-1.02010200	-2.17314500
C	0.76959000	1.44947900	0.80349600
H	0.85926800	0.71077700	1.60460200
C	0.91363700	2.85457400	1.37701900
H	0.80647800	3.62463300	0.60917500
H	1.90421800	2.96631700	1.82929000
H	0.16477800	3.03751700	2.15296900
C	4.10207500	-0.59445400	1.85340900
H	3.42679400	-1.38473200	2.14690400
C	3.95231000	0.77944700	2.20487900
H	3.18355000	1.18338100	2.84857600
C	4.94808100	1.53007500	1.50799000
H	5.07152900	2.60410800	1.53571800
C	5.71700200	0.61738800	0.72429200
H	6.52704000	0.87856400	0.05712900
C	5.19485600	-0.69457100	0.93875100
H	5.54560800	-1.60020200	0.46539100
C	-1.30279400	2.48760000	-0.96470900
C	-1.13166900	2.30384300	-2.34619000
H	-0.84349500	1.32467200	-2.71621600
C	-1.31485200	3.36343000	-3.23427100
H	-1.17600600	3.20446100	-4.29946800
C	-1.67901300	4.62174100	-2.75299000
H	-1.83157400	5.44600900	-3.44332400
C	-1.83878400	4.82035700	-1.38020000
H	-2.10973400	5.80073500	-0.99958200
C	-1.64183600	3.76476800	-0.48982100
H	-1.74411800	3.94059900	0.57435400
C	-1.96995000	1.09126600	1.60391300
C	-1.63452300	0.13988600	2.58597300

H	-0.79262100	-0.53196700	2.42214500
C	-2.39833800	0.03595900	3.74684900
H	-2.12849300	-0.69882300	4.49985000
C	-3.51222900	0.85818700	3.93688200
H	-4.10772200	0.77028500	4.84083300
C	-3.86243800	1.78518000	2.95529800
H	-4.73472800	2.41851600	3.08832900
C	-3.09704500	1.90191000	1.79283300
H	-3.39754200	2.60946700	1.02927600
C	1.66823300	-3.21296700	-0.73264600
C	3.10926100	-3.38206500	-0.22889900
H	3.77822200	-2.62012400	-0.63101800
H	3.49406300	-4.36433100	-0.52985500
H	3.14705100	-3.32607500	0.86202000
C	1.60884100	-3.29186100	-2.26353500
H	0.58356100	-3.16741600	-2.62742400
H	1.96259200	-4.27517200	-2.59699400
H	2.22708700	-2.53562900	-2.75182600
C	0.80372300	-4.33684900	-0.13529800
H	0.79486300	-4.28738600	0.95656200
H	1.20390300	-5.31211500	-0.43722200
H	-0.23122600	-4.27740500	-0.48845200
H	-3.73052100	0.18902500	0.07212200
H	-6.03100400	-2.57081500	0.71829300
C	-5.25239200	-1.79396700	0.69204800
H	-3.69284400	-2.29167900	2.16688200
H	-4.09940800	-3.41324500	-1.46871500
C	-3.92358400	-2.38002000	1.10712700
H	-5.53779300	-1.07044900	1.46524300
C	-2.99877900	-2.95318600	0.33086900
H	-2.45916900	-4.02923300	-1.42749100
C	-3.07664700	-3.16534100	-1.16211000
H	-2.07080900	-3.27717700	0.79707200
H	-5.39000700	-1.78026400	-1.49559900
C	-5.30087800	-1.07032700	-0.66894400
H	-6.22367500	-0.47871100	-0.68853500
C	-2.57679500	-1.97097600	-1.96135400
Ni	-1.03535000	-0.96899300	-0.85707200
H	-2.08254500	-2.21259800	-2.89947000
C	-4.10031700	-0.12599700	-0.90353400
C	-2.97638100	-0.65772600	-1.78401800
H	-0.64115400	-2.30830400	-1.21515400
H	-4.45668900	0.78799700	-1.39117000
H	-2.68808300	0.01830800	-2.58533900

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Fe	-3.65938300	-0.23369700	-0.38496500
P	-0.87754200	1.50052600	0.85739400
P	0.84246100	-1.23610000	0.27004300
O	-1.36235300	1.03839200	2.23588000
C	-1.75935500	0.57669100	-0.46464500
C	-1.71657900	-0.86732000	-0.45869500
C	-2.41379500	-1.34200600	-1.61059500
H	-2.57663300	-2.37795600	-1.86905300
C	-2.91320000	-0.21393100	-2.32211100
H	-3.52661000	-0.24339800	-3.21223600
C	-2.51151300	0.96274700	-1.62474500
H	-2.77327100	1.96825400	-1.91325600
C	-0.96685700	-1.67740000	0.55549000
H	-1.18468600	-1.26357000	1.54449500
C	-1.27008100	-3.17139600	0.51006900
H	-1.01082200	-3.60751300	-0.45833800
H	-2.33902700	-3.33707200	0.67773400
H	-0.71547400	-3.70917600	1.28273000
C	-4.45902600	0.29894800	1.44420300
H	-3.85423600	0.82918100	2.16590800
C	-4.48614800	-1.11840600	1.28417800
H	-3.95861400	-1.83110400	1.90219300
C	-5.27281900	-1.42344200	0.13086900
H	-5.45225100	-2.40955000	-0.27517400
C	-5.73369800	-0.19121500	-0.42390200
H	-6.32662200	-0.08067600	-1.32150900
C	-5.23101200	0.87154100	0.38788300
H	-5.37756100	1.92713700	0.21029000
C	1.11063000	-1.93363400	-1.39991400
C	0.84130000	-1.08259500	-2.48379700
H	0.56365700	-0.05132000	-2.29177400
C	0.90778100	-1.55835400	-3.79278800
H	0.69365100	-0.88866100	-4.62017800
C	1.24875900	-2.89003200	-4.03536700
H	1.30835000	-3.26014600	-5.05453000
C	1.50474300	-3.74751800	-2.96391900
H	1.75790700	-4.78763600	-3.14706100
C	1.42661400	-3.27677800	-1.65253200
H	1.60607400	-3.95841600	-0.82891500
C	1.76202500	-2.27901400	1.46014300
C	1.28390400	-2.35709500	2.77913100
H	0.34639500	-1.88139900	3.04841000

C	2.01303600	-3.03019800	3.75813500
H	1.62589900	-3.08544600	4.77114100
C	3.23566800	-3.62521200	3.44052100
H	3.80250200	-4.14880800	4.20436200
C	3.72834500	-3.53630600	2.13834400
H	4.68225000	-3.98868600	1.88354000
C	3.00018500	-2.86482300	1.15503900
H	3.40041000	-2.79907200	0.14964200
C	-1.29904000	3.31495500	0.58868500
C	-2.82009600	3.52571500	0.63423100
H	-3.33741800	3.02979300	-0.18689900
H	-3.04831600	4.59739900	0.57825800
H	-3.23248800	3.14378400	1.57213400
C	-0.69696200	3.81564800	-0.73057400
H	0.38276300	3.63252400	-0.76045200
H	-0.85682100	4.89627300	-0.83152000
H	-1.13889000	3.33173100	-1.60496300
C	-0.67504200	4.08635600	1.76370000
H	-1.05518700	3.71580300	2.71944300
H	-0.92106400	5.15161700	1.67847000
H	0.41620700	3.99461700	1.77570500
H	2.74552100	3.51928600	-0.24879300
H	5.87314600	3.03492400	-2.05085400
C	4.85920000	3.22693800	-1.66969300
H	3.42018800	2.63264500	-3.22726600
H	5.09969800	0.43143700	-0.58571100
C	3.88156400	2.27013600	-2.30896300
H	4.60463400	4.23440500	-2.02196100
C	3.50396400	1.06020100	-1.88345400
H	3.86060600	-0.76670500	-0.87456900
C	4.01331400	0.29987800	-0.68287100
H	2.76448000	0.53126900	-2.47643500
H	5.48458600	2.42098500	0.26050200
C	4.88962400	3.25204300	-0.12882400
H	5.41576800	4.16276000	0.17828000
C	3.36770500	0.62761800	0.65250300
Ni	1.24826900	0.93785200	0.58843300
H	3.41378400	-0.17383200	1.38502800
C	3.47810100	3.22821400	0.50665100
C	3.10587200	1.89413100	1.14489500
H	1.07253100	2.33037000	0.91139700
H	3.41557000	3.98422100	1.29570900
H	2.92419300	1.94194800	2.21677900

TS17

Fe	-3.67842900	-0.22286100	-0.37910600
P	-0.87772800	1.50246200	0.83718500
P	0.82710100	-1.23819200	0.26803800
O	-1.38217300	1.06719300	2.22108800
C	-1.77825600	0.58130900	-0.47366300
C	-1.73665700	-0.86257800	-0.45756000
C	-2.44124300	-1.34563400	-1.60180800
H	-2.60799300	-2.38324800	-1.85124800
C	-2.94222300	-0.22217200	-2.31958100
H	-3.55995300	-0.25770500	-3.20655500
C	-2.53487800	0.95936400	-1.63299800
H	-2.79665300	1.96325200	-1.92756100
C	-0.98444800	-1.66555200	0.56114000
H	-1.19542000	-1.24104900	1.54746200
C	-1.29474000	-3.15853700	0.53344500
H	-1.04705800	-3.60568600	-0.43293200
H	-2.36317300	-3.31607600	0.71141300
H	-0.73692000	-3.69136400	1.30729300
C	-4.46120900	0.33551300	1.45045000
H	-3.84403600	0.86736600	2.16065800
C	-4.50217600	-1.08313900	1.30486900
H	-3.97807600	-1.79406800	1.92787100
C	-5.29906100	-1.39316700	0.15996200
H	-5.49120900	-2.38190600	-0.23374300
C	-5.75202800	-0.16246500	-0.40485900
H	-6.35034700	-0.05582500	-1.29935700
C	-5.23423500	0.90401600	0.39278100
H	-5.37067200	1.95920300	0.20433900
C	1.08788200	-1.90862200	-1.41115800
C	0.86996000	-1.02382000	-2.47911400
H	0.64404900	0.01605500	-2.26705600
C	0.92365900	-1.47689100	-3.79668600
H	0.74934000	-0.78182600	-4.61236300
C	1.20142500	-2.81879400	-4.06282700
H	1.25003400	-3.17169200	-5.08864400
C	1.40949500	-3.70831400	-3.00715400
H	1.61581800	-4.75518900	-3.20930500
C	1.34395300	-3.25986000	-1.68737800
H	1.48741200	-3.96431300	-0.87603800
C	1.74584100	-2.28739900	1.45063400
C	1.29671300	-2.31601700	2.78199100
H	0.38504600	-1.79652900	3.06013600
C	2.02274400	-2.99496600	3.75890400

H	1.65931600	-3.01165500	4.78199300
C	3.21331200	-3.64481700	3.42589500
H	3.77847300	-4.17229700	4.18831600
C	3.67562800	-3.60689800	2.11038500
H	4.60365200	-4.10391400	1.84343400
C	2.94957300	-2.93075700	1.12837200
H	3.32462100	-2.90799300	0.11171900
C	-1.25844800	3.32289700	0.54789300
C	-2.77364500	3.56965600	0.60455400
H	-3.30882000	3.07638800	-0.20712500
H	-2.97997400	4.64546300	0.53957600
H	-3.18527400	3.20513200	1.54982100
C	-0.65622800	3.78899500	-0.78342400
H	0.41922000	3.58289500	-0.81740000
H	-0.79334800	4.87103000	-0.90296500
H	-1.11477000	3.29921900	-1.64595800
C	-0.60373500	4.09384600	1.70566900
H	-0.98024900	3.74351200	2.67048100
H	-0.82467400	5.16393400	1.61158900
H	0.48510400	3.97685700	1.70567300
H	2.76402900	3.42761300	-0.49332500
H	6.06808700	2.85212500	-1.88004300
C	5.02091000	3.07966300	-1.63173400
H	3.74629600	2.35117300	-3.27443000
H	5.13396600	0.41056300	-0.30043400
C	4.10665200	2.07009700	-2.28510500
H	4.81809700	4.05136400	-2.09924100
C	3.67463900	0.90378200	-1.79411100
H	3.93826900	-0.82505500	-0.60001300
C	4.06179800	0.25644400	-0.48691500
H	2.99403100	0.32425200	-2.41055600
H	5.43036900	2.45465100	0.41912700
C	4.88388400	3.24437400	-0.10412000
H	5.37601600	4.18208600	0.17625400
C	3.29301700	0.67886300	0.75536400
Ni	1.24844600	0.90817600	0.58561300
H	3.36528600	-0.03190000	1.57642600
C	3.41079100	3.26421600	0.37056700
C	2.99201500	2.00194300	1.12498400
H	1.29344400	2.31938700	0.93050100
H	3.24332600	4.11190700	1.04216300
H	2.87066200	2.15026000	2.19660200

Fe	3.70963700	-0.31168800	0.38322200
P	0.96285100	1.47978800	-0.87029700
P	-0.83947600	-1.18261000	-0.26860300
O	1.50114400	1.04792500	-2.24891300
C	1.83993100	0.55986100	0.45645800
C	1.74290800	-0.88095500	0.46072700
C	2.42709700	-1.37618500	1.61291400
H	2.55533000	-2.41577300	1.87671500
C	2.96494200	-0.26272500	2.31912900
H	3.57740800	-0.30988300	3.20926000
C	2.60410000	0.92392700	1.61498600
H	2.90228100	1.92136800	1.89735100
C	0.96253900	-1.67017100	-0.54844400
H	1.18623400	-1.27078300	-1.54283100
C	1.22259300	-3.17265100	-0.49621900
H	0.96715300	-3.59483400	0.47933600
H	2.28546600	-3.36472500	-0.67426000
H	0.64742700	-3.70274600	-1.25859200
C	4.51346500	0.21327500	-1.44671800
H	3.91063900	0.75699200	-2.16064400
C	4.51597700	-1.20532000	-1.29051400
H	3.97439800	-1.90677900	-1.90939800
C	5.30018400	-1.52874600	-0.14046000
H	5.46566700	-2.51960100	0.26008500
C	5.78260300	-0.30643600	0.41860100
H	6.37937700	-0.20946600	1.31528600
C	5.29574000	0.76799000	-0.38853300
H	5.45517600	1.82090300	-0.20443600
C	-1.09286700	-1.63331900	1.47991500
C	-0.98109700	-0.59758200	2.42074000
H	-0.84459600	0.42116400	2.07142900
C	-1.03527600	-0.87439600	3.78533300
H	-0.94374800	-0.06516000	4.50331600
C	-1.21096700	-2.18810900	4.22484600
H	-1.25939400	-2.40409800	5.28796500
C	-1.32227200	-3.22445600	3.29630400
H	-1.45568600	-4.24759900	3.63483000
C	-1.25574700	-2.95196500	1.92934300
H	-1.33169100	-3.76562500	1.21708600
C	-1.80006600	-2.32008700	-1.32558600
C	-1.43288700	-2.39642700	-2.68005400
H	-0.57133000	-1.84216700	-3.04115500
C	-2.17379300	-3.17187400	-3.56931200
H	-1.87554900	-3.22566500	-4.61200300

C	-3.29720100	-3.87235300	-3.12267500
H	-3.87505200	-4.47490300	-3.81688500
C	-3.67576400	-3.79036200	-1.78306200
H	-4.55131200	-4.32693800	-1.42968400
C	-2.93361600	-3.01777900	-0.88714000
H	-3.24327700	-2.96083600	0.14997500
C	1.34651600	3.30069300	-0.57099600
C	2.86062300	3.55035700	-0.62499900
H	3.39437000	3.05691600	0.18815500
H	3.06985900	4.62618900	-0.56178000
H	3.27224700	3.18132700	-1.56874400
C	0.73877200	3.75486700	0.76215000
H	-0.33566600	3.54050000	0.79757200
H	0.86519100	4.83738300	0.89122100
H	1.20068600	3.26257100	1.62137800
C	0.69070800	4.07531800	-1.72641400
H	1.05796400	3.71842600	-2.69243700
H	0.92095700	5.14428200	-1.63940300
H	-0.39964600	3.97276800	-1.72238400
H	-2.76986200	3.09028300	0.83101400
H	-6.29131100	2.68348200	1.58432900
C	-5.20160700	2.82625000	1.53883200
H	-4.32230900	1.59905400	3.14219200
H	-5.18455500	0.61446000	-0.43277100
C	-4.49852100	1.59693000	2.06654800
H	-4.99019100	3.64530300	2.23849400
C	-4.04555700	0.54169100	1.38128500
H	-4.21881900	-0.81934300	-0.23230400
C	-4.19891500	0.26623600	-0.09347100
H	-3.52226800	-0.22781300	1.94232200
H	-5.30769300	2.68453000	-0.63500600
C	-4.80878400	3.29466500	0.12282100
H	-5.19846200	4.30937600	-0.01292800
C	-3.12420400	0.80442700	-1.02939000
Ni	-1.21041200	0.89042400	-0.69461700
H	-3.19850000	0.31963800	-2.00722400
C	-3.28226300	3.28382400	-0.11458300
C	-2.81182500	2.25988900	-1.15893200
H	-1.63086300	2.41927200	-1.15698800
H	-2.94522400	4.27057700	-0.44965900
H	-2.99242400	2.61912100	-2.17808400
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Fe	3.87810200	0.34819500	-0.15195400

P	0.97976100	-1.62786100	0.12049800
P	-0.73335800	1.11407400	0.24281700
O	1.28133700	-1.61212000	1.63462800
C	2.05240600	-0.40691200	-0.74417900
C	1.93722200	0.98219500	-0.36376300
C	2.78609100	1.75650400	-1.21160600
H	2.94736000	2.82297400	-1.14615800
C	3.44115700	0.86458300	-2.11109700
H	4.18353000	1.13734800	-2.84885000
C	2.99020300	-0.45983800	-1.82910700
H	3.34361100	-1.34998300	-2.32589200
C	1.04828400	1.45450300	0.74626100
H	1.18189100	0.76142800	1.58205300
C	1.31298300	2.88156300	1.21397100
H	1.18128800	3.60898200	0.40936200
H	2.34306600	2.96113500	1.57502500
H	0.64489300	3.15325500	2.03639500
C	4.40658700	-0.72350200	1.53492400
H	3.71764100	-1.44579800	1.94950700
C	4.39277500	0.67450300	1.81925300
H	3.74487500	1.16374800	2.53320600
C	5.33508200	1.31684300	0.95809700
H	5.53360900	2.37882200	0.90957800
C	5.93213400	0.31346100	0.13619500
H	6.66213700	0.48223800	-0.64372100
C	5.35764900	-0.94573800	0.49253000
H	5.57255500	-1.89533800	0.02330700
C	-1.20350800	2.51913600	-0.82171900
C	-1.26632600	2.28764600	-2.20414300
H	-1.09438000	1.28512300	-2.58089600
C	-1.54300200	3.33154900	-3.08633400
H	-1.58498900	3.13801200	-4.15392700
C	-1.76825600	4.61863100	-2.59632700
H	-1.99140500	5.43096900	-3.28149800
C	-1.70078000	4.86162900	-1.22303300
H	-1.86764200	5.86305600	-0.83775200
C	-1.41141800	3.82203000	-0.33978900
H	-1.34452200	4.02848000	0.72179000
C	-1.63815900	1.19615100	1.82797300
C	-1.23497500	0.25802600	2.79805600
H	-0.40835500	-0.42227600	2.58982400
C	-1.91086900	0.18393600	4.01428100
H	-1.59219700	-0.53979400	4.75870400
C	-2.99582800	1.02573000	4.27318900

H	-3.52134700	0.96166100	5.22146100
C	-3.40824200	1.94218100	3.30611300
H	-4.25783600	2.59154200	3.49625100
C	-2.73522300	2.02758100	2.08564900
H	-3.07897200	2.73124200	1.33699300
C	1.43023000	-3.31281200	-0.58986300
C	2.90425000	-3.63767100	-0.30830200
H	3.58302900	-2.95845600	-0.82770400
H	3.13580200	-4.66063800	-0.63215200
H	3.11227800	-3.56693100	0.76289500
C	1.11871400	-3.37513200	-2.09085200
H	0.07769200	-3.09930200	-2.29405300
H	1.26926500	-4.39540300	-2.46552900
H	1.75272900	-2.70931900	-2.67992300
C	0.54836800	-4.32794700	0.15728300
H	0.70966800	-4.26511700	1.23691800
H	0.78537900	-5.34740600	-0.17124400
H	-0.51691300	-4.15726800	-0.03429700
H	-6.10088100	0.39619400	-0.57819000
H	-6.46781300	-3.30696700	-0.40438600
C	-5.85377000	-2.42197100	-0.17928800
H	-4.78098500	-3.49763900	1.37550200
H	-2.85226900	-2.65949000	-2.02872800
C	-4.58995700	-2.92902900	0.46445200
H	-6.42630500	-1.87812000	0.58762100
C	-3.30353100	-2.83342700	0.10803900
H	-1.53571500	-2.39052500	-0.98827500
C	-2.69186800	-2.13071600	-1.08128400
H	-2.58348700	-3.31807600	0.76394700
H	-5.08980300	-2.02239300	-2.16744200
C	-5.75960000	-1.55269200	-1.43928500
H	-6.74884400	-1.53834000	-1.91258700
C	-2.84946500	-0.64447900	-1.20878300
Ni	-1.05633000	-0.87292200	-0.50380900
H	-2.73583900	-0.30597500	-2.24399800
C	-5.33266900	-0.10115800	-1.18648700
C	-3.96717900	0.07141500	-0.49259200
H	-4.02796100	-0.26387600	0.54602900
H	-5.30876500	0.42712900	-2.14909900
H	-3.74230300	1.14299100	-0.45996400

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Fe	-3.84812700	-0.37436300	-0.14605300
P	-0.97297900	1.63876100	0.12534100

P	0.75407500	-1.09629500	0.24684700
O	-1.21709800	1.58069300	1.64387900
C	-2.02573700	0.39927500	-0.73391400
C	-1.90468300	-0.99010700	-0.35594500
C	-2.74348900	-1.76532600	-1.21221300
H	-2.89822000	-2.83293500	-1.15114300
C	-3.40299800	-0.87390200	-2.10874100
H	-4.14155900	-1.14816400	-2.84968600
C	-2.96251500	0.45185800	-1.81997300
H	-3.31917700	1.34128100	-2.31542600
C	-1.01910000	-1.46414300	0.75572700
H	-1.16088900	-0.77875300	1.59608100
C	-1.27450900	-2.89714200	1.20874600
H	-1.13463800	-3.61580300	0.39762700
H	-2.30458900	-2.99030400	1.56682900
H	-0.60533500	-3.17094400	2.02958600
C	-4.39387900	0.64813600	1.56673700
H	-3.72269100	1.36993700	2.00949800
C	-4.36324600	-0.75593800	1.81523000
H	-3.71039900	-1.25572000	2.51716700
C	-5.29587500	-1.38679200	0.93539200
H	-5.47909500	-2.44972500	0.85711900
C	-5.90429900	-0.36982200	0.13923500
H	-6.63079800	-0.52716500	-0.64628000
C	-5.34668400	0.88637800	0.52942900
H	-5.57817000	1.84576200	0.08951900
C	1.20396700	-2.48512700	-0.85044600
C	1.21830100	-2.22262300	-2.22927800
H	1.02182300	-1.21379600	-2.57702500
C	1.47243400	-3.24323400	-3.14504500
H	1.47661300	-3.02462900	-4.20865000
C	1.72273700	-4.53964800	-2.69330900
H	1.92822400	-5.33427700	-3.40430200
C	1.70082200	-4.81486100	-1.32463700
H	1.88461700	-5.82426300	-0.96881900
C	1.43411900	-3.79809700	-0.40808400
H	1.39877500	-4.03179200	0.64918700
C	1.66503100	-1.21883800	1.82883000
C	1.28022900	-0.28185400	2.80727900
H	0.46611200	0.41417200	2.60335700
C	1.95460200	-0.23172200	4.02584900
H	1.64914400	0.49222600	4.77561700
C	3.02167600	-1.09722700	4.27974500
H	3.54678900	-1.05194600	5.22934300

C	3.41677600	-2.01343900	3.30515800
H	4.25257700	-2.68178500	3.49089900
C	2.74404400	-2.07476300	2.08309800
H	3.07684000	-2.77853000	1.32947700
C	-1.50419400	3.32525500	-0.52232700
C	-2.98874300	3.56282900	-0.20975100
H	-3.63933200	2.87986900	-0.75812200
H	-3.27002000	4.58855900	-0.47996700
H	-3.18089700	3.42999500	0.85806800
C	-1.22206400	3.46582500	-2.02299700
H	-0.16759400	3.27216500	-2.24644000
H	-1.45013300	4.48721700	-2.35249400
H	-1.81842400	2.78150800	-2.63010200
C	-0.66620500	4.35582100	0.25174900
H	-0.81826500	4.25478200	1.32954000
H	-0.95183700	5.37143600	-0.04808300
H	0.40341500	4.23603400	0.04800400
H	6.04542300	-0.46995900	-0.39897500
H	6.54375000	3.19004900	-0.27545200
C	5.82574500	2.37411400	-0.10910000
H	4.69750400	3.75805800	1.12309200
H	2.47280200	2.61073200	-2.12883400
C	4.54227500	3.03729000	0.31893800
H	6.23193900	1.82416700	0.75418200
C	3.27962200	2.94979900	-0.12255900
H	1.12241700	2.37577100	-0.82982900
C	2.70008300	2.08698100	-1.19923600
H	2.56379500	3.61629500	0.35344800
H	5.23231500	1.91986400	-2.13836900
C	5.82781300	1.46048600	-1.34130400
H	6.85363200	1.40397100	-1.72435700
C	2.91562900	0.68920100	-1.28927100
Ni	1.05147600	0.95510500	-0.50377200
H	2.73403400	0.25003400	-2.27113600
C	5.33800500	0.03418500	-1.07110200
C	3.93119600	-0.04482700	-0.45140700
H	3.94638100	0.35609200	0.56557200
H	5.34720300	-0.52995200	-2.01318700
H	3.65492900	-1.09959800	-0.37036900

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Fe	-3.87723500	-0.15116400	-0.12498000
P	-0.83384600	1.59864000	0.24775700
P	0.65341100	-1.22269500	0.11660100

O	-0.94430600	1.30902600	1.75278400
C	-2.01581600	0.55935800	-0.68836400
C	-1.99589700	-0.87238000	-0.49455900
C	-2.91931900	-1.45924100	-1.41163500
H	-3.15742400	-2.51055200	-1.48505600
C	-3.53561400	-0.40905200	-2.15370300
H	-4.31711200	-0.52659100	-2.89195600
C	-2.98273500	0.82897300	-1.71256000
H	-3.28248500	1.80242000	-2.06682700
C	-1.14615700	-1.56302200	0.53237900
H	-1.26074400	-1.01056700	1.46850300
C	-1.49480800	-3.03119700	0.75162400
H	-1.37811300	-3.62106300	-0.16069200
H	-2.53685200	-3.11690800	1.07566700
H	-0.86208900	-3.47034600	1.52807200
C	-4.30918100	0.64780900	1.73312900
H	-3.59281800	1.26254400	2.25786600
C	-4.35902700	-0.77655300	1.78121900
H	-3.71724900	-1.40909200	2.37832500
C	-5.35317200	-1.21997700	0.85588100
H	-5.60295000	-2.24841000	0.63376000
C	-5.91963000	-0.06633800	0.23411100
H	-6.67582700	-0.06795400	-0.53888700
C	-5.27488800	1.08703700	0.77654500
H	-5.46277400	2.11138000	0.48828000
C	1.05214000	-2.41035100	-1.21614900
C	1.18067100	-1.88263400	-2.51051600
H	1.08548500	-0.80993500	-2.65327800
C	1.41815100	-2.72010600	-3.60044700
H	1.51192000	-2.29764400	-4.59632800
C	1.53627200	-4.09718100	-3.40746100
H	1.72649800	-4.75119000	-4.25323100
C	1.40687400	-4.63418400	-2.12464200
H	1.49376000	-5.70583200	-1.97169600
C	1.16065900	-3.79888300	-1.03543500
H	1.05423200	-4.22849200	-0.04620800
C	1.53290000	-1.73784100	1.63231200
C	1.16873900	-1.06596200	2.81446500
H	0.37061500	-0.32620300	2.78896300
C	1.87020300	-1.30240900	3.99490600
H	1.58205200	-0.77957700	4.90220600
C	2.94960400	-2.19010700	4.01025100
H	3.49723000	-2.36669000	4.93128000
C	3.33049200	-2.83672400	2.83463300

H	4.17792000	-3.51614200	2.83535600
C	2.62795100	-2.61148700	1.64857600
H	2.94571200	-3.10806100	0.73899900
C	-1.27860900	3.39910500	-0.06042900
C	-2.70375900	3.65967600	0.45007500
H	-3.44790900	3.10233700	-0.12211200
H	-2.94031000	4.72760200	0.36668300
H	-2.79654600	3.37300600	1.50062000
C	-1.14717700	3.79627300	-1.53517400
H	-0.14607100	3.57389200	-1.91775900
H	-1.31360800	4.87540600	-1.64014500
H	-1.86991300	3.28833300	-2.17720800
C	-0.28183900	4.21973500	0.77665300
H	-0.35080200	3.95875100	1.83588600
H	-0.49873100	5.28915700	0.66661900
H	0.74875900	4.04564700	0.44857700
H	5.70869900	0.92747200	1.81527000
H	6.55476300	3.40192700	-0.77821700
C	5.71338200	2.87609500	-0.30622900
H	4.49467600	4.43783500	-1.18859100
H	2.71167100	0.91593800	-2.49933700
C	4.47768200	3.35913800	-1.02713900
H	5.69026600	3.26714900	0.72345700
C	3.40467000	2.73301300	-1.54010300
H	0.99824800	2.28880800	-0.85271300
C	3.03342500	1.30291400	-1.53129700
H	2.70891700	3.35945300	-2.09424800
H	5.81188900	0.93248800	-1.25041300
C	6.04095800	1.37474800	-0.27454400
H	7.12289400	1.26311400	-0.13652200
C	3.23608200	0.38944200	-0.52274700
Ni	1.11476300	0.90241200	-0.46138200
H	3.23086700	-0.66626900	-0.78186800
C	5.33236200	0.59607500	0.83917900
C	3.80325300	0.75988300	0.81990800
H	3.53874200	1.79736700	1.04880000
H	5.58229900	-0.46946000	0.75406000
H	3.36490700	0.13444900	1.60029100

TS19

Ni	0.78734200	0.18418500	-1.24365400
Fe	-3.82007300	-1.05379200	0.74457700
P	-1.03576200	-1.09415900	-1.38245900
P	-0.13003200	1.70785500	0.04846500

O	-1.94041600	-0.39078500	-2.40611000
C	-1.80997200	-1.07712900	0.27714600
C	-2.19928100	0.18797600	0.85352200
C	-2.69818500	-0.05542600	2.16949100
H	-3.09379500	0.68847400	2.84526600
C	-2.64522300	-1.45731100	2.41158800
H	-2.99925300	-1.96276500	3.29964700
C	-2.09904300	-2.08645100	1.25551600
H	-1.96478500	-3.14988900	1.13625000
C	-2.00297900	1.51661400	0.18512000
H	-2.32982200	1.42913500	-0.85546200
C	-2.72048800	2.66603800	0.88650300
H	-2.37775900	2.79083900	1.91699300
H	-3.79511700	2.45899900	0.91645800
H	-2.57059100	3.61166200	0.36155000
C	-4.84131000	-1.22311300	-1.04104200
H	-4.29944000	-1.23958700	-1.97556500
C	-5.24363500	-0.04169700	-0.34955800
H	-5.11168600	0.97065500	-0.70503700
C	-5.78579200	-0.42590000	0.91509300
H	-6.14347000	0.24439500	1.68476300
C	-5.71887400	-1.84931200	1.00646700
H	-6.01911200	-2.44644200	1.85660400
C	-5.13640400	-2.34082200	-0.20189600
H	-4.91965600	-3.37575300	-0.42399200
C	0.39852900	1.49471400	1.78623800
C	0.89904900	0.23303100	2.14776900
H	1.01961400	-0.52818600	1.38242600
C	1.22605100	-0.04715600	3.47327900
H	1.61445500	-1.02637000	3.73576400
C	1.05598000	0.93145300	4.45453900
H	1.31271400	0.71662200	5.48756800
C	0.55343000	2.18680400	4.10663200
H	0.41638100	2.94864900	4.86832200
C	0.22127100	2.46789800	2.78070000
H	-0.17359400	3.44429400	2.52309700
C	0.12556800	3.45901400	-0.40291600
C	-0.59607300	3.95687700	-1.50145100
H	-1.32444300	3.32607700	-2.00293000
C	-0.37614800	5.25325600	-1.96336500
H	-0.94465400	5.62532600	-2.81027000
C	0.57584000	6.06698300	-1.34433100
H	0.74828700	7.07592700	-1.70628100
C	1.30561100	5.57651100	-0.26162400

H	2.04962400	6.20202100	0.22270100
C	1.08382900	4.28009700	0.20760900
H	1.65733900	3.91259100	1.05110600
C	-0.80429200	-2.90066300	-1.84479100
C	-2.15823300	-3.62765900	-1.83381800
H	-2.59729700	-3.68008800	-0.83722000
H	-2.03062400	-4.65338900	-2.20171200
H	-2.87201000	-3.12203100	-2.48995800
C	0.21134700	-3.57521600	-0.91311200
H	1.19477600	-3.09985300	-0.98343500
H	0.33858600	-4.62624200	-1.20052800
H	-0.09966700	-3.55474400	0.13449000
C	-0.26309700	-2.91177700	-3.28446100
H	-0.94666600	-2.39647500	-3.96456900
H	-0.14299800	-3.94670000	-3.62617700
H	0.71675900	-2.42855200	-3.35373200
H	1.20396700	-1.03927300	-1.92666400
C	4.60148900	-1.39239200	0.63873400
C	4.47456100	-2.57386900	-0.14005000
C	5.03877700	-3.77020600	0.31888000
C	5.70472400	-3.75265400	1.54147900
C	5.81682100	-2.57152500	2.30265900
C	5.26773700	-1.36767500	1.86478600
C	3.45281000	-1.02204200	-1.22141700
H	4.94920300	-4.67903300	-0.26756500
H	6.14731900	-4.66847200	1.92151800
H	6.34155000	-2.60063100	3.25286200
H	5.35023500	-0.45981200	2.45386300
N	3.95148300	-0.41310400	-0.08941000
N	3.74881300	-2.30670200	-1.29274400
C	3.73630200	0.98116900	0.27655700
H	2.92134100	1.03669300	1.00228900
H	4.64349500	1.35372000	0.76099000
C	3.41214600	1.81086700	-0.96311500
H	3.00892600	2.77447200	-0.64196500
H	4.34562400	2.03038000	-1.50491900
C	2.02059200	1.99767500	-3.09994100
H	1.29812900	1.47271500	-3.73280700
H	1.55757200	2.92652100	-2.75765400
H	2.88102100	2.27210700	-3.72964100
C	2.45901300	1.14023000	-1.93556200
C	2.60049600	-0.26438200	-2.15079700
H	2.56634500	-0.66407000	-3.16161600

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Ni	1.13420900	0.36597500	-1.16883100
Fe	-3.85651700	-0.80708300	0.67402700
P	-1.18171500	-1.31520100	-1.38955600
P	0.04788500	1.77873300	0.05369700
O	-1.76618900	-0.42658700	-2.45990400
C	-1.86286900	-1.02756300	0.24807400
C	-2.12851000	0.29913000	0.76735200
C	-2.65679300	0.13770600	2.08300900
H	-2.98283700	0.93896100	2.72891700
C	-2.74230700	-1.25155400	2.37786700
H	-3.15171100	-1.68539400	3.27942800
C	-2.25487900	-1.97427800	1.25616000
H	-2.22254300	-3.04842000	1.16981900
C	-1.83903000	1.60561000	0.08271500
H	-2.10380200	1.50146900	-0.97339500
C	-2.58191800	2.78672200	0.70475700
H	-2.29218200	2.94362900	1.74685900
H	-3.66113300	2.60535500	0.68093300
H	-2.37883700	3.70984100	0.15856100
C	-4.92403600	-1.03246200	-1.08529300
H	-4.44720700	-1.20600900	-2.03874200
C	-5.17583800	0.24965600	-0.51374600
H	-4.94241500	1.20002000	-0.97245600
C	-5.73382200	0.05329400	0.78622800
H	-6.00050600	0.83104500	1.48832600
C	-5.82550900	-1.35249900	1.01819600
H	-6.17397200	-1.82455100	1.92641500
C	-5.32519200	-2.02379100	-0.13902500
H	-5.23256000	-3.09345600	-0.26196200
C	0.45799900	1.69003000	1.83824900
C	0.93290300	0.45663800	2.31229700
H	1.09679200	-0.35280100	1.60656500
C	1.18674900	0.26548300	3.67012200
H	1.55658100	-0.69403800	4.01871900
C	0.97255400	1.30977400	4.57146900
H	1.17407000	1.16616500	5.62891600
C	0.50272000	2.54191200	4.11084600
H	0.33693500	3.35646800	4.80993200
C	0.24360200	2.73215800	2.75295700
H	-0.11719900	3.69401200	2.40496100
C	0.35645200	3.50499500	-0.46758000
C	-0.32264900	4.00211500	-1.59229000
H	-1.09057800	3.40252600	-2.07237800

C	-0.00625300	5.25512300	-2.11457900
H	-0.54393600	5.62676300	-2.98182900
C	1.00275500	6.02542100	-1.53159000
H	1.25123200	6.99964900	-1.94144200
C	1.69378300	5.53264100	-0.42410400
H	2.48381500	6.12212200	0.03208600
C	1.37546300	4.28061200	0.10459900
H	1.92418700	3.90784000	0.96273700
C	-1.10447500	-3.12060200	-1.80557700
C	-2.50767300	-3.74468500	-1.79180800
H	-2.95479300	-3.73540300	-0.79589100
H	-2.44248800	-4.78699400	-2.12418600
H	-3.18333400	-3.21952700	-2.47318900
C	-0.14414600	-3.83966600	-0.84358200
H	0.86834100	-3.42921700	-0.90998400
H	-0.08587700	-4.89762200	-1.12392100
H	-0.46865100	-3.79325900	0.19864200
C	-0.51905100	-3.17097700	-3.23008800
H	-1.15402500	-2.64134000	-3.94436800
H	-0.43245400	-4.21666800	-3.54558900
H	0.48236700	-2.72980200	-3.26126000
H	0.24788600	-1.15165500	-1.18379600
C	4.36982400	-1.82041000	0.69594300
C	3.97943800	-2.97087000	-0.04333400
C	4.25108300	-4.24346500	0.47083800
C	4.89124800	-4.33316600	1.70734400
C	5.26051400	-3.18327200	2.42888800
C	5.00506400	-1.90223500	1.93352400
C	3.34051800	-1.26374700	-1.20110700
H	3.96366400	-5.13112200	-0.08431400
H	5.10856100	-5.31182300	2.12547500
H	5.75337800	-3.29274400	3.39041500
H	5.28676700	-1.01432700	2.49109400
N	3.97420400	-0.74630100	-0.08046700
N	3.34164400	-2.59229600	-1.21564500
C	3.99219100	0.66473800	0.28415200
H	3.17017800	0.86309300	0.98070200
H	4.93190100	0.87642800	0.80322100
C	3.85401900	1.54357000	-0.96026000
H	3.60311400	2.56071300	-0.64262300
H	4.82710200	1.60364100	-1.47330200
C	2.55396800	1.98054200	-3.10927800
H	1.82586800	1.55985500	-3.80885500
H	2.16647200	2.94053900	-2.75428500

H	3.47930100	2.18780100	-3.66943000
C	2.82445700	1.03987500	-1.95808500
C	2.70092400	-0.36634300	-2.14490300
H	2.40246000	-0.79197100	-3.09920300

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Ni	0.57929600	0.19944700	-0.53811300
C	2.15123700	1.54903700	-0.19549900
C	2.48147100	1.82764400	-1.60800500
H	1.71705700	2.45499500	0.23814900
C	3.22574000	1.03985100	0.75702600
C	3.61045400	1.62037500	-2.32158700
H	1.65946400	2.28522800	-2.15986200
H	3.73087900	0.17059700	0.33773300
H	2.74068600	0.67606300	1.67036800
C	4.26835600	2.09143800	1.19629100
H	3.58613100	1.91683100	-3.37000200
C	4.94184200	1.12294600	-1.81188100
H	3.77615900	2.78829900	1.88913200
H	5.05227200	1.58560100	1.78001800
C	4.91767600	2.92770400	0.08394100
C	5.72594200	2.16769100	-0.97717900
H	5.56602500	0.83313100	-2.66541200
H	4.81826900	0.21123000	-1.22568600
H	4.13876800	3.51014100	-0.41964500
H	5.58727800	3.65953400	0.55553800
H	6.57937300	1.66304000	-0.50227300
H	6.15360200	2.91148800	-1.66241100
H	0.51831200	0.38331400	2.20394400
C	0.25218700	1.34052300	2.63987900
C	-0.34651400	2.31236600	1.82380900
C	0.51584700	1.60048800	3.98343900
P	-0.72290700	1.82604200	0.09884200
C	-0.68896600	3.55052500	2.38768200
H	0.98309000	0.83736400	4.59789300
C	0.18663800	2.84189900	4.53037700
C	-2.57820400	1.51960700	0.14493900
C	-0.58150200	3.28027200	-0.99664600
C	-0.41651600	3.81423200	3.73078900
H	-1.16744200	4.31093000	1.78194400
H	0.39792800	3.05102900	5.57491000
C	-2.80395400	0.17195100	0.76267900
H	-2.81840800	1.43201600	-0.91758000
C	-3.39047100	2.64638900	0.77510100

C	-1.07964400	3.10211000	-2.30087300
C	0.09481300	4.46294300	-0.67226400
H	-0.67904600	4.78005100	4.15231500
C	-2.35055200	-1.05810200	0.15747900
C	-3.47389400	-0.14317100	1.98458200
H	-3.16646300	2.77329200	1.83689700
H	-4.45769700	2.42228200	0.68329900
H	-3.20006800	3.59638100	0.26784300
H	-1.53829500	2.15272600	-2.57502000
C	-0.93172500	4.11547200	-3.24588500
C	0.24421100	5.46998400	-1.62797700
H	0.52082300	4.59820800	0.31489800
P	-1.27779600	-0.93740200	-1.33570800
C	-2.78035900	-2.12289400	1.01706400
H	-3.95584000	0.56323500	2.64508800
C	-3.46962200	-1.56167100	2.13531000
H	-1.31847800	3.97080000	-4.25048800
C	-0.27423000	5.30255200	-2.91178700
H	0.77216900	6.38254800	-1.36696900
O	-2.00127900	-0.09293600	-2.41184700
C	-1.14277600	-2.69935400	-2.02310000
H	-2.65136100	-3.17923400	0.83619900
H	-3.94501000	-2.11738400	2.93236600
H	-0.15615800	6.08748200	-3.65311300
C	-2.55188900	-3.22710200	-2.32679500
C	-0.40593000	-3.67112500	-1.09056600
C	-0.37284200	-2.57089900	-3.34686200
H	-3.13413800	-3.38341100	-1.41727500
H	-2.48304100	-4.18662200	-2.85626800
H	-3.09564300	-2.52578100	-2.96329900
H	0.66040000	-3.45266900	-1.04735600
H	-0.51418400	-4.69594500	-1.46928600
H	-0.79738800	-3.65694100	-0.07024300
H	-0.89371000	-1.89775900	-4.03251700
H	-0.28040500	-3.55430100	-3.82525700
H	0.63549800	-2.18165800	-3.18802500
Fe	-4.41737500	-1.02852700	0.37313700
C	-6.38984500	-0.39107400	0.36692100
C	-5.69795600	0.10674800	-0.77932200
H	-6.83699900	0.20576000	1.15017000
C	-6.33954400	-1.81727300	0.32395100
C	-5.21786100	-1.00657700	-1.52995300
H	-5.52281800	1.14678200	-1.01585000
H	-6.74400100	-2.49043600	1.06746700

C	-5.61571500	-2.19691800	-0.84723600
H	-4.57160800	-0.93961500	-2.39245600
H	-5.38003200	-3.20848000	-1.14429400
C	3.49458300	-2.85814000	-0.53607000
C	2.78438600	-1.87164200	-1.25992300
C	3.10167800	-1.60585300	-2.59566900
C	4.13480600	-2.34042300	-3.16702800
C	4.84059600	-3.31784000	-2.43499700
C	4.53432200	-3.59702600	-1.10639800
C	1.93381500	-1.94554400	0.73740600
H	2.57482200	-0.83521800	-3.14244000
H	4.40916500	-2.15486000	-4.20054500
H	5.64191500	-3.86646300	-2.92010000
H	5.07384700	-4.35293800	-0.54590900
H	1.33436300	-1.73394700	1.60535700
N	2.92756900	-2.87795500	0.73289900
N	1.81804100	-1.32318000	-0.42238700
C	3.34362700	-3.75342400	1.82960300
H	3.20241000	-4.78921600	1.50471000
H	4.41561600	-3.60300500	1.99362500
C	2.57013800	-3.52237900	3.12393400
H	1.49573000	-3.65722900	2.93779200
H	2.83961200	-4.34128800	3.80405400
C	1.89599400	-2.01043800	5.04444200
H	2.14176400	-1.09195900	5.58352500
H	0.84146100	-1.96094700	4.74225500
H	1.97815800	-2.84959000	5.74721700
C	2.79171600	-2.21047900	3.84953000
C	3.69724900	-1.29809800	3.48377700
H	3.82914400	-0.38122700	4.05067600
H	4.33611400	-1.41704300	2.61531200

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Fe	-4.19208300	-1.50732800	0.38806400
P	-1.19033800	-1.02595600	-1.41507000
P	-0.93897400	1.88638900	0.20887500
O	-1.87104000	-0.07813700	-2.39927100
C	-2.16220800	-1.25673300	0.09876700
C	-2.73570200	-0.11353700	0.77458100
C	-3.29775000	-0.56899600	2.00456000
H	-3.83597800	0.04068100	2.71542500
C	-3.10487100	-1.97891800	2.09167900
H	-3.46937000	-2.62215900	2.88066300
C	-2.40974200	-2.40611200	0.92374500

H	-2.15388200	-3.42738600	0.68906200
C	-2.72161900	1.28360800	0.22918100
H	-2.95320200	1.21911200	-0.83585400
C	-3.70126300	2.23288000	0.91357300
H	-3.49221000	2.34376100	1.97984700
H	-4.71971800	1.84760900	0.80803800
H	-3.66483900	3.22409100	0.45342900
C	-5.33292100	-2.81530700	-0.74860100
H	-5.00892900	-3.79666400	-1.06431700
C	-5.12793900	-1.59298100	-1.45822900
H	-4.59461600	-1.47082600	-2.38857000
C	-5.67323900	-0.53361600	-0.67593200
H	-5.63768600	0.51689100	-0.92734100
C	-6.21661700	-1.09795100	0.51823100
H	-6.66902200	-0.54976500	1.33311300
C	-6.00627300	-2.50909100	0.47276700
H	-6.27255700	-3.21573200	1.24670400
C	-0.64450600	2.47607500	1.91377300
C	0.13605900	1.65730700	2.74020100
H	0.57128600	0.76087600	2.31669400
C	0.36330100	1.99560300	4.07315700
H	0.97609200	1.35206100	4.69722100
C	-0.18864100	3.16635500	4.59523300
H	-0.00849300	3.43916700	5.63074000
C	-0.97142500	3.98925800	3.78201600
H	-1.40282500	4.90065900	4.18509300
C	-1.20407600	3.64656900	2.45017100
H	-1.81350000	4.29401200	1.83044500
C	-0.99008100	3.34899800	-0.88368300
C	-1.51003100	3.16127000	-2.17711300
H	-1.88966400	2.18577700	-2.46919700
C	-1.47538900	4.20448600	-3.10022900
H	-1.87782700	4.04995600	-4.09698700
C	-0.90857700	5.43395400	-2.75566200
H	-0.87795600	6.24219100	-3.48032800
C	-0.36610000	5.61435800	-1.48357900
H	0.09314200	6.56101300	-1.21480100
C	-0.40282700	4.57721200	-0.55013200
H	0.03841800	4.72568800	0.42852100
C	-0.87788500	-2.68014800	-2.24947900
C	-2.23139600	-3.29978600	-2.62600400
H	-2.80901500	-3.58034100	-1.74272800
H	-2.06113200	-4.20262800	-3.22479700
H	-2.82682500	-2.60614500	-3.22433700

C	-0.05974400	-3.66044900	-1.39613800
H	0.96354800	-3.31841900	-1.24508300
H	-0.00105500	-4.62010100	-1.92304500
H	-0.50580900	-3.85478800	-0.41877500
C	-0.08851600	-2.33682500	-3.52790100
H	-0.65398600	-1.65490100	-4.16715500
H	0.10472000	-3.25940100	-4.08804300
H	0.87649000	-1.87488500	-3.29665100
H	0.57203300	-1.01204400	-1.00057200
Ni	0.60262700	0.43125300	-0.45670400
N	2.78678200	-1.17678600	-1.68563300
C	3.66491500	-2.18143300	-1.32256900
C	1.96591100	-1.01090400	-0.66026900
C	3.33800400	-2.66773100	-0.02958900
C	4.73219300	-2.74406300	-2.03715500
N	2.25447500	-1.90501700	0.37522200
C	4.03471100	-3.72805500	0.55745800
C	5.43334100	-3.79132100	-1.44973900
H	4.98646600	-2.36705400	-3.02282400
C	1.43901700	-2.10320800	1.56308500
C	5.08324300	-4.28019800	-0.17410600
H	3.78458000	-4.10345900	1.54156100
H	6.26372000	-4.24697400	-1.98109700
H	0.46056800	-1.66482900	1.34867400
H	1.29140400	-3.17922000	1.70497500
C	1.99907100	-1.45536500	2.84312300
H	5.64817500	-5.10416400	0.25192900
H	2.20708700	-0.40726100	2.62517700
H	1.19362900	-1.48559200	3.59000100
C	3.23825800	-2.10663200	3.40727500
C	3.03910300	-3.42043200	4.11639300
C	4.43935500	-1.53627200	3.27590000
H	3.98898200	-3.86163200	4.42977500
H	2.41114100	-3.28972000	5.00763200
H	2.52006700	-4.14898500	3.48031900
H	5.33990200	-2.00596600	3.66248500
H	4.56349500	-0.58630800	2.76402200
C	2.01603000	1.85073300	-0.21882400
C	2.13767400	2.13937200	-1.66329900
H	1.50104900	2.68311800	0.27141000
C	3.23097700	1.48367700	0.62105900
C	3.17482900	1.97559700	-2.51216100
H	1.23127500	2.55290200	-2.10385400
H	3.74276700	0.61611000	0.20826500

H	2.87296600	1.17184600	1.60845700
C	4.23522000	2.63364700	0.86287000
H	3.00222900	2.26053000	-3.54947600
C	4.57524100	1.54360700	-2.16762600
H	3.77792900	3.34547100	1.56435300
H	5.11033400	2.21605300	1.38152000
C	4.70353000	3.43253000	-0.36227900
C	5.41336800	2.65139300	-1.47577600
H	5.09572200	1.24461700	-3.08467700
H	4.54825900	0.65226400	-1.54270900
H	3.84444500	3.95707300	-0.79367200
H	5.38929900	4.21431600	-0.00899100
H	6.33208600	2.19500500	-1.08218800
H	5.73251000	3.37665200	-2.23579800

c1

Ni	0.41236800	0.97049600	1.54743300
Fe	-3.41163400	-1.88494300	-0.97611200
P	-0.59019800	-1.62381300	0.90118700
P	-0.72758900	1.88470500	-0.05092400
O	0.28797100	-1.80754700	-0.31631900
C	-2.26550500	-1.09077000	0.52912100
C	-2.57670700	-0.07934400	-0.46129100
C	-3.99573400	0.05331800	-0.49964000
H	-4.54430000	0.70653700	-1.16140600
C	-4.56891000	-0.86512900	0.42490700
H	-5.62527000	-1.03116300	0.58361100
C	-3.51340300	-1.57232700	1.06079500
H	-3.63821600	-2.35725200	1.78936700
C	-1.58318700	0.71199000	-1.25959700
H	-0.78280200	0.02737000	-1.55458800
C	-2.18695900	1.38306000	-2.49151500
H	-2.95755400	2.10835900	-2.21830400
H	-2.64557300	0.63279700	-3.14315000
H	-1.42005800	1.90953300	-3.06393200
C	-3.52820300	-3.91754700	-1.36513700
H	-3.60878600	-4.68030000	-0.60388600
C	-2.31392100	-3.38007700	-1.89023800
H	-1.30987500	-3.62921300	-1.58118200
C	-2.65299200	-2.36745600	-2.83543400
H	-1.94927800	-1.75064300	-3.37643300
C	-4.07701600	-2.27774400	-2.89679700
H	-4.64599700	-1.57925100	-3.49466800
C	-4.61817100	-3.23572800	-1.98729100

H	-5.66774100	-3.38937200	-1.77739200
C	-2.05247000	3.08431900	0.34998000
C	-2.73989000	2.88245500	1.55613800
H	-2.42086800	2.08040300	2.21584200
C	-3.81507200	3.69967300	1.90529100
H	-4.34127600	3.53094300	2.84023700
C	-4.20459000	4.73862600	1.05824800
H	-5.03594100	5.38154300	1.33212700
C	-3.51849700	4.95563400	-0.13896900
H	-3.81587600	5.76685500	-0.79714800
C	-2.45126200	4.13101200	-0.49525500
H	-1.92180800	4.30703700	-1.42547600
C	0.47532900	2.78867500	-1.09779600
C	1.19750300	2.10860800	-2.09182600
H	0.95962900	1.07811700	-2.33435600
C	2.24378900	2.73829800	-2.76617500
H	2.79166600	2.19602600	-3.53111300
C	2.58964700	4.05423600	-2.45467700
H	3.40579500	4.54260700	-2.97842900
C	1.88466500	4.73565500	-1.46038100
H	2.15039000	5.75794000	-1.20705100
C	0.83989800	4.10729300	-0.78300200
H	0.30872600	4.64125400	-0.00152500
C	-0.58127300	-3.05385900	2.08760300
C	-1.29852700	-4.27486300	1.49425000
H	-2.36146500	-4.09337900	1.32787100
H	-1.20275100	-5.12009200	2.18521600
H	-0.84966800	-4.57086500	0.54221300
C	-1.19761700	-2.62460700	3.42885200
H	-0.70982300	-1.72753600	3.82518600
H	-1.05961400	-3.42673600	4.16234600
H	-2.26801500	-2.42145400	3.35860500
C	0.90866800	-3.38421100	2.29702100
H	1.39344300	-3.66403900	1.35923600
H	0.99737700	-4.22225600	2.99691300
H	1.45184700	-2.53495900	2.72293200
H	-0.06030700	-0.66180900	1.86639400
C	5.29202300	-0.71213000	-0.48347100
C	5.60376800	-1.86739600	-1.24707100
C	6.93673500	-2.13773900	-1.58192600
C	7.91567700	-1.24936300	-1.14586000
C	7.58689000	-0.10566600	-0.38933200
C	6.26886400	0.18415600	-0.04371600
C	3.47427700	-1.86620800	-0.99328300

H	7.18694900	-3.01794800	-2.16596900
H	8.95668200	-1.43774900	-1.39158600
H	8.37955800	0.56335600	-0.06751900
H	6.01652100	1.06384200	0.53998800
H	2.41525300	-2.09803200	-1.00298600
N	3.91605900	-0.73904400	-0.33946200
N	4.44075700	-2.56628600	-1.54789100
C	3.08215900	0.21502800	0.37791400
H	3.38413200	1.22459600	0.08739900
H	2.05846800	0.06786500	0.02520200
C	3.13388500	0.02691000	1.90120200
H	2.97201100	-1.03667600	2.11012700
H	4.14803900	0.25335100	2.26553700
C	1.88534000	0.40472100	4.09689200
H	1.10182200	0.99288200	4.58503000
H	1.60046300	-0.65234400	4.15784700
H	2.80584200	0.51888100	4.69061600
C	2.09979000	0.84885700	2.66344200
C	1.79286700	2.16934700	2.27679500
H	1.34248400	2.84892600	3.00079200
H	2.30606600	2.66273100	1.45370400

c1-2

Ni	0.32796600	1.15515600	-1.23885300
Fe	-2.63942600	-2.54185600	1.11251800
P	-1.02323500	-1.34334400	-1.65307500
P	-1.28550600	1.83614800	0.04747200
O	-2.32158700	-0.95711500	-2.31565100
C	-1.14293500	-1.53154700	0.13161100
C	-1.91836800	-0.62607200	0.95706100
C	-1.78990200	-1.06747000	2.30636200
H	-2.27277100	-0.61614600	3.16027700
C	-0.97949200	-2.23796900	2.33181500
H	-0.74710300	-2.83103300	3.20542500
C	-0.57912700	-2.53072600	0.99933700
H	0.01013400	-3.38187100	0.69823700
C	-2.64234600	0.59592500	0.47346900
H	-3.08407200	0.34974600	-0.49640400
C	-3.71442300	1.10323900	1.43545600
H	-3.29309700	1.37306200	2.40678900
H	-4.47281600	0.33138100	1.59977500
H	-4.21171600	1.98826100	1.03095800
C	-3.35723700	-4.39451000	0.51200000
H	-2.73901600	-5.21099300	0.16723800

C	-3.91314000	-3.35908400	-0.29882500
H	-3.77003400	-3.22378200	-1.36033800
C	-4.62679400	-2.46707300	0.55409800
H	-5.12810600	-1.56259000	0.24029500
C	-4.51137200	-2.94802200	1.89387800
H	-4.91241500	-2.47223200	2.77811700
C	-3.72558200	-4.13930100	1.86762000
H	-3.42785000	-4.72283400	2.72795000
C	-0.70608900	2.35041800	1.71271800
C	0.43362700	1.70845800	2.21922100
H	0.95383200	0.99093200	1.59338100
C	0.89714100	1.98752900	3.50480100
H	1.77976300	1.48015000	3.88327600
C	0.23071900	2.92403500	4.29693000
H	0.59339800	3.14979700	5.29540300
C	-0.90117800	3.57442800	3.80019100
H	-1.42088300	4.30551900	4.41273000
C	-1.37063500	3.28735400	2.51803300
H	-2.24986500	3.79820400	2.14039400
C	-2.17388900	3.29635600	-0.61084900
C	-3.34180700	3.15041300	-1.37446500
H	-3.78623300	2.17031800	-1.51282900
C	-3.93871900	4.26006600	-1.97398800
H	-4.84540800	4.13077300	-2.55772900
C	-3.37492900	5.52803500	-1.82676800
H	-3.84149000	6.39044500	-2.29335400
C	-2.20409400	5.68070500	-1.08117000
H	-1.75477100	6.66291300	-0.96621400
C	-1.60480300	4.57388500	-0.48194200
H	-0.69306100	4.70164000	0.09282200
C	-0.15704300	-2.78949700	-2.43882400
C	-0.93382400	-4.09116900	-2.20044100
H	-0.97198800	-4.35625800	-1.14212700
H	-0.44287000	-4.90985700	-2.73891800
H	-1.95886200	-4.01474900	-2.57216500
C	1.28486600	-2.89739500	-1.92311600
H	1.82270700	-1.95354100	-2.04689100
H	1.82200300	-3.65961600	-2.49824600
H	1.33401700	-3.18643800	-0.87159100
C	-0.13704400	-2.45675800	-3.94313300
H	-1.14901400	-2.35348800	-4.34141900
H	0.37297200	-3.26051800	-4.48531900
H	0.40140200	-1.52324300	-4.14104300
H	0.08475800	-0.41012500	-1.89744700

C	5.56062400	-0.25801800	0.47327600
C	6.24977300	-1.44911100	0.81761900
C	7.61265500	-1.39528000	1.13696800
C	8.24341000	-0.15552700	1.10258200
C	7.54157200	1.01867500	0.75937900
C	6.18699700	0.99011000	0.43758100
C	4.22309900	-2.01366100	0.42389400
H	8.14983900	-2.30040500	1.40199800
H	9.29978500	-0.08626000	1.34439200
H	8.07052700	1.96684700	0.74391300
H	5.64917800	1.89427400	0.17117000
H	3.30087000	-2.56250600	0.28562200
N	4.25591800	-0.65423200	0.22782300
N	5.37791000	-2.53131500	0.77612300
C	3.15280600	0.19726400	-0.19911200
H	2.22016800	-0.33968800	-0.00287000
H	3.14942700	1.08791800	0.43474700
C	1.94609500	1.48294500	-3.68027800
H	1.79469900	0.47725600	-4.09027800
H	2.84753600	1.89100300	-4.16474100
C	3.23474400	0.57503000	-1.68154500
H	3.25317400	-0.35218300	-2.26694500
H	4.20290200	1.06344500	-1.87060600
C	2.09592600	1.45962600	-2.17019600
C	1.66213400	2.57304200	-1.41385500
H	2.10784800	2.81859300	-0.45041900
H	1.19663900	3.41960800	-1.91911100
H	1.09641800	2.09976700	-3.98821000

c1-3

Ni	-0.41289000	-1.19726500	0.96289600
Fe	4.38254700	0.56636600	-0.91725900
P	2.32476400	-1.77035700	0.47211800
P	-0.05643000	0.91843600	0.67403800
O	2.71725400	-1.35613800	1.86889100
C	2.65179200	-0.52440100	-0.77958700
C	2.38046900	0.88327400	-0.56832600
C	2.76779700	1.56953100	-1.75764800
H	2.72065100	2.63770600	-1.90629200
C	3.28689300	0.62506700	-2.68714700
H	3.70438400	0.85277300	-3.65800500
C	3.21963900	-0.66446100	-2.09382700
H	3.57129900	-1.57917500	-2.54391200
C	1.75001000	1.49872900	0.64773400

H	2.18411500	1.02267100	1.53144100
C	1.93115500	3.01442400	0.71096500
H	1.44134600	3.51386900	-0.12923000
H	2.99562800	3.26828500	0.67868100
H	1.51111400	3.42181900	1.63238600
C	6.26023000	-0.28479600	-0.68878500
H	6.55150000	-1.24300200	-1.09446300
C	5.65839900	-0.06134900	0.58686400
H	5.37580400	-0.81346000	1.30846600
C	5.39529600	1.33488100	0.71028400
H	4.90920000	1.81320500	1.54894700
C	5.83421000	1.97679700	-0.48758600
H	5.73903100	3.02909100	-0.71739400
C	6.36805700	0.97501800	-1.35313600
H	6.74864400	1.13631500	-2.35228200
C	-0.66800400	1.61059600	-0.91264900
C	-0.65143000	0.74205000	-2.01662100
H	-0.34107600	-0.28886800	-1.87112500
C	-1.02223800	1.19059000	-3.28376200
H	-1.00450100	0.50579200	-4.12623400
C	-1.43242000	2.51352600	-3.46214700
H	-1.74046400	2.86120200	-4.44340700
C	-1.45285400	3.38627400	-2.37225400
H	-1.77220700	4.41548500	-2.50600100
C	-1.06245200	2.94254100	-1.10739400
H	-1.07468000	3.63329400	-0.27171500
C	-0.81736000	1.91392800	2.01061900
C	-0.15148500	2.00037200	3.24464300
H	0.84180800	1.57651100	3.35718500
C	-0.76396800	2.60402700	4.34143700
H	-0.23265600	2.66412900	5.28669500
C	-2.05766600	3.11891300	4.22983500
H	-2.53636100	3.58394900	5.08624100
C	-2.73322400	3.02474400	3.01291700
H	-3.74219200	3.41481200	2.91633900
C	-2.11933000	2.42625800	1.91150000
H	-2.66291400	2.35601900	0.97660800
C	2.92778500	-3.44846100	-0.04675400
C	4.44815500	-3.45269900	-0.25906200
H	4.74946500	-2.81702800	-1.09385900
H	4.78360500	-4.47412200	-0.47250100
H	4.97324700	-3.11035700	0.63717100
C	2.17607200	-3.90697200	-1.30632400
H	1.09170500	-3.88904000	-1.15177200

H	2.45869800	-4.93900400	-1.54234300
H	2.40209700	-3.29326000	-2.18093900
C	2.55957200	-4.37266800	1.13038800
H	3.06696000	-4.06885800	2.04892900
H	2.85471000	-5.40021200	0.89037900
H	1.48065000	-4.36659400	1.32032700
H	0.91229400	-2.09308300	0.29073200
C	-5.81949000	-0.93730700	-0.94798300
C	-6.48855100	0.07968500	-1.67656900
C	-7.87970200	0.02308300	-1.83071700
C	-8.55905000	-1.04524000	-1.25311400
C	-7.87741100	-2.04766900	-0.53243100
C	-6.49523700	-2.01251900	-0.36555900
C	-4.40487400	0.57700800	-1.71584200
H	-8.40132500	0.79540400	-2.38714800
H	-9.63796300	-1.11219700	-1.35704500
H	-8.44369400	-2.86517100	-0.09626200
H	-5.97301700	-2.78407800	0.19103400
H	-3.44931800	1.04986900	-1.89828800
N	-4.47880500	-0.59135600	-0.99407600
N	-5.56948800	1.01229100	-2.14290100
C	-3.37652200	-1.29217800	-0.34671500
H	-3.46836200	-2.35748200	-0.57864200
H	-2.44592100	-0.93693800	-0.79484200
C	-3.34370500	-1.05254300	1.16403200
H	-3.37729600	0.02799600	1.34090200
H	-4.26332400	-1.45930100	1.61279800
C	-2.06479200	-1.20356700	3.34134400
H	-1.15052600	-1.56633700	3.81957800
H	-2.09540500	-0.11591900	3.44934300
H	-2.92142200	-1.61084600	3.90093400
C	-2.13539400	-1.62157600	1.88547200
C	-1.47254100	-2.79815500	1.46742800
H	-0.93924000	-3.39759900	2.20493700
H	-1.79938900	-3.34752200	0.58551200

c1-4

Ni	0.53331000	-0.32552700	1.22308700
Fe	-4.43849300	-0.47236800	-0.68743700
P	-1.49548000	-2.02754300	0.04066000
P	-0.13867000	1.35885500	0.02764100
O	-1.11451000	-2.07778600	-1.41865900
C	-2.74680400	-0.79726500	0.42792300
C	-2.72511100	0.53035700	-0.15123500

C	-3.85866400	1.23206100	0.35440800
H	-4.14075800	2.23923600	0.08665700
C	-4.59036400	0.36345700	1.21289300
H	-5.52449400	0.59541900	1.70515100
C	-3.91320400	-0.88564700	1.26397800
H	-4.24430700	-1.75346700	1.81144800
C	-1.66335800	1.07580300	-1.06032500
H	-1.36245900	0.26755100	-1.73286800
C	-2.11885700	2.29157200	-1.86519400
H	-2.39389100	3.12702400	-1.21711000
H	-2.99314200	2.03246300	-2.47021000
H	-1.32964900	2.63530500	-2.53737100
C	-5.66357100	-1.98550800	-1.39882200
H	-5.96085100	-2.85133900	-0.82436200
C	-4.49144900	-1.87471000	-2.20638700
H	-3.72483900	-2.62406300	-2.33490200
C	-4.45340500	-0.55642900	-2.74957900
H	-3.66445400	-0.15420300	-3.36884600
C	-5.60271100	0.14939300	-2.27989400
H	-5.84085500	1.18434000	-2.48321300
C	-6.35024000	-0.73380400	-1.44351400
H	-7.25454200	-0.48522600	-0.90532900
C	-0.69487100	2.76692600	1.06741300
C	-1.18926200	2.44883400	2.34161300
H	-1.15401200	1.41534400	2.67488700
C	-1.71097800	3.44133800	3.17055200
H	-2.09034900	3.17971400	4.15394900
C	-1.73452200	4.76880400	2.73900800
H	-2.13247800	5.54502000	3.38601200
C	-1.23921700	5.09765200	1.47540500
H	-1.25320500	6.12954800	1.13682600
C	-0.72724200	4.10328500	0.64122500
H	-0.34552700	4.37025800	-0.33806300
C	1.09118800	2.07384500	-1.13210900
C	1.18950500	1.58820100	-2.44592200
H	0.50631700	0.82159300	-2.79694500
C	2.16356200	2.08256000	-3.31473200
H	2.21921100	1.70287900	-4.33053200
C	3.06590700	3.05543300	-2.87951700
H	3.82632400	3.43578900	-3.55426400
C	2.99721500	3.52017400	-1.56463800
H	3.70587100	4.26358400	-1.21215500
C	2.02040300	3.03203000	-0.69662500
H	1.97385300	3.40532700	0.32102900

C	-1.88974500	-3.67248300	0.80664200
C	-3.20418100	-4.24418500	0.25638400
H	-4.06492200	-3.62209000	0.51005600
H	-3.37089300	-5.24155400	0.67934200
H	-3.16632800	-4.34677400	-0.83170100
C	-1.92244800	-3.54449900	2.33798100
H	-0.99862600	-3.09819900	2.72055700
H	-2.01873300	-4.54177100	2.78197100
H	-2.75984100	-2.94180400	2.69555100
C	-0.71396700	-4.58144800	0.39793100
H	-0.63615300	-4.66839300	-0.68837900
H	-0.86504900	-5.58146000	0.81921600
H	0.23937300	-4.19764000	0.77795900
H	-0.37469400	-1.74510700	0.92938000
C	5.88754800	-1.22316100	-0.25469300
C	6.78934600	-0.78505400	-1.25852500
C	8.12676900	-1.19909700	-1.21826600
C	8.52253200	-2.03408600	-0.17740400
C	7.61243100	-2.45825600	0.81260000
C	6.27766900	-2.06024200	0.79319300
C	4.88825900	0.08276400	-1.72936100
H	8.82506900	-0.87189700	-1.98217100
H	9.55434200	-2.36844400	-0.12287800
H	7.96057700	-3.10901700	1.60922100
H	5.57893000	-2.38572700	1.55731000
H	4.08077500	0.64094500	-2.18296000
N	4.67076900	-0.65117900	-0.58916100
N	6.12730500	0.03330400	-2.16644900
C	3.42663900	-0.76353000	0.16188600
H	3.31512500	-1.80830600	0.46146600
H	2.59645900	-0.52948400	-0.51035600
C	3.39857700	0.17080700	1.37577300
H	3.45127700	1.20284300	1.01082600
H	4.31297400	0.00907900	1.96699700
C	2.02785800	1.15196700	3.26998400
H	1.15804400	1.00930500	3.91682800
H	1.91510700	2.11744800	2.76556900
H	2.91614500	1.22534200	3.91663000
C	2.18441400	0.01585500	2.27945500
C	1.64368100	-1.25869400	2.57232800
H	1.08885600	-1.39681200	3.50084300
H	2.09439500	-2.16861700	2.17891100

Ni	0.89746800	0.56214600	0.13161000
P	-0.74817700	1.83620900	-0.02494500
N	2.63464500	-0.20950600	0.29786400
C	-2.37390300	1.14229700	-0.74293000
C	-1.37505000	2.63079200	1.51522600
C	-0.38386200	3.24626400	-1.15328600
C	3.19595400	-0.80883400	1.42708800
C	3.57812700	-0.24393200	-0.63248400
C	-2.79442200	0.01402100	0.15141800
H	-2.07490200	0.71382500	-1.70539600
C	-3.47669200	2.17600600	-0.97067200
C	-1.21286100	1.91075400	2.70818100
C	-2.06352300	3.85290800	1.55401600
C	-0.57384300	3.11196400	-2.53825500
C	0.22913300	4.41438100	-0.67263700
C	4.51499800	-1.21419000	1.12451500
C	2.65352800	-1.04477400	2.69393400
H	3.47822600	0.14213500	-1.63538500
N	4.72652200	-0.84076200	-0.19583200
C	-2.24193800	-1.32166500	0.14257500
C	-3.74902000	0.07689700	1.21015800
H	-3.79682300	2.63591300	-0.03302400
H	-4.35022300	1.69816900	-1.42384400
H	-3.13699800	2.97360400	-1.63504400
H	-0.67441000	0.96773100	2.67807100
C	-1.73402600	2.39139200	3.90923500
C	-2.57431000	4.34108100	2.75750500
H	-2.19500600	4.42869500	0.64443100
H	-1.02122800	2.20866800	-2.94142500
C	-0.18497000	4.12620300	-3.41345200
C	0.61679600	5.42814800	-1.54818700
H	0.40482200	4.52993800	0.39217300
C	5.32700300	-1.86102800	2.05968000
C	3.45717100	-1.68907700	3.62854700
H	1.64085300	-0.72973000	2.92058600
C	5.96571000	-0.99214900	-0.94824300
P	-1.00170800	-1.82487900	-1.07260100
C	-2.88039100	-2.05848600	1.19889100
H	-4.35385900	0.93607200	1.45932800
C	-3.80436300	-1.19400900	1.85060700
H	-1.60316100	1.81891400	4.82312200
C	-2.41448900	3.61024700	3.93664900
H	-3.10026600	5.29156000	2.77325200
H	-0.34664000	4.00480600	-4.48088500

C	0.40868200	5.29020600	-2.92220600
H	1.08399800	6.32697600	-1.15538700
C	4.77227500	-2.09190700	3.31534900
H	6.33963200	-2.16952800	1.82244600
H	3.06710700	-1.88690400	4.62200700
H	6.33846500	-2.00774500	-0.78632900
H	5.72109400	-0.89683000	-2.00871200
C	7.01202500	0.04507400	-0.53665600
O	-1.47191300	-1.81669500	-2.51320600
C	-0.22099300	-3.42461500	-0.54791200
H	0.05015700	-0.86474600	-0.79088700
H	-2.72472200	-3.09861800	1.43800900
H	-4.46592300	-1.46902200	2.66050000
H	-2.81426400	3.99132400	4.87197100
H	0.70998800	6.08037600	-3.60361500
H	5.36750800	-2.59193400	4.07311600
H	6.59774800	1.04904300	-0.70224600
H	7.17776700	-0.02269800	0.54681700
C	8.34361700	-0.06172600	-1.24311500
C	-1.20440800	-4.58718200	-0.74695800
C	0.28025600	-3.33018400	0.90026300
C	0.98398100	-3.60063800	-1.49257200
C	9.36147300	0.96173800	-0.81127500
C	8.61706400	-0.97841400	-2.17726500
H	-2.08202400	-4.50207900	-0.10107000
H	-0.70907000	-5.53794900	-0.51585500
H	-1.55293300	-4.62933200	-1.78300300
H	0.88365200	-2.43092900	1.05141300
H	0.91281400	-4.19624700	1.12948000
H	-0.53536500	-3.31127100	1.62560800
H	0.67067700	-3.61239900	-2.54003300
H	1.49197100	-4.54677400	-1.27210400
H	1.70853200	-2.79015500	-1.36072900
H	10.30520200	0.84629900	-1.35054000
H	8.99088800	1.98056300	-0.98208400
H	9.56813200	0.88150300	0.26369200
H	9.59104200	-1.01284800	-2.65740100
H	7.89840100	-1.72299400	-2.50399100
Fe	-4.27171600	-1.40019000	-0.16116000
C	-6.18201600	-2.18337500	-0.31818800
C	-5.23678000	-3.06264200	-0.93200600
C	-6.10788100	-0.92315400	-0.98569300
H	-6.81471200	-2.41845600	0.52678000
H	-5.02776500	-4.07949900	-0.62932200

C	-4.57752000	-2.34647800	-1.97560800
C	-5.11495800	-1.02551700	-2.00787300
H	-6.67222500	-0.03629200	-0.73177100
H	-3.74153400	-2.68785600	-2.56812200
H	-4.78714200	-0.23134400	-2.66307900

c2-2

Ni	0.66866800	1.23253300	-0.02008800
P	-1.32350300	1.85516900	0.08108800
N	2.55697200	1.02233900	-0.11558800
C	-2.68566800	0.60661000	-0.37881900
C	-1.93343300	2.43751000	1.72020500
C	-1.66833800	3.25729900	-1.06229500
C	3.25246700	0.73386400	-1.29232400
C	3.47375800	1.08095700	0.83832000
C	-2.47840900	-0.57631900	0.51754600
H	-2.42967700	0.29651700	-1.39636200
C	-4.11206000	1.15240700	-0.35583600
C	-1.32598200	1.88061000	2.85557600
C	-3.00344200	3.32799200	1.89672800
C	-2.00691800	3.00758300	-2.40188200
C	-1.45846000	4.58623600	-0.66142800
C	4.62689400	0.60702500	-0.99408200
C	2.78777300	0.57315200	-2.60138200
H	3.27921200	1.29568800	1.87785400
N	4.73526700	0.84064100	0.37092100
C	-1.47651500	-1.60209000	0.33859700
C	-3.15440100	-0.84434500	1.74478300
H	-4.41049700	1.46371300	0.64766100
H	-4.81298300	0.38125100	-0.68951400
H	-4.21286100	2.01542000	-1.01853900
H	-0.49099500	1.19940700	2.71536000
C	-1.78288300	2.19323200	4.13592700
C	-3.45309500	3.65153700	3.17767500
H	-3.48133900	3.77733000	1.03303700
H	-2.14812100	1.98826900	-2.74781700
C	-2.15463900	4.05837200	-3.30753600
C	-1.60694500	5.63586000	-1.56734400
H	-1.17763500	4.80045400	0.36481400
C	5.57498000	0.31069000	-1.97687700
C	3.72844400	0.27807500	-3.58341800
H	1.73078800	0.67467300	-2.82304900
C	5.95448800	0.75666800	1.16454300
P	-0.41716400	-1.63230800	-1.12548800

C	-1.55941000	-2.48604600	1.46904400
H	-3.97868300	-0.27328100	2.14563100
C	-2.59452500	-2.01761200	2.32613400
H	-1.30477500	1.74900500	5.00443000
C	-2.84762200	3.08153200	4.29958800
H	-4.27900200	4.34684900	3.29906200
H	-2.42192700	3.84408400	-4.33847200
C	-1.95918600	5.37694800	-2.89354000
H	-1.44516700	6.65791300	-1.23614200
C	5.09868100	0.14802300	-3.27515100
H	6.63040000	0.21397200	-1.74517700
H	3.40200800	0.14259300	-4.60955200
H	6.74697300	1.28054100	0.62263400
H	5.78122900	1.29755800	2.09769400
C	6.35182900	-0.69422600	1.44139800
O	-1.17541500	-1.57593700	-2.43553600
C	0.78362500	-3.04309800	-1.00004100
H	0.41017500	-0.46691100	-0.88914700
H	-0.97551100	-3.37819300	1.63023700
H	-2.92753600	-2.49735000	3.23622900
H	-3.20074100	3.33277200	5.29567000
H	-2.07489800	6.19471200	-3.59877600
H	5.80028000	-0.08280400	-4.07073000
H	5.53447900	-1.18676000	1.98607900
H	6.42695800	-1.23263300	0.48708100
C	7.63940600	-0.87921500	2.21052300
C	0.04173100	-4.38855600	-0.98799100
C	1.67282800	-2.86348000	0.24076800
C	1.65600600	-2.96014400	-2.26695800
C	8.01062500	-2.31659200	2.46758900
C	8.40162600	0.13360900	2.63588200
H	-0.60919400	-4.50151700	-0.11927500
H	0.76927400	-5.20919000	-0.97516800
H	-0.57318200	-4.50196600	-1.88551700
H	2.16136600	-1.88429100	0.23408100
H	2.45644200	-3.63077800	0.24473700
H	1.11588500	-2.95051600	1.17611900
H	1.04731800	-3.03031400	-3.17210500
H	2.37706200	-3.78610800	-2.26832300
H	2.21848200	-2.02331400	-2.30899000
H	8.94577700	-2.39916600	3.02754200
H	7.22424400	-2.83019300	3.03544000
H	8.12529600	-2.86753300	1.52524300
H	9.32058100	-0.05185000	3.18501800

H	8.15240900	1.17565200	2.46224700
Fe	-3.33891900	-2.45355500	0.43757000
C	-4.82540400	-3.88132900	0.63925800
C	-3.76058400	-4.38971600	-0.16690800
C	-5.34393600	-2.71539900	-0.00163100
H	-5.15372600	-4.28426200	1.58753300
H	-3.14181900	-5.24551300	0.06450000
C	-3.62064700	-3.53733500	-1.30301300
C	-4.59782000	-2.50374100	-1.20088200
H	-6.13429800	-2.08246400	0.37751900
H	-2.86546000	-3.60156500	-2.07214000
H	-4.71878400	-1.68398700	-1.89452800

c3

Ni	0.50491000	-0.26902400	-0.59249200
Fe	-4.90157500	-1.70290900	0.47071600
P	-3.01590000	0.21516500	-1.68477000
P	-0.60047100	0.28442300	1.25626500
O	-3.56129500	1.49625200	-1.08522300
C	-3.22881700	-1.22519100	-0.62053600
C	-2.92804500	-1.17781900	0.79369600
C	-3.16624300	-2.47800200	1.32591000
H	-3.07416100	-2.75410900	2.36634300
C	-3.61752400	-3.32631100	0.27373100
H	-3.92490500	-4.35787400	0.37571500
C	-3.65692600	-2.56248200	-0.92540200
H	-3.99621300	-2.92412400	-1.88300600
C	-2.46278200	0.03462000	1.53997100
H	-2.91390400	0.89485200	1.04290700
C	-2.86967700	0.05158800	3.01315900
H	-2.42738700	-0.77459000	3.57420500
H	-3.95620600	-0.02499800	3.10116600
H	-2.55454500	0.98527800	3.48685500
C	-6.40941900	-0.37715800	-0.03411900
H	-6.27937300	0.40009800	-0.77134000
C	-6.09153100	-0.25635400	1.35006100
H	-5.70288500	0.63172100	1.82749600
C	-6.31834200	-1.52323500	1.96878500
H	-6.13203900	-1.76769900	3.00541800
C	-6.77874700	-2.42757800	0.96426500
H	-7.00401700	-3.47527500	1.10826000
C	-6.83528800	-1.71835500	-0.27474500
H	-7.11536900	-2.13551100	-1.23186200
C	0.14828900	-0.60735100	2.68718400

C	0.67893100	-1.87989200	2.42007600
H	0.62321700	-2.26301400	1.40772100
C	1.27290700	-2.63674300	3.43064600
H	1.68083400	-3.61711700	3.20170000
C	1.34986200	-2.12918200	4.72834400
H	1.82215200	-2.70984000	5.51525500
C	0.81220800	-0.87162500	5.01119500
H	0.85888000	-0.47472800	6.02127900
C	0.20937000	-0.12016200	4.00225300
H	-0.20888000	0.85019700	4.24171700
C	-0.45818900	2.08359300	1.65510600
C	-1.33302800	2.97700300	1.00770200
H	-2.12209100	2.60643400	0.35735000
C	-1.18705900	4.35526300	1.16773200
H	-1.88170700	5.02526900	0.66842100
C	-0.15848000	4.87321000	1.95833800
H	-0.04834600	5.94678600	2.08113000
C	0.73215400	3.99748800	2.57902400
H	1.55042300	4.38180800	3.18126600
C	0.58489900	2.61771800	2.42709700
H	1.30028300	1.96157500	2.90509600
C	-3.62485700	-0.11224200	-3.40919400
C	-5.14310400	-0.34237300	-3.40404900
H	-5.41884600	-1.22941000	-2.82914100
H	-5.49495100	-0.48134100	-4.43301000
H	-5.67218400	0.51722400	-2.98401400
C	-2.89407300	-1.29727100	-4.05893600
H	-1.80970700	-1.16637000	-4.04707700
H	-3.20424000	-1.37708900	-5.10748300
H	-3.11965900	-2.24926300	-3.57644300
C	-3.29787000	1.17610900	-4.18986100
H	-3.78117400	2.04712000	-3.74070100
H	-3.64787000	1.07686300	-5.22349100
H	-2.21814900	1.36328900	-4.22053300
H	-1.60707800	0.25261600	-1.85925300
C	4.91620200	-4.02098300	-0.78048300
C	6.28513100	-3.89657800	-0.42919100
C	7.17799800	-4.93039600	-0.73980900
C	6.67793200	-6.05320300	-1.39240600
C	5.31397900	-6.15850800	-1.73558400
C	4.40756500	-5.14416000	-1.43715400
C	5.32005000	-2.10707600	0.24415200
H	8.22716500	-4.84665600	-0.47423600
H	7.34964500	-6.86806600	-1.64578900

H	4.96310300	-7.05017800	-2.24661300
H	3.35914500	-5.22416800	-1.70639600
H	5.10125800	-1.13660900	0.67073100
N	4.32017100	-2.85613800	-0.32781000
N	6.50196300	-2.68259400	0.21175100
C	2.92039400	-2.47786000	-0.48200200
H	2.31260400	-3.36305900	-0.27648900
H	2.68669500	-1.74020000	0.28603600
C	2.61218300	-1.90286500	-1.86444200
H	3.30289800	-1.06792300	-2.04179500
H	2.85964200	-2.66369400	-2.62320800
C	0.99634600	-0.76046600	-3.41365900
H	0.00223700	-0.31840100	-3.52160200
H	1.72950700	0.04116700	-3.57051400
H	1.13092700	-1.47802900	-4.23991500
C	1.18316300	-1.41593000	-2.05734000
C	0.07609100	-2.02660600	-1.39496300
H	-0.89335500	-2.04818000	-1.88650300
H	0.22481400	-2.87915400	-0.73263900
C	3.32039500	2.84090700	-0.05195400
C	2.76232500	1.57838000	0.25110500
C	3.21832000	0.84890600	1.35398300
C	4.23580100	1.40617900	2.12261000
C	4.78860900	2.66503100	1.80736600
C	4.33884800	3.40718500	0.71857800
C	1.69942900	2.34028600	-1.47350100
H	2.75968600	-0.09596900	1.61815100
H	4.60509800	0.86682600	2.98913700
H	5.58076400	3.06673900	2.43132800
H	4.75854600	4.38006800	0.48613500
H	1.01465600	2.45179000	-2.30083900
N	2.62611000	3.29737700	-1.16370900
N	1.74636600	1.30085600	-0.66054800
C	2.72578300	4.62549300	-1.75669200
H	3.78576500	4.87982500	-1.84388900
H	2.31673100	4.57024200	-2.76846200
C	1.97457700	5.66069500	-0.91829300
H	0.92563000	5.34868300	-0.83395600
H	2.35682200	5.63003100	0.11034000
C	1.26051800	8.06626400	-0.57851400
H	1.32832800	9.08232000	-0.97597200
H	0.19988500	7.78944000	-0.52286100
H	1.63537300	8.07586500	0.45310400
C	2.02952500	7.08234500	-1.42201300

C	2.69376300	7.45955600	-2.51937700
H	2.70065700	8.49780800	-2.83953700
H	3.25173300	6.76549000	-3.14009100

c3-2

Ni	-0.31587500	0.12470000	-1.12085800
Fe	5.29421200	0.21687300	0.44820800
P	2.86804600	-1.71034100	-0.95190600
P	0.54141400	0.91049800	0.78456600
O	2.83236300	-2.55539000	0.30581600
C	3.63429500	-0.09756700	-0.71535700
C	3.29639400	0.75735500	0.40172300
C	4.11245700	1.92380400	0.30432200
H	4.12044900	2.74178800	1.00819600
C	4.94569800	1.80736800	-0.84450300
H	5.70163600	2.51464100	-1.15625800
C	4.65508900	0.56776800	-1.47754800
H	5.15550800	0.18122500	-2.35101900
C	2.26754800	0.47621100	1.45854300
H	2.23901900	-0.60785900	1.59882100
C	2.58046900	1.16981600	2.78797800
H	2.58554000	2.25711400	2.68273500
H	3.56442900	0.86261500	3.15168200
H	1.83921100	0.91796500	3.54843300
C	6.98541400	-0.97932300	0.36899500
H	7.43118200	-1.34605300	-0.54471900
C	5.95862000	-1.62492200	1.12187400
H	5.45100300	-2.54392500	0.87074700
C	5.62858100	-0.78573500	2.22562100
H	4.85987000	-0.98906200	2.95668000
C	6.44821700	0.38188500	2.15721900
H	6.40857900	1.22859000	2.82860200
C	7.28771600	0.26201000	1.00833600
H	7.99698100	1.00056600	0.66084300
C	0.64612300	2.75024800	0.84396600
C	1.23346700	3.38488800	-0.26412900
H	1.55695000	2.78447000	-1.10641700
C	1.39446000	4.77016200	-0.28997300
H	1.85463000	5.24290000	-1.15312500
C	0.95613400	5.54595900	0.78553300
H	1.06764900	6.62605500	0.76175900
C	0.37186200	4.92531500	1.89019500
H	0.02845200	5.52100400	2.73104300
C	0.22560500	3.53758900	1.92433300

H	-0.22184300	3.07012000	2.79357700
C	-0.54452700	0.44635900	2.20015400
C	-0.23515700	-0.64401000	3.02874000
H	0.71195300	-1.16055000	2.92773900
C	-1.14865200	-1.10537500	3.97643000
H	-0.88891300	-1.95681000	4.59780200
C	-2.39352600	-0.49040900	4.11044800
H	-3.10601500	-0.85248700	4.84619000
C	-2.71654700	0.58903500	3.28632800
H	-3.68359200	1.07610700	3.37745900
C	-1.80604800	1.05054900	2.33525200
H	-2.08587700	1.88124700	1.69540600
C	3.59198800	-2.59660400	-2.41482800
C	5.07195300	-2.92262400	-2.16355500
H	5.68150200	-2.02089200	-2.07710600
H	5.46062000	-3.51543700	-2.99985800
H	5.19870400	-3.51022200	-1.25031700
C	3.41967700	-1.79262200	-3.71353800
H	2.37448300	-1.53815100	-3.90233900
H	3.76793500	-2.39871200	-4.55832900
H	3.99426600	-0.86453200	-3.71699400
C	2.78871800	-3.90946700	-2.51142000
H	2.87442800	-4.49346900	-1.59187200
H	3.17100600	-4.51087000	-3.34392100
H	1.72542600	-3.72196400	-2.69566800
H	1.56716800	-1.36136900	-1.40207000
C	-4.11519900	2.10732900	-1.70684900
C	-4.21590500	2.57686200	-0.37002300
C	-5.40422200	2.38723500	0.34752700
C	-6.45628600	1.73167200	-0.28787200
C	-6.34043500	1.27255400	-1.61667100
C	-5.17005300	1.45414000	-2.35148100
C	-2.22575700	3.03417000	-1.03089400
H	-5.49020800	2.74323600	1.36939000
H	-7.38326600	1.55633000	0.24830300
H	-7.18334700	0.76562800	-2.07616000
H	-5.08267000	1.09385800	-3.37094200
H	-1.19629200	3.35714600	-1.07692800
N	-2.82102900	2.41258400	-2.09934200
N	-3.01344800	3.15300400	0.01849200
C	-2.22884700	2.13508000	-3.40369100
H	-2.93834200	2.48762400	-4.15953300
H	-1.33361200	2.75310400	-3.49282700
C	-1.90851100	0.65901900	-3.65777600

H	-2.77164800	0.05535000	-3.34759000
H	-1.86171600	0.54792800	-4.75497200
C	-0.45171500	-1.35939300	-3.58331900
H	0.42163900	-1.84725200	-3.14820900
H	-1.32134500	-1.97995600	-3.33209200
H	-0.33920100	-1.39099700	-4.68095700
C	-0.63102900	0.06166000	-3.07358000
C	0.50403800	0.86756200	-2.74855800
H	1.50943300	0.47762700	-2.90440700
H	0.45424300	1.95045000	-2.85827800
C	-2.75937000	-2.55521600	1.07249600
C	-1.52981700	-2.23472200	0.44809000
C	-0.38374900	-2.98974700	0.71228300
C	-0.50888900	-4.05786800	1.59537500
C	-1.73907300	-4.37346100	2.20666100
C	-2.88827300	-3.62704900	1.95668400
C	-2.97633400	-0.75784100	-0.19871300
H	0.58033100	-2.74109300	0.28516100
H	0.36867300	-4.65433900	1.82492500
H	-1.79252800	-5.21518500	2.89067500
H	-3.83319500	-3.86367300	2.43463500
H	-3.44730100	0.09388600	-0.65999100
N	-3.65831900	-1.58934900	0.64102500
N	-1.70697900	-1.09490000	-0.33648900
C	-5.05517000	-1.44046300	1.02585400
H	-5.16260100	-1.82579000	2.04253500
H	-5.27614500	-0.37185600	1.05033100
C	-6.00055600	-2.15458500	0.06068800
H	-5.82455100	-1.76477700	-0.95099400
H	-5.73782200	-3.22044300	0.01552500
C	-8.38564800	-2.72595900	-0.58849100
H	-9.43738900	-2.60260700	-0.31700700
H	-8.24776400	-2.34392400	-1.60837600
H	-8.16408900	-3.80023600	-0.62606500
C	-7.47133300	-2.01836500	0.37752600
C	-7.94677200	-1.32078400	1.41493000
H	-9.01563800	-1.24980200	1.59728300
H	-7.30612300	-0.80013600	2.11922200

c3-3

Ni	0.58555200	-0.51616500	-1.06525600
Fe	-5.11127400	-1.30449500	-0.29671600
P	-3.03323900	1.42687300	-0.16740100
P	-0.40105600	-1.41507300	0.69392200

O	-3.22295000	1.57200000	1.32780700
C	-3.44716800	-0.21078300	-0.80069400
C	-3.05017900	-1.42332700	-0.11996100
C	-3.52816500	-2.52231700	-0.89078400
H	-3.42764400	-3.56433600	-0.62356600
C	-4.21483800	-2.01573500	-2.03182800
H	-4.72740200	-2.60464800	-2.77986500
C	-4.16604100	-0.59551500	-1.98403500
H	-4.62657800	0.06760100	-2.69915600
C	-2.24492000	-1.48934600	1.14049700
H	-2.42582900	-0.55835100	1.67967100
C	-2.60547500	-2.65844600	2.05741500
H	-2.43990300	-3.62641700	1.57914900
H	-3.65770100	-2.59878000	2.34358300
H	-2.00293000	-2.62918800	2.96938600
C	-7.06408600	-0.60441000	-0.29698300
H	-7.49310900	0.00332300	-1.08140200
C	-6.36946500	-0.12468500	0.85363800
H	-6.15953500	0.90527100	1.09639000
C	-5.92860300	-1.25144100	1.60625100
H	-5.34605900	-1.20536300	2.51431000
C	-6.34715800	-2.43214400	0.92131600
H	-6.13227400	-3.44984500	1.21660900
C	-7.04952100	-2.03235700	-0.25595300
H	-7.46035200	-2.69441200	-1.00564400
C	0.07212300	-3.19581900	0.62237200
C	0.19054800	-3.75398900	-0.66176900
H	0.01855800	-3.11619200	-1.52470600
C	0.53217600	-5.09677700	-0.82953800
H	0.61489000	-5.51235000	-1.82993800
C	0.77088100	-5.90079300	0.28646000
H	1.04385800	-6.94442900	0.15940000
C	0.65574600	-5.35792700	1.56807300
H	0.83618800	-5.97952600	2.44052800
C	0.30303000	-4.01829800	1.73541300
H	0.20950900	-3.61218600	2.73624500
C	0.30950900	-0.76785400	2.26584000
C	-0.26460500	0.37648300	2.84910800
H	-1.19009500	0.79506600	2.46158300
C	0.35937400	1.01470200	3.92080000
H	-0.09743600	1.90066100	4.35212300
C	1.56601200	0.53051100	4.42814400
H	2.05417400	1.03567200	5.25616700
C	2.14786100	-0.59835000	3.85160900

H	3.09717800	-0.97299600	4.22332800
C	1.52976500	-1.23684300	2.77719500
H	2.01237900	-2.09409400	2.32292500
C	-3.83902500	2.76942800	-1.16966200
C	-5.36915400	2.65753700	-1.11013400
H	-5.73285700	1.71950700	-1.53371300
H	-5.81494100	3.48306800	-1.67694100
H	-5.72889200	2.73042700	-0.08071800
C	-3.34226500	2.74569600	-2.62345300
H	-2.25494300	2.84770400	-2.67888600
H	-3.77733100	3.59286200	-3.16621700
H	-3.61821800	1.83383700	-3.15584100
C	-3.39795800	4.08814100	-0.50427300
H	-3.70642000	4.12828900	0.54311700
H	-3.85431400	4.93160000	-1.03458800
H	-2.31215200	4.22239500	-0.54072600
H	-1.67999600	1.56405200	-0.54841900
C	1.21900700	4.27599600	-0.13851900
C	2.18780400	5.30400000	-0.01878800
C	2.20911400	6.10583500	1.12982500
C	1.26439000	5.85571600	2.12185700
C	0.30837600	4.82778300	1.98535200
C	0.26657100	4.01909200	0.85205100
C	2.56743000	4.32281800	-1.88578500
H	2.94878000	6.89328800	1.23494900
H	1.26066900	6.46331400	3.02193800
H	-0.41321900	4.66045300	2.77901700
H	-0.46614300	3.22482400	0.76074500
H	2.98149000	4.02793400	-2.83977100
N	1.49485400	3.65554900	-1.34554200
N	3.01477000	5.30684800	-1.13557500
C	0.74385700	2.52635900	-1.88240700
H	0.39192500	1.94771100	-1.02355800
H	-0.14122400	2.89982000	-2.40804700
C	1.55237200	1.59057800	-2.78165200
H	1.66254400	2.03819100	-3.78371600
H	2.56578000	1.49940400	-2.37138900
C	1.75445500	-0.74087100	-3.74938200
H	1.32554500	-1.74855800	-3.76167500
H	1.79905400	-0.39080800	-4.79383100
H	2.79207100	-0.82200800	-3.39982000
C	0.94335000	0.19543000	-2.87723200
C	-0.44921300	-0.04439900	-2.67846600
H	-0.90583700	-0.91265800	-3.15480600

H	-1.14654200	0.77676400	-2.53860200
C	4.44226900	-0.17295400	0.67531300
C	3.11888200	0.26352800	0.44446100
C	2.65328500	1.45035500	1.01236200
C	3.53878900	2.19009500	1.78497900
C	4.86277100	1.75322300	1.99962700
C	5.33928700	0.56313500	1.45482500
C	3.34209600	-1.63161500	-0.58079500
H	1.62781900	1.76067300	0.87783200
H	3.20104300	3.11886600	2.23217800
H	5.52722800	2.35852300	2.60857500
H	6.35627500	0.22794600	1.62974900
H	3.15230500	-2.52259300	-1.16056100
N	4.55080900	-1.39170300	0.01524900
N	2.46107200	-0.67523600	-0.34879900
C	5.75186500	-2.20701000	-0.10304600
H	6.22109400	-2.26378500	0.88341200
H	5.44054100	-3.21797500	-0.37708500
C	6.72517600	-1.63749900	-1.13632100
H	6.21274100	-1.57719800	-2.10646000
H	6.96066700	-0.59821600	-0.87058500
C	8.95352100	-1.81976200	-2.33361400
H	9.87174600	-2.40602400	-2.42315200
H	8.47721900	-1.77493600	-3.32140400
H	9.22796700	-0.78944600	-2.07338500
C	8.01619300	-2.40337100	-1.30831000
C	8.32350100	-3.50789000	-0.62013000
H	9.26734600	-4.02121400	-0.78186000
H	7.66516200	-3.94573300	0.12367400

c3-4

Ni	0.42495500	0.56416300	-1.03859100
Fe	-3.95271800	-1.60904000	1.13558900
P	-4.58443300	1.06056400	-0.86088600
P	-0.13368200	1.20497700	0.99257900
O	-5.27366400	1.70742400	0.31736500
C	-3.53277300	-0.34008900	-0.43521400
C	-2.48266100	-0.21706700	0.54909900
C	-1.91433800	-1.51274700	0.72347500
H	-1.13208900	-1.76285900	1.42206400
C	-2.56686200	-2.42421300	-0.15588600
H	-2.36612800	-3.48330100	-0.23278700
C	-3.56739100	-1.71004700	-0.87213900
H	-4.25175400	-2.14015200	-1.58608700

C	-2.01476600	1.09314000	1.14046700
H	-2.33436000	1.86998500	0.44160100
C	-2.60020400	1.45006700	2.50608900
H	-2.34219300	0.70276500	3.25825200
H	-3.68692300	1.51178800	2.41475800
H	-2.22844800	2.42390400	2.83948100
C	-5.88499000	-2.29728200	1.40093100
H	-6.56590400	-2.50883300	0.58875200
C	-5.72731700	-1.03925100	2.05693700
H	-6.22531800	-0.11507600	1.80092300
C	-4.70045800	-1.18291500	3.03447200
H	-4.33184300	-0.40250900	3.68128500
C	-4.21373900	-2.52314700	2.97904300
H	-3.40496000	-2.93094600	3.56964500
C	-4.94951500	-3.21497700	1.97039200
H	-4.79397500	-4.23926400	1.66043100
C	0.46199500	0.39857100	2.54976900
C	1.04989300	-0.87079900	2.43829300
H	1.15077400	-1.31706600	1.45712300
C	1.49326300	-1.56037100	3.56834900
H	1.94171000	-2.54373700	3.45832700
C	1.36290200	-0.98474700	4.83245400
H	1.71044200	-1.51545300	5.71408900
C	0.78373300	0.28031300	4.95891400
H	0.67766900	0.73448100	5.94000500
C	0.33620000	0.96488600	3.82923800
H	-0.10432400	1.94846300	3.94334100
C	0.16236900	2.99247100	1.33082300
C	-0.64801000	3.97376200	0.73472900
H	-1.51362300	3.68721600	0.14876700
C	-0.35298500	5.32973900	0.87577700
H	-1.00000400	6.06891400	0.41229700
C	0.76363000	5.73595300	1.60799800
H	0.99221100	6.79170000	1.71880000
C	1.58361700	4.77171200	2.19574400
H	2.45637800	5.07441200	2.76773000
C	1.28856500	3.41548000	2.05501700
H	1.94255100	2.68026600	2.50935800
C	-5.70620500	0.62725400	-2.26953500
C	-6.72381600	-0.43703100	-1.83095700
H	-6.25147300	-1.39816000	-1.61832300
H	-7.45890600	-0.59384500	-2.62889800
H	-7.26299300	-0.11755500	-0.93452000
C	-4.88794000	0.16991600	-3.48665200

H	-4.13348000	0.91308700	-3.76501600
H	-5.55556500	0.04040900	-4.34648200
H	-4.37600000	-0.77938400	-3.31786900
C	-6.44705100	1.93507500	-2.61100800
H	-7.01864700	2.30479900	-1.75595200
H	-7.13943500	1.75642200	-3.44139500
H	-5.75032400	2.72206700	-2.92041900
H	-3.67491400	1.93613300	-1.50882300
C	3.92337400	1.87203800	-1.58218400
C	5.08725800	1.06415600	-1.48180300
C	5.89038200	1.12362100	-0.33489200
C	5.50274700	1.98759200	0.68501000
C	4.33774100	2.77539300	0.57490900
C	3.52340900	2.73054200	-0.55461800
C	4.16195000	0.57379200	-3.35083500
H	6.77472300	0.50040700	-0.24733000
H	6.10571200	2.05860400	1.58540200
H	4.06328100	3.43361500	1.39122700
H	2.61413900	3.31745000	-0.61231700
H	3.93286500	0.14326900	-4.31596600
N	3.34845100	1.53062300	-2.79626300
N	5.19889900	0.25356300	-2.60427800
C	2.23114800	2.20258700	-3.46536500
H	1.84418700	2.94878300	-2.77146100
H	2.64100300	2.74578400	-4.32408700
C	1.11508400	1.26174100	-3.93229900
H	0.66727800	1.72892800	-4.82670000
H	1.56789600	0.32993200	-4.29469100
C	-0.97672000	-0.06554800	-3.55640900
H	-1.77039000	-0.33145500	-2.85256100
H	-1.45986300	0.34248200	-4.46155100
H	-0.47356100	-0.99051400	-3.86033100
C	-0.00239800	0.93199700	-2.95161300
C	-0.52883600	1.91555400	-2.05699200
H	-1.60308900	1.92575900	-1.87014900
H	-0.07944700	2.90713700	-1.98605900
C	2.66994000	-3.03373700	-1.21504000
C	1.46334800	-2.31725700	-1.40796200
C	0.34843300	-2.94496800	-1.97182300
C	0.47909100	-4.27752900	-2.34924800
C	1.69069100	-4.97698500	-2.17090300
C	2.80609000	-4.36979500	-1.60079000
C	2.86253700	-0.96242100	-0.46211100
H	-0.57933900	-2.40254900	-2.09392200

H	-0.36822000	-4.79231600	-2.79205700
H	1.75526100	-6.01485100	-2.48299500
H	3.73458100	-4.91404300	-1.46369600
H	3.30503800	-0.09290900	-0.00793300
N	3.53912700	-2.13975400	-0.60376500
N	1.62809100	-1.01779700	-0.93268300
C	4.95287000	-2.34394300	-0.29200200
H	5.17977300	-3.39531300	-0.47732600
H	5.54249200	-1.74276800	-0.98946000
C	5.26324700	-1.98313300	1.15969800
H	4.93112000	-0.95681000	1.35851300
H	4.66358600	-2.62125400	1.82342200
C	6.99542500	-1.71983500	2.98930300
H	8.06009900	-1.78977600	3.22692400
H	6.66085100	-0.69743100	3.20735200
H	6.44617800	-2.37954300	3.67329400
C	6.71820000	-2.07803600	1.55235500
C	7.69644600	-2.42628100	0.70943500
H	8.73025900	-2.46840800	1.04120500
H	7.51683500	-2.68055200	-0.32998900

c4

Ni	-1.03339200	-0.11996800	1.70344400
Fe	3.41139800	-1.69053300	-2.05126800
P	0.80433800	0.52550700	-1.86433700
P	-0.30721200	-2.07235100	0.98286900
O	-0.01936600	-0.31251500	-2.81817500
C	2.14285400	-0.39890300	-1.08284700
C	1.96184000	-1.74300100	-0.57560800
C	3.21610400	-2.16684100	-0.04044700
H	3.42013200	-3.13865600	0.38264300
C	4.16317600	-1.11542300	-0.20461400
H	5.21016400	-1.15585400	0.06263200
C	3.50928700	-0.02573800	-0.84435500
H	3.97535100	0.90512600	-1.12356100
C	0.68189800	-2.53218500	-0.57475600
H	0.07752600	-2.16037100	-1.40726200
C	0.90598400	-4.04054700	-0.71519600
H	1.52641300	-4.43284600	0.09310100
H	1.40568500	-4.26150600	-1.66104300
H	-0.04051500	-4.58520900	-0.69441000
C	4.38297700	-1.26113900	-3.83191800
H	4.85282300	-0.31405900	-4.05643100
C	3.02114900	-1.60539200	-4.08518900

H	2.26060500	-0.96677000	-4.50697900
C	2.80218800	-2.92656300	-3.59882800
H	1.85918200	-3.45238900	-3.62244600
C	4.02648000	-3.40233200	-3.03886200
H	4.17608400	-4.35527700	-2.55027900
C	5.00472000	-2.37226400	-3.18412500
H	6.02472800	-2.41052000	-2.82719200
C	0.62497400	-3.03713100	2.24373200
C	1.72056000	-2.40195200	2.84909800
H	1.94408100	-1.37313700	2.58864200
C	2.51433400	-3.07593900	3.77614900
H	3.36082100	-2.56976400	4.23135700
C	2.21255800	-4.39356700	4.12722800
H	2.82226200	-4.91700600	4.85789300
C	1.12004100	-5.03252500	3.53862300
H	0.87935800	-6.05742300	3.80663800
C	0.33581700	-4.36192600	2.59810600
H	-0.50321600	-4.87364800	2.13925600
C	-1.87700900	-3.00883100	0.76403400
C	-2.40353700	-3.31366900	-0.50162300
H	-1.82028500	-3.12957000	-1.39698900
C	-3.69452100	-3.83324000	-0.63246800
H	-4.08098400	-4.06291400	-1.62145900
C	-4.48167800	-4.05688800	0.49728900
H	-5.48462200	-4.46027400	0.39484100
C	-3.96807600	-3.75916000	1.76299000
H	-4.57139000	-3.93086600	2.64985600
C	-2.68408300	-3.23491000	1.89460000
H	-2.30170200	-2.99193300	2.88052500
C	1.41079100	2.12736300	-2.58215900
C	2.49781000	1.89629100	-3.64076900
H	3.38839700	1.42179200	-3.22510900
H	2.79578300	2.86099500	-4.06771900
H	2.12696600	1.27220600	-4.45802500
C	1.91818700	3.05194700	-1.46508000
H	1.15343200	3.21622400	-0.70269400
H	2.17005100	4.03124800	-1.88742500
H	2.81074000	2.67055300	-0.96859000
C	0.17298800	2.75517500	-3.25361300
H	-0.21765200	2.11000300	-4.04427400
H	0.45243200	3.71879200	-3.69520800
H	-0.62886500	2.94068700	-2.53464400
H	0.07976800	0.97373900	-0.74084600
C	2.77999700	3.42027900	1.97495500

C	3.02638800	4.79679300	1.74457900
C	4.23804000	5.19499400	1.16460800
C	5.16414900	4.20717700	0.84098700
C	4.90287500	2.84281600	1.08554800
C	3.70278400	2.42243800	1.65517300
C	1.06502500	4.66044500	2.60125200
H	4.43816100	6.24510300	0.97685200
H	6.11175600	4.49015000	0.39234200
H	5.65313900	2.10294600	0.82272300
H	3.49580500	1.37136000	1.82409000
H	0.08845400	4.89333600	3.00001300
N	1.50789600	3.36064300	2.51913400
N	1.93024100	5.54630200	2.15340700
C	0.81877600	2.10566900	2.81538400
H	0.75102200	1.52717000	1.88266200
H	1.45287400	1.53072700	3.49704600
C	-0.58409900	2.26334900	3.39961100
H	-0.51192000	2.65033200	4.42947100
H	-1.13970800	3.01649000	2.83152800
C	-2.84142700	1.12781900	3.67814000
H	-3.36762900	0.16874400	3.63081900
H	-3.00050000	1.54310400	4.68741000
H	-3.32992900	1.80952100	2.97049100
C	-1.36974400	0.95789700	3.36225400
C	-0.71266900	-0.27283900	3.63497300
H	-1.28890800	-1.10035900	4.05229500
H	0.33623500	-0.30226500	3.92278500
C	-3.37539400	2.14762000	-1.05015100
C	-2.28082800	2.04872200	-0.15914200
C	-1.49914400	3.17431100	0.11616000
C	-1.84667600	4.37650900	-0.49197500
C	-2.94485300	4.46229000	-1.37175100
C	-3.72652000	3.34884800	-1.67053600
C	-3.14804600	0.07240600	-0.31796600
H	-0.63925600	3.10107000	0.76622900
H	-1.24979300	5.26174100	-0.29676600
H	-3.18142500	5.41566600	-1.83352500
H	-4.56434400	3.41395900	-2.35651900
H	-3.33781300	-0.98446200	-0.21377500
N	-3.90575600	0.86759000	-1.12663000
N	-2.16542100	0.72863200	0.27700700
C	-5.07978600	0.45278600	-1.88307600
H	-5.01336800	0.89229800	-2.88223000
H	-5.02824600	-0.63253300	-1.99601200

C	-6.37750000	0.86536400	-1.18707700
H	-6.39441400	0.42039600	-0.18260900
H	-6.36611000	1.95101200	-1.02106000
C	-8.91343800	0.92507200	-1.21301800
H	-9.80579700	0.63071300	-1.77151900
H	-8.97696300	0.48655300	-0.20886100
H	-8.93599900	2.01420800	-1.07892800
C	-7.65020300	0.49318800	-1.91152000
C	-7.67726800	-0.16585400	-3.07458500
H	-8.62038900	-0.41099300	-3.55516200
H	-6.78008000	-0.48666600	-3.59435900

c4-2

Ni	0.39790800	-0.94898100	-1.26451300
Fe	-5.22032900	0.51053400	0.68543700
P	-2.28362000	1.92999100	-0.40802900
P	-1.02506700	-1.78507500	0.20122300
O	-1.82902800	2.21218800	1.00741300
C	-3.55973100	0.65866800	-0.51263500
C	-3.50147500	-0.56000000	0.26510300
C	-4.64953000	-1.33669700	-0.07732900
H	-4.91240900	-2.29028200	0.35521900
C	-5.41447700	-0.62463800	-1.04340600
H	-6.36164800	-0.93742700	-1.46058900
C	-4.74842500	0.60155100	-1.31835000
H	-5.10515300	1.37022600	-1.98586300
C	-2.41409600	-0.96633500	1.21924800
H	-1.96624200	-0.04861600	1.61163800
C	-2.93844300	-1.83299600	2.36724900
H	-3.39272100	-2.75529400	1.99945000
H	-3.70171500	-1.28705300	2.92692100
H	-2.13980000	-2.10910400	3.05835600
C	-6.49541000	2.08552500	1.12764600
H	-6.84271100	2.80991500	0.40467000
C	-5.30492100	2.18105500	1.90951500
H	-4.57094400	2.97118600	1.87477200
C	-5.19965000	0.99968800	2.69917700
H	-4.38786600	0.76758800	3.37279000
C	-6.32265400	0.16833500	2.40564600
H	-6.51081600	-0.81543400	2.81310300
C	-7.12430700	0.84001300	1.43370800
H	-8.02592200	0.45412300	0.97830200
C	-1.89770600	-3.30989600	-0.34533400
C	-2.46424500	-3.28462900	-1.62886500

H	-2.30955100	-2.41218000	-2.25566800
C	-3.21550800	-4.36102800	-2.09912800
H	-3.65030600	-4.32225400	-3.09366700
C	-3.40004400	-5.48805700	-1.29565800
H	-3.97749200	-6.33151800	-1.66284600
C	-2.83382900	-5.52917300	-0.02022700
H	-2.97144500	-6.40402100	0.60891100
C	-2.09235800	-4.44562900	0.45451300
H	-1.66344300	-4.48855900	1.44975000
C	0.12928200	-2.34956900	1.52096900
C	0.39993300	-1.52623700	2.62892200
H	-0.16447800	-0.61068300	2.77629500
C	1.38526300	-1.87135100	3.55558100
H	1.57479500	-1.22173200	4.40520400
C	2.11983400	-3.04844800	3.39599000
H	2.88772700	-3.31602900	4.11496000
C	1.86289300	-3.87328800	2.29901100
H	2.43103200	-4.78878200	2.16198700
C	0.88287300	-3.52567900	1.36874800
H	0.70037200	-4.17282300	0.51794200
C	-2.76118600	3.43881200	-1.38110800
C	-4.08987100	4.03354200	-0.89408900
H	-4.92660300	3.34217700	-1.00740000
H	-4.31604900	4.93804200	-1.47103200
H	-4.02849600	4.32083700	0.15893400
C	-2.81714700	3.09085100	-2.87767400
H	-1.86412500	2.68144600	-3.22601600
H	-3.01602500	4.00002600	-3.45684600
H	-3.60186400	2.36866900	-3.11555100
C	-1.62945500	4.45532100	-1.13308800
H	-1.53737200	4.69139800	-0.07028300
H	-1.84761500	5.38091700	-1.67854800
H	-0.66558100	4.08139700	-1.48432000
H	-1.27695800	1.37949400	-1.22609000
C	5.82658100	-1.42595700	-0.55178500
C	6.43290500	-0.77713400	0.55613400
C	7.76985100	-0.36653800	0.47974500
C	8.46434200	-0.61963800	-0.69885700
C	7.85001700	-1.27122500	-1.78827500
C	6.52214500	-1.68642800	-1.73555100
C	4.41335000	-1.20708900	1.12997800
H	8.24067100	0.13080400	1.32183700
H	9.50212600	-0.31171200	-0.78529800
H	8.42632000	-1.45339300	-2.69041400

H	6.05230700	-2.18594500	-2.57553400
H	3.48162900	-1.30593900	1.67067800
N	4.52488100	-1.68475100	-0.15058800
N	5.51608900	-0.65650000	1.59443700
C	3.43489500	-2.25304800	-0.93968100
H	3.67451300	-3.29328200	-1.18417400
H	2.56185500	-2.26347300	-0.28523600
C	3.12930400	-1.44246900	-2.20608100
H	3.37918400	-0.39144400	-2.01562200
H	3.80637900	-1.76659700	-3.01245200
C	1.51074300	-0.89641200	-4.05698800
H	0.45407900	-0.81239200	-4.33273800
H	1.95690300	0.10186200	-4.10883000
H	2.00543300	-1.50282000	-4.83365800
C	1.68680700	-1.52338000	-2.68606800
C	0.79635200	-2.56499900	-2.29897000
H	0.00144500	-2.85525500	-2.98571200
H	1.12534300	-3.38498000	-1.66073000
C	1.94653300	2.96309600	-0.66196800
C	1.30306900	1.99633000	-1.47078800
C	0.99704800	2.28634600	-2.80431000
C	1.37863400	3.52871800	-3.30234000
C	2.03828500	4.47527300	-2.49162700
C	2.32927800	4.21235300	-1.15565200
C	1.48392400	1.14853500	0.51099600
H	0.47354700	1.56360800	-3.41654400
H	1.15576000	3.78011600	-4.33451800
H	2.31751700	5.43454700	-2.91594000
H	2.82537400	4.94650700	-0.52982400
H	1.43130300	0.48394800	1.35940100
N	2.04412500	2.38823000	0.59648800
N	1.03369300	0.86498500	-0.70059800
C	2.70605200	2.95082400	1.76889000
H	2.47824600	4.01942100	1.79916400
H	2.25322700	2.49588800	2.65321400
C	4.21275700	2.69204800	1.74137100
H	4.38663900	1.61607900	1.62494500
H	4.64506900	3.15437900	0.84281400
C	6.39755900	2.66374900	3.01397200
H	6.93113900	3.05517300	3.88443800
H	6.41082200	1.56759700	3.05050000
H	6.95103200	2.95125000	2.11058400
C	4.97642600	3.16005000	2.95764600
C	4.44907200	3.92393000	3.92031300

H	5.04049700	4.22792400	4.77978400
H	3.42194700	4.27516900	3.89957500

c4-3

Ni	-0.14091800	-2.22355200	0.26478300
Fe	-2.57641500	3.26517800	-1.01155000
P	-0.60904700	2.17313900	1.53251300
P	-2.17354500	-1.42983200	0.07192200
O	-1.76043700	2.42448200	2.47947700
C	-1.08740900	2.10419500	-0.20670000
C	-2.17746000	1.26049900	-0.63776000
C	-2.35141300	1.46847600	-2.03890700
H	-3.11313200	1.00830500	-2.65031600
C	-1.38571400	2.41822700	-2.48233200
H	-1.29280400	2.80892900	-3.48620800
C	-0.60545300	2.81601200	-1.35896900
H	0.17613200	3.55906800	-1.37276900
C	-2.93792200	0.31048900	0.23876200
H	-2.74706700	0.60343800	1.27362000
C	-4.45257900	0.33977600	0.01670600
H	-4.71815100	0.16156600	-1.02713300
H	-4.84849700	1.31529300	0.30438400
H	-4.94896700	-0.41841900	0.62768800
C	-2.80835000	5.32896900	-1.03777200
H	-2.04069100	6.02285200	-1.35190300
C	-2.99761800	4.82603500	0.28356400
H	-2.40075000	5.05694800	1.15193100
C	-4.08252200	3.90210000	0.25555200
H	-4.41970800	3.31985500	1.09940900
C	-4.56630700	3.83054800	-1.08535400
H	-5.35509500	3.18467200	-1.44480900
C	-3.77669400	4.71058400	-1.88649200
H	-3.86995700	4.85311700	-2.95436900
C	-2.94026300	-1.94328200	-1.52630300
C	-2.14258000	-1.82205800	-2.67546300
H	-1.11622400	-1.48547800	-2.57377700
C	-2.64810400	-2.12528900	-3.93899100
H	-2.01368000	-2.01764200	-4.81419900
C	-3.96333600	-2.57414700	-4.07492700
H	-4.35837600	-2.82072300	-5.05607300
C	-4.76574100	-2.70834800	-2.94093200
H	-5.78975800	-3.05804800	-3.03658100
C	-4.26113600	-2.38935900	-1.67870200
H	-4.90327800	-2.49002000	-0.81146200

C	-3.11077900	-2.31495500	1.38957700
C	-3.22654500	-1.72533600	2.66090400
H	-2.86470100	-0.71665300	2.83374400
C	-3.80262100	-2.42175900	3.72336400
H	-3.88426700	-1.94272800	4.69485200
C	-4.27322300	-3.72289300	3.53993500
H	-4.72308100	-4.26449000	4.36666200
C	-4.16042400	-4.32107600	2.28403900
H	-4.52219500	-5.33348000	2.12786200
C	-3.58197500	-3.62672600	1.22119100
H	-3.49783600	-4.11041200	0.25530300
C	0.84036300	3.30015600	1.76675700
C	0.46253400	4.75574900	1.46057500
H	0.15319700	4.89567200	0.42210300
H	1.32579800	5.40540100	1.64743000
H	-0.35300900	5.09220900	2.10663000
C	2.01432700	2.82615200	0.90090800
H	2.24990800	1.77844200	1.09825800
H	2.90591900	3.41744200	1.13814600
H	1.82431200	2.92665300	-0.16858400
C	1.21660800	3.16489900	3.25543600
H	0.38430100	3.45463100	3.90179300
H	2.07102000	3.81520600	3.47696200
H	1.50121900	2.13897400	3.50902300
H	-0.00409100	0.91345800	1.71286900
C	2.93274800	-0.94957400	-2.85471700
C	4.27884400	-0.71648100	-3.24145500
C	4.74388000	0.59677600	-3.39468900
C	3.85013900	1.63803000	-3.16181700
C	2.51411200	1.38851000	-2.78119100
C	2.02926700	0.09320400	-2.61929100
C	4.04987100	-2.84105700	-3.09339300
H	5.77340300	0.78240700	-3.68310100
H	4.18201700	2.66512400	-3.28138400
H	1.84091300	2.22190600	-2.61330900
H	1.00623700	-0.08445900	-2.30390800
H	4.22314100	-3.90895800	-3.09224300
N	2.81886200	-2.32998000	-2.75991200
N	4.94674700	-1.92509800	-3.38803700
C	1.66052400	-3.06637600	-2.25394900
H	0.89653200	-2.32118700	-2.02301400
H	1.26297600	-3.70801700	-3.04569400
C	1.97311800	-3.86374400	-0.97522700
H	2.34525700	-4.86500600	-1.24754100

H	2.80798000	-3.37392700	-0.46013600
C	1.17806400	-4.62868500	1.30563300
H	0.32163000	-4.66405100	1.98614900
H	1.53064700	-5.66315900	1.16103100
H	1.98383800	-4.08499700	1.81481400
C	0.80619900	-3.97496700	-0.00974800
C	-0.53609000	-4.02469900	-0.46488000
H	-1.27010900	-4.55447100	0.13963000
H	-0.77245500	-4.01046600	-1.52738500
C	2.79220500	-0.54139400	2.78122300
C	1.46864800	-0.96602800	2.50696900
C	0.52062900	-1.05022100	3.53151300
C	0.92537800	-0.69016300	4.81248800
C	2.24425800	-0.26383200	5.07559400
C	3.20181600	-0.18208400	4.06741400
C	2.53822700	-0.97736000	0.62680700
H	-0.48995000	-1.38096400	3.31902700
H	0.21151800	-0.73382900	5.62876700
H	2.51917700	0.01097400	6.08910800
H	4.21366400	0.15011800	4.27408600
H	2.79908900	-1.06067600	-0.41386400
N	3.45126700	-0.57170700	1.55831100
N	1.34632800	-1.22822900	1.14160900
C	4.85674100	-0.28531600	1.27631400
H	5.42149700	-0.46882100	2.19308000
H	5.19735500	-1.00835100	0.53034800
C	5.06973100	1.13799100	0.76455500
H	4.40651100	1.30497500	-0.09368200
H	4.74132700	1.85038900	1.53220900
C	6.63058400	2.84891600	-0.25388100
H	7.66845600	3.06558100	-0.51995100
H	6.01588700	2.94034400	-1.15820000
H	6.28466900	3.62537900	0.44085000
C	6.48137000	1.47630000	0.34859000
C	7.51906300	0.64438900	0.48133400
H	8.51450100	0.93724700	0.15923100
H	7.42830300	-0.35130800	0.90368200

c4-4

Ni	-1.00073200	-0.20073900	1.36253200
Fe	4.70669000	-1.71481700	-0.68612900
P	2.58913400	0.91304200	-0.90162600
P	0.01419700	-1.95248900	0.46390300
O	2.38492700	0.58324600	-2.36230400

C	3.29529000	-0.43405600	0.06772400
C	2.74842900	-1.77045900	0.00591200
C	3.57216500	-2.60474100	0.81963400
H	3.44324000	-3.66750100	0.95950100
C	4.60947600	-1.81164600	1.38651700
H	5.41184200	-2.17066600	2.01617500
C	4.44480700	-0.47402600	0.93065800
H	5.09809900	0.35069400	1.16768100
C	1.50314000	-2.18417000	-0.72146400
H	1.33283200	-1.46367300	-1.52712900
C	1.60526800	-3.58826700	-1.32388800
H	1.81553000	-4.34161000	-0.56241900
H	2.41762600	-3.62087000	-2.05305000
H	0.67981300	-3.87029600	-1.83016900
C	6.43418800	-1.11775900	-1.65962500
H	7.07458900	-0.31635200	-1.31819600
C	5.30957500	-0.98226800	-2.52774200
H	4.91035800	-0.06711900	-2.93717700
C	4.71576300	-2.26835000	-2.68253800
H	3.82621600	-2.47774400	-3.25766200
C	5.46927900	-3.20252000	-1.90923900
H	5.24951200	-4.25425600	-1.78865200
C	6.53302000	-2.49074400	-1.27576600
H	7.26049800	-2.90994600	-0.59424500
C	0.42608400	-3.22202100	1.73218600
C	0.94480800	-2.74490700	2.94586000
H	1.01153300	-1.67209000	3.10137000
C	1.36328300	-3.62646500	3.94153500
H	1.76742700	-3.23838400	4.87207200
C	1.25414500	-5.00477700	3.74481600
H	1.57200500	-5.69401800	4.52171600
C	0.72592300	-5.49269000	2.54853700
H	0.63066400	-6.56336200	2.39144600
C	0.31893800	-4.60836800	1.54734900
H	-0.08935200	-5.00354700	0.62432900
C	-1.33906200	-2.67559200	-0.55890000
C	-1.51721400	-2.19791600	-1.86934800
H	-0.76711100	-1.55413400	-2.31838000
C	-2.65013300	-2.53461100	-2.60942500
H	-2.77183700	-2.14131400	-3.61441300
C	-3.62514400	-3.36977700	-2.06045100
H	-4.51486900	-3.62055400	-2.62938300
C	-3.44369000	-3.88005900	-0.77454300
H	-4.19007700	-4.53966800	-0.34117600

C	-2.31372600	-3.53569000	-0.03002700
H	-2.20092800	-3.92712600	0.97385700
C	3.51847600	2.48917500	-0.59582900
C	4.97003300	2.38962200	-1.08605600
H	5.54496700	1.63953100	-0.53945700
H	5.46809000	3.35772200	-0.95517000
H	5.00819100	2.13727800	-2.14915000
C	3.45252900	2.85528300	0.89486000
H	2.41931600	2.86688100	1.25683200
H	3.87213500	3.85683500	1.04710100
H	4.01613300	2.16259600	1.52341100
C	2.77302200	3.55129500	-1.42717100
H	2.78527100	3.29945600	-2.49029200
H	3.25440200	4.52730100	-1.29446200
H	1.72724700	3.64308200	-1.12175800
H	1.38846900	1.16786000	-0.21210400
C	-6.26125300	-0.46118900	-0.56517800
C	-6.95652600	0.21270500	-1.60232600
C	-8.30422300	-0.08615300	-1.84136400
C	-8.91367200	-1.04740100	-1.04035200
C	-8.20496400	-1.70930400	-0.01588300
C	-6.86560800	-1.42800100	0.24163300
C	-4.95252000	0.96926600	-1.61965200
H	-8.84675800	0.42234500	-2.63225600
H	-9.95778000	-1.29686500	-1.20503900
H	-8.71656000	-2.45390600	0.58688600
H	-6.32009400	-1.93524200	1.03098000
H	-4.03992200	1.50086100	-1.85633900
N	-4.97532900	0.04820800	-0.60164700
N	-6.10343600	1.10339200	-2.24325400
C	-3.86722100	-0.32920600	0.26711800
H	-3.94560900	-1.40174900	0.44461100
H	-2.93901800	-0.17173200	-0.28429200
C	-3.82904700	0.45101000	1.58410500
H	-3.78943800	1.52246400	1.34696300
H	-4.77958500	0.29519900	2.12013900
C	-2.49240900	1.02182300	3.66240000
H	-1.60673000	0.77363900	4.25736000
H	-2.41483400	2.07266800	3.35695800
H	-3.36500200	0.96020800	4.33247700
C	-2.64591600	0.09292200	2.47543800
C	-2.17497800	-1.24260100	2.56897900
H	-1.65111600	-1.55131900	3.47367900
H	-2.69627400	-2.05630000	2.07237000

C	-0.89630400	3.59395200	-0.48931000
C	-0.95698300	2.18237700	-0.53280500
C	-1.20382300	1.52216700	-1.73956600
C	-1.39505400	2.30166500	-2.87560400
C	-1.34590500	3.70982400	-2.81788100
C	-1.09301100	4.38278200	-1.62591000
C	-0.51428700	2.73129300	1.51481400
H	-1.23784400	0.44121500	-1.77503500
H	-1.58249700	1.81738800	-3.82837300
H	-1.50408400	4.28230100	-3.72618600
H	-1.04907500	5.46576800	-1.58620100
H	-0.31706700	2.70033600	2.57518900
N	-0.60914800	3.91296800	0.83150800
N	-0.71975500	1.67403700	0.74517400
C	-0.42883800	5.25403500	1.37642200
H	-1.23756500	5.88366400	0.99463900
H	-0.54699600	5.18960900	2.46065200
C	0.93681700	5.83696600	1.01196900
H	1.71745300	5.16851400	1.39631500
H	1.05625100	5.81753900	-0.07896400
C	2.56449100	7.77322900	1.13721100
H	2.71742300	8.78754000	1.51454200
H	3.36103300	7.13424800	1.54022100
H	2.69818400	7.78846600	0.04782000
C	1.20532000	7.23816100	1.50682300
C	0.32943600	7.95876400	2.21425600
H	0.57297500	8.96390100	2.54704300
H	-0.65360600	7.59015400	2.48959600

c5

Ni	1.32647200	1.06626300	-0.34576500
Fe	-3.75184800	-2.09733400	-0.37592000
P	-2.52064300	-1.32549000	2.67504700
P	0.90603700	-1.09097500	-0.71472300
O	-2.36641700	-2.80750300	2.91876800
C	-2.73851900	-0.87699700	0.93988700
C	-1.81312100	-1.32952800	-0.07777800
C	-2.33987500	-0.91303300	-1.33823900
H	-1.90990500	-1.13606300	-2.30136900
C	-3.54313000	-0.18141700	-1.11720300
H	-4.17857900	0.24612500	-1.87996100
C	-3.79708500	-0.15713000	0.28175200
H	-4.65435600	0.29989100	0.74855200
C	-0.47893400	-1.98666300	0.20749100

H	-0.23520400	-1.75730600	1.24909600
C	-0.46509400	-3.51060900	0.07337200
H	-0.76782200	-3.82431100	-0.92675500
H	-1.16091500	-3.92593300	0.80530100
H	0.53170500	-3.90971200	0.28229400
C	-5.55475800	-2.93694200	0.18708000
H	-6.27648000	-2.43901500	0.81923100
C	-4.47843800	-3.76304700	0.63183900
H	-4.20255600	-3.96335500	1.65685400
C	-3.74311800	-4.17680400	-0.51656000
H	-2.85618600	-4.79055200	-0.51001600
C	-4.35467600	-3.60210500	-1.67058600
H	-4.00543700	-3.69624500	-2.68954100
C	-5.47866500	-2.83734700	-1.23606500
H	-6.12801700	-2.24675300	-1.86754200
C	0.77387600	-1.73030200	-2.43385400
C	0.31566700	-0.85589900	-3.43084700
H	0.09645100	0.17404100	-3.17168500
C	0.12803800	-1.29769600	-4.74052400
H	-0.23167600	-0.60712200	-5.49745000
C	0.40855300	-2.62337700	-5.07536000
H	0.26776500	-2.96976000	-6.09481800
C	0.87867000	-3.50106800	-4.09639100
H	1.10497600	-4.53195400	-4.35217500
C	1.05915100	-3.05975700	-2.78547500
H	1.43275600	-3.75029600	-2.03839700
C	2.41846300	-1.89079100	-0.04350500
C	2.58439000	-1.98663200	1.34875900
H	1.76377700	-1.74382800	2.01620900
C	3.80727400	-2.37134500	1.89670800
H	3.91616100	-2.43511300	2.97528100
C	4.89187600	-2.65987600	1.06619200
H	5.85012300	-2.93693800	1.49352800
C	4.73696000	-2.57887500	-0.31770500
H	5.57568200	-2.79782600	-0.97114800
C	3.51235500	-2.19763300	-0.86908200
H	3.41472000	-2.12449600	-1.94643200
C	-3.79361900	-0.49134700	3.72952100
C	-5.18942900	-1.05816600	3.42950500
H	-5.51612100	-0.82908800	2.41301500
H	-5.91859300	-0.62476100	4.12353900
H	-5.20761400	-2.14429500	3.55686400
C	-3.74476200	1.03010700	3.52392700
H	-2.72427800	1.41900600	3.61884400

H	-4.35658600	1.52316500	4.28781400
H	-4.13284400	1.32651500	2.54866000
C	-3.39754100	-0.83177500	5.17952100
H	-3.37910100	-1.91206600	5.34431000
H	-4.12372400	-0.38781700	5.86948700
H	-2.40908000	-0.43161300	5.43125700
H	-1.36253900	-0.59010800	3.03831800
C	6.75181700	0.61244900	0.61684000
C	7.71068300	0.70068500	1.65769600
C	9.04236300	0.34515200	1.40581200
C	9.37235600	-0.08856100	0.12535000
C	8.40373800	-0.17225100	-0.89679800
C	7.07494200	0.17781800	-0.67073500
C	5.83923500	1.31001400	2.50097800
H	9.78540600	0.40784900	2.19452900
H	10.39747300	-0.37032300	-0.09595500
H	8.70213400	-0.51527700	-1.88302600
H	6.32927900	0.11249200	-1.45607300
H	5.05623900	1.64263600	3.17013700
N	5.55662500	1.01110900	1.19101500
N	7.10177200	1.14330800	2.82653900
C	4.26187600	1.05586600	0.52441900
H	4.21559900	0.18830600	-0.13163800
H	3.48457800	0.92036700	1.27827800
C	4.02429200	2.35258400	-0.25509900
H	3.97088700	3.18454700	0.45354700
H	4.90239800	2.54981000	-0.88815800
C	2.32384000	3.70528500	-1.58575200
H	1.42110100	3.64982400	-2.20133200
H	2.12517800	4.38029600	-0.74903800
H	3.10719000	4.18140300	-2.19467500
C	2.77950300	2.33442800	-1.13481300
C	2.51322500	1.22711600	-1.95266900
H	1.91966100	1.36872300	-2.85214200
H	3.19141500	0.37877200	-1.99944600
C	-3.54777000	3.71991600	-0.70852500
C	-4.24645200	4.38127100	-1.75021300
C	-5.51233200	4.92664000	-1.49886400
C	-6.04054500	4.79201500	-0.21829800
C	-5.32989100	4.13219900	0.80617400
C	-4.06875200	3.58616200	0.58050900
C	-2.40092900	3.69918300	-2.59374400
H	-6.05687500	5.43500400	-2.28817300
H	-7.01995700	5.20589300	0.00192000

H	-5.77311400	4.05328000	1.79445000
H	-3.51697700	3.08903500	1.37000000
H	-1.58031100	3.47301700	-3.26251400
N	-2.36239700	3.29200800	-1.28210500
N	-3.49468900	4.35057500	-2.91915800
C	-1.33065000	2.49235100	-0.63735500
H	-1.82627900	1.64884100	-0.15701200
H	-0.68703500	2.07952600	-1.42000000
C	-0.48307400	3.27943600	0.36486400
H	-0.01345300	4.11967400	-0.15618800
H	-1.13972000	3.72734600	1.12577400
C	1.55732200	3.23184300	1.88657400
H	2.31530500	2.59097400	2.34499700
H	2.06632900	4.00893100	1.31110500
H	1.02388800	3.74193500	2.70276000
C	0.57850700	2.43417600	1.05612700
C	0.30678400	1.10259300	1.38895100
H	0.89725800	0.62042800	2.16665700
H	-0.67355100	0.67369600	1.22949200

c6

Ni	0.32794400	0.92063400	0.22475200
Fe	-0.32107900	-4.50497100	-0.51774900
P	-0.02726800	-1.34970200	-1.81520500
P	-0.42520300	-0.28923700	1.73554800
O	-1.51285500	-1.36998500	-2.14024200
C	0.49081800	-2.62638200	-0.65168600
C	-0.13113400	-2.80288600	0.64297700
C	0.52506100	-3.89628400	1.28367100
H	0.26922500	-4.29761900	2.25269100
C	1.53288000	-4.40255000	0.41491300
H	2.16753200	-5.25695600	0.60589700
C	1.51959500	-3.62491100	-0.77573500
H	2.14885600	-3.79334400	-1.63478200
C	-1.22058500	-1.95824300	1.23162600
H	-1.89759400	-1.68024400	0.41848900
C	-1.99563200	-2.67605000	2.33657000
H	-1.35410500	-2.90792500	3.19014700
H	-2.41176500	-3.61769400	1.96256600
H	-2.81933000	-2.06000500	2.70319100
C	-0.73040300	-5.66721400	-2.18131300
H	-0.06253900	-5.76928600	-3.02536700
C	-1.73050100	-4.66076700	-2.02088400
H	-1.93161500	-3.83594800	-2.68871300

C	-2.34239000	-4.84908500	-0.74561300
H	-3.10661900	-4.21741100	-0.31567200
C	-1.72321200	-5.97259300	-0.11687100
H	-1.93959400	-6.34670000	0.87431300
C	-0.72555900	-6.47864100	-1.00454900
H	-0.05698700	-7.30464200	-0.80401900
C	0.53913700	-0.88138400	3.21187200
C	1.86899300	-1.26325000	2.97441600
H	2.26573900	-1.16276900	1.96742800
C	2.66809500	-1.76867500	3.99986300
H	3.69142700	-2.06997700	3.79172000
C	2.15453600	-1.88001800	5.29423600
H	2.77724600	-2.26013100	6.09917900
C	0.83618600	-1.49678600	5.54776500
H	0.42930800	-1.58160700	6.55195700
C	0.03235800	-1.01161000	4.51363300
H	-0.99396900	-0.72862100	4.72200000
C	-1.83999400	0.61026500	2.50473600
C	-3.14337000	0.49361700	1.99314400
H	-3.36253800	-0.24779400	1.23199500
C	-4.16766500	1.32967900	2.43844100
H	-5.16901800	1.21215500	2.03439700
C	-3.91159900	2.31308600	3.39470500
H	-4.70745000	2.96924500	3.73433600
C	-2.61825900	2.44994800	3.90304900
H	-2.40184300	3.21833900	4.64021400
C	-1.59646600	1.61156100	3.46129900
H	-0.59289200	1.74011600	3.85620700
C	1.05102500	-1.37515700	-3.32850200
C	0.88792500	-2.69159800	-4.10213100
H	1.24237500	-3.55515900	-3.53584700
H	1.45830200	-2.64538700	-5.03794200
H	-0.16133000	-2.86562400	-4.35838900
C	2.51248400	-1.10681200	-2.93687000
H	2.59984200	-0.17793000	-2.36464000
H	3.12146100	-0.99819300	-3.84234600
H	2.94403400	-1.91196900	-2.33873900
C	0.54213500	-0.20682300	-4.19553100
H	-0.50921500	-0.33916000	-4.46348500
H	1.13210700	-0.15174900	-5.11772800
H	0.64774500	0.75037200	-3.67492700
H	0.40209100	-0.12162600	-1.17016200
C	3.81026500	2.92969600	-1.09044500
C	2.44079200	2.59251900	-1.19330100

C	1.67140500	3.06236100	-2.26187600
C	2.30636000	3.85596700	-3.21222500
C	3.67478400	4.18070400	-3.10457000
C	4.45242700	3.72610300	-2.04224900
C	3.18310300	1.65102000	0.60674800
H	0.61906300	2.81067000	-2.31954100
H	1.73837100	4.23755900	-4.05511900
H	4.13327900	4.80259900	-3.86739500
H	5.50385200	3.98162600	-1.96119500
H	3.25475600	1.07825800	1.51942900
N	4.25385000	2.32058100	0.07608800
N	2.08427600	1.78176100	-0.11489500
C	5.62114600	2.30750800	0.57785600
H	6.01515000	3.32647000	0.52123800
H	5.58333400	2.02752500	1.63333400
C	6.50516400	1.33844400	-0.20989900
H	6.06914300	0.33187900	-0.14486700
H	6.46298500	1.60154200	-1.27535000
C	8.80220600	0.32509100	-0.57607400
H	9.83812100	0.31685100	-0.22727500
H	8.41073800	-0.69837700	-0.51269800
H	8.80037100	0.59394600	-1.64024700
C	7.95162400	1.27807700	0.22292000
C	8.45542400	2.00002600	1.22919700
H	9.50377400	1.92056300	1.50337400
H	7.85942300	2.69072800	1.81694800
C	-2.92448000	3.50613300	-0.51669700
C	-1.61794300	3.20938700	-0.06258100
C	-0.95925300	4.07219100	0.81739800
C	-1.63230800	5.22247700	1.21791900
C	-2.93390800	5.51025200	0.75794000
C	-3.60516600	4.65818900	-0.11616700
C	-2.21360500	1.57805700	-1.35711000
H	0.03513700	3.82537200	1.17330400
H	-1.15127000	5.91190600	1.90519000
H	-3.42770700	6.41594300	1.09734600
H	-4.61005600	4.88032300	-0.46040400
H	-2.22797700	0.63106300	-1.88702400
N	-3.27275900	2.45132200	-1.34843600
N	-1.20553500	1.99575400	-0.60890200
C	-4.56676700	2.24070200	-1.97970700
H	-4.89599400	3.19096400	-2.41055900
H	-4.42405300	1.53656300	-2.80292200
C	-5.60056000	1.70845300	-0.98571900

H	-5.23429300	0.75670400	-0.57806100
H	-5.64837000	2.38927800	-0.12580400
C	-7.98368400	0.97701500	-0.52603000
H	-8.97690500	0.84543300	-0.96354900
H	-7.65547500	0.00983800	-0.12388700
H	-8.07369800	1.65709300	0.33105800
C	-6.99360700	1.50524900	-1.53169600
C	-7.34172200	1.76286900	-2.79656000
H	-8.35883900	1.59810000	-3.14164300
H	-6.64199700	2.14080000	-3.53523300

c6-2

Ni	0.42092400	-0.26751000	0.16696200
Fe	-5.13540100	-0.26627800	-0.77469300
P	-1.97968900	-0.94707200	-1.89882600
P	-0.95447800	0.79683500	1.29761000
O	-2.25365000	0.03651600	-3.02343700
C	-3.22644800	-1.00631900	-0.59333800
C	-3.43107800	0.07093400	0.34913400
C	-4.50744000	-0.31370600	1.20438400
H	-4.91732900	0.28497500	2.00374400
C	-4.97443600	-1.59844400	0.80917100
H	-5.80727400	-2.13364300	1.24393000
C	-4.19233000	-2.03000800	-0.29736200
H	-4.33050400	-2.95278900	-0.83833600
C	-2.60967700	1.32160700	0.47630700
H	-2.31126500	1.64732100	-0.52542400
C	-3.37496000	2.44706900	1.17338900
H	-3.63631700	2.17635300	2.19928600
H	-4.30537400	2.65949000	0.63595400
H	-2.78591400	3.36454800	1.21472200
C	-6.36560400	-0.61160500	-2.40490600
H	-6.49461100	-1.57854500	-2.87162000
C	-5.36577100	0.35127500	-2.73636500
H	-4.55842200	0.23030500	-3.44384400
C	-5.50859200	1.45662400	-1.84563800
H	-4.86594400	2.32522700	-1.81463700
C	-6.59974200	1.18081000	-0.96524100
H	-6.93734200	1.80866000	-0.15226300
C	-7.12925300	-0.10021900	-1.30970200
H	-7.93882200	-0.60906800	-0.80455000
C	-1.64712300	0.20112000	2.91655400
C	-1.87483300	-1.17912900	3.02392700
H	-1.58686100	-1.81637800	2.19187200

C	-2.45628700	-1.72552400	4.16786400
H	-2.62893500	-2.79659900	4.22770500
C	-2.80828000	-0.89651900	5.23519800
H	-3.25228300	-1.31879200	6.13233400
C	-2.58193200	0.47872800	5.14559000
H	-2.85247100	1.12935000	5.97301500
C	-2.01200100	1.02386800	3.99308300
H	-1.84500000	2.09422700	3.93441300
C	-0.16798800	2.40006900	1.76862800
C	-0.19900500	3.50512500	0.90251100
H	-0.79000400	3.46847500	-0.00610200
C	0.54821100	4.65163300	1.17513200
H	0.50270900	5.49090200	0.48782300
C	1.35857300	4.71386800	2.30999400
H	1.93846900	5.60769600	2.52247600
C	1.41560500	3.61408000	3.17092000
H	2.04463500	3.64703300	4.05670600
C	0.66272700	2.47200500	2.90204500
H	0.71735400	1.62506300	3.57911500
C	-1.62525500	-2.66333900	-2.50481700
C	-2.78757300	-3.18507100	-3.36254700
H	-3.70653300	-3.31168400	-2.78511700
H	-2.52586000	-4.15945000	-3.79268900
H	-3.00175000	-2.49692100	-4.18541100
C	-1.31456300	-3.58858200	-1.31865000
H	-0.58473300	-3.13304700	-0.64162300
H	-0.89653900	-4.53383500	-1.68617500
H	-2.20720000	-3.82264700	-0.73482300
C	-0.37288600	-2.50757600	-3.38993800
H	-0.56599600	-1.84209500	-4.23562000
H	-0.06922600	-3.48608200	-3.78045800
H	0.46268500	-2.09035400	-2.81991800
H	-0.78101800	-0.63933100	-1.13788600
C	2.84470600	-3.57844500	1.22481400
C	1.91004200	-2.55641700	1.51244000
C	1.43276700	-2.38061100	2.81420000
C	1.90335900	-3.24610400	3.79671200
C	2.83182300	-4.26496300	3.49825600
C	3.32208400	-4.44960600	2.20795500
C	2.35865100	-2.42039400	-0.59900600
H	0.71600100	-1.59709300	3.02714000
H	1.54706200	-3.13677200	4.81643700
H	3.17453600	-4.92023900	4.29334000
H	4.03864600	-5.23224100	1.98137000

H	2.37839300	-2.11544500	-1.63467500
N	3.10615700	-3.47016200	-0.13485800
N	1.62015400	-1.85406200	0.34083600
C	4.05438500	-4.26714700	-0.90097300
H	3.90995400	-5.31805700	-0.63316300
H	3.79894500	-4.15974100	-1.95800100
C	5.49997200	-3.83559700	-0.64607300
H	5.60328200	-2.77486900	-0.91408700
H	5.70184500	-3.88147100	0.43254800
C	7.97073700	-4.19152700	-1.10039300
H	8.69745300	-4.79619900	-1.64909200
H	8.11663200	-3.14076600	-1.38215000
H	8.20362400	-4.26247800	-0.03009900
C	6.55649200	-4.63274500	-1.37535200
C	6.28242900	-5.64844100	-2.20044400
H	7.07910400	-6.19092800	-2.70188500
H	5.27156500	-5.98172600	-2.41226800
C	2.05651800	3.16133200	-1.52628100
C	1.18403000	2.07090500	-1.75600100
C	0.07246300	2.21837800	-2.59280700
C	-0.12770200	3.46745400	-3.17655400
C	0.74742200	4.54779700	-2.94007100
C	1.85823400	4.41418000	-2.11032900
C	2.68087100	1.39555300	-0.34775500
H	-0.62173200	1.40169400	-2.77292700
H	-0.98349800	3.61273300	-3.82904600
H	0.55094900	5.50528000	-3.41342700
H	2.52346200	5.24875600	-1.91479900
H	3.24584300	0.80403500	0.35771800
N	2.99791900	2.70015600	-0.61734400
N	1.60186600	0.97902300	-0.99094200
C	4.07573000	3.47730700	-0.02496800
H	3.65664800	4.43178400	0.30556800
H	4.41269600	2.94657200	0.86866400
C	5.23303000	3.69440500	-1.00038900
H	5.62157600	2.71516100	-1.31326000
H	4.84598400	4.15535700	-1.91911200
C	7.49439500	4.74825900	-1.46431600
H	8.29752300	5.35727600	-1.04103100
H	7.92342200	3.79067100	-1.78654600
H	7.12828100	5.24605600	-2.37151100
C	6.37548900	4.53412900	-0.47792900
C	6.41263700	5.05548200	0.75286300
H	7.25882300	5.65360700	1.07989300

H	5.61852800	4.91516400	1.47921500
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c6-3

Ni	-0.62405700	0.53284300	0.31336100
Fe	3.65157800	-2.78397200	-0.74661100
P	1.42308800	-0.46157600	-1.87677100
P	-0.38850100	-1.27639900	1.30413300
O	0.80333400	-1.55310200	-2.73002500
C	2.50296900	-1.08751800	-0.57446300
C	2.06753200	-2.08095300	0.38280900
C	3.17811300	-2.36756000	1.23218300
H	3.18130000	-3.09050300	2.03384100
C	4.29064200	-1.58068600	0.81760400
H	5.28548500	-1.61293000	1.24012000
C	3.88169500	-0.79034100	-0.29270400
H	4.51842500	-0.12112100	-0.84908900
C	0.68346700	-2.64593100	0.50671100
H	0.27209200	-2.74392800	-0.50271400
C	0.65430600	-3.99826600	1.21928800
H	1.03535200	-3.92213300	2.24040500
H	1.27119100	-4.72660600	0.68258200
H	-0.36252300	-4.39123600	1.27866100
C	4.77695900	-3.21898800	-2.43183600
H	5.37559600	-2.49496200	-2.96665500
C	3.39846800	-3.50604600	-2.66801300
H	2.74358200	-3.01249100	-3.37074200
C	2.98330900	-4.47961700	-1.71176500
H	1.98030100	-4.86777100	-1.60606600
C	4.10374200	-4.79739200	-0.88447400
H	4.10083700	-5.47345300	-0.04054100
C	5.21338600	-4.01615800	-1.32885800
H	6.19903300	-4.00253700	-0.88402300
C	0.27540500	-1.38706500	3.04000900
C	1.36688700	-0.56215900	3.35224300
H	1.74269700	0.11017600	2.58668300
C	1.97266800	-0.60956200	4.60757900
H	2.82425500	0.03038900	4.82354600
C	1.48089300	-1.47518400	5.58742900
H	1.94082800	-1.50671000	6.57110900
C	0.39326700	-2.29959600	5.29375500
H	0.00677000	-2.97909100	6.04877300
C	-0.19729000	-2.26306700	4.02862200
H	-1.03267500	-2.91955600	3.81062000
C	-2.04044500	-2.08909200	1.47704200

C	-2.51471300	-3.02681600	0.54530400
H	-1.85870300	-3.40107500	-0.23240200
C	-3.83665600	-3.47099100	0.58059900
H	-4.17744800	-4.19117300	-0.15684400
C	-4.72159800	-2.97813200	1.54076400
H	-5.75132200	-3.32326500	1.56630700
C	-4.27034000	-2.03208900	2.46494700
H	-4.94930600	-1.63758100	3.21678600
C	-2.94827700	-1.59088200	2.42962700
H	-2.61257000	-0.84984200	3.14959100
C	2.30681900	0.82511500	-2.88467000
C	3.46699200	0.18616700	-3.66279300
H	4.24856100	-0.19737400	-3.00324800
H	3.92047500	0.93173900	-4.32734300
H	3.11167300	-0.64302400	-4.28107800
C	2.78130600	1.98912800	-2.00177300
H	1.95194600	2.40662100	-1.42807300
H	3.17990300	2.79057500	-2.63544900
H	3.56643500	1.69557400	-1.30235100
C	1.24662200	1.34338100	-3.87639300
H	0.85958800	0.53439100	-4.50106900
H	1.69406200	2.10362400	-4.52705900
H	0.40455300	1.80610500	-3.35223800
H	0.43561800	0.31460900	-1.14973200
C	0.73777000	4.50061200	-0.05881800
C	-0.13955600	3.44213100	-0.39218000
C	-0.93678900	3.51609300	-1.53921200
C	-0.83252100	4.66191800	-2.32216200
C	0.04615600	5.71124600	-1.98057800
C	0.85018900	5.64993800	-0.84525900
C	0.90841600	2.84536500	1.40382100
H	-1.59333200	2.69170200	-1.79294500
H	-1.43407500	4.74958000	-3.22163900
H	0.10168600	6.58574600	-2.62165500
H	1.53280800	6.45415700	-0.59096800
H	1.25792100	2.29013500	2.26075300
N	1.38539000	4.09268100	1.09992600
N	0.00534800	2.41379000	0.54174800
C	2.49726300	4.77203100	1.75090900
H	2.27430400	5.84220000	1.77550400
H	2.54437200	4.42163100	2.78487900
C	3.81772600	4.50363500	1.02502100
H	3.99229500	3.41902400	1.00625300
H	3.71089400	4.79561600	-0.02853900

C	6.31953700	4.88578100	0.87569500
H	7.17074600	5.40328100	1.32560300
H	6.53071700	3.80865100	0.88147400
H	6.25377000	5.18470800	-0.17836800
C	5.03475200	5.18648000	1.60312900
C	4.99967000	5.99238900	2.66939500
H	5.90558800	6.45928700	3.04601000
H	4.08619900	6.22133200	3.20907300
C	-4.38972600	-0.47640000	-1.21608100
C	-2.99897000	-0.36712200	-1.44870800
C	-2.36562600	-1.20562700	-2.37061900
C	-3.16139000	-2.12534600	-3.04937700
C	-4.54857000	-2.22119300	-2.81681700
C	-5.18936600	-1.39942500	-1.89267700
C	-3.48995600	1.05685600	0.10417400
H	-1.29159200	-1.16801800	-2.53070400
H	-2.69807900	-2.79277600	-3.76998900
H	-5.13056000	-2.95623600	-3.36518400
H	-6.25299100	-1.48775000	-1.69717300
H	-3.42924200	1.81375200	0.87230400
N	-4.67214500	0.44043600	-0.21336800
N	-2.46445700	0.60225800	-0.59659400
C	-5.96990400	0.66936500	0.40106100
H	-6.40999800	-0.30683300	0.62481900
H	-5.80024400	1.17625200	1.35406400
C	-6.89479200	1.49434500	-0.49536900
H	-6.41537200	2.46087500	-0.70389800
H	-6.98030400	1.00037300	-1.47255000
C	-9.17199200	2.55721900	-0.84940800
H	-10.16491700	2.70203200	-0.41546700
H	-8.73434100	3.54525900	-1.04186600
H	-9.29206700	2.07420400	-1.82769700
C	-8.28226000	1.73914400	0.05048100
C	-8.70795200	1.27798900	1.23116300
H	-9.71712500	1.48099500	1.57910000
H	-8.08436000	0.68659100	1.89390800

c7

Ni	1.53464200	-0.00552600	1.50784300
Fe	-3.92317900	-0.14125200	-1.08117200
P	-1.78894800	-2.14616500	0.68041600
P	0.54690800	1.22831600	0.01602400
O	-2.44814300	-3.34735700	0.04243500
C	-2.57956800	-0.54344400	0.42109900

C	-2.10409100	0.55438700	-0.39448400
C	-3.08075700	1.59532000	-0.30885000
H	-3.03096100	2.54437500	-0.82004800
C	-4.14906100	1.16034800	0.52293300
H	-5.05258500	1.71428800	0.73662500
C	-3.85135400	-0.15595600	0.96915600
H	-4.49373000	-0.77959900	1.57227300
C	-0.81838700	0.64912200	-1.17425900
H	-0.50304900	-0.35704900	-1.46909800
C	-0.97460100	1.52103000	-2.42521700
H	-1.22780600	2.55162600	-2.16772500
H	-1.78119200	1.12714500	-3.04799800
H	-0.06017600	1.54392400	-3.01798700
C	-5.50671200	-1.35609100	-1.62681600
H	-6.18242700	-1.81022600	-0.91520900
C	-4.27932600	-1.91782900	-2.08645100
H	-3.83057100	-2.83513500	-1.73189200
C	-3.66446200	-0.96991300	-2.95859800
H	-2.70529500	-1.08922900	-3.44279500
C	-4.51317200	0.17683400	-3.04029900
H	-4.31137200	1.08282800	-3.59489900
C	-5.65309300	-0.06177300	-2.21444200
H	-6.46174000	0.63285800	-2.03323000
C	-0.16815200	2.79029900	0.66367800
C	-0.72884000	2.75546900	1.94829500
H	-0.65263100	1.84355200	2.53142900
C	-1.38034800	3.87280000	2.47028400
H	-1.81606200	3.82930800	3.46418600
C	-1.46659200	5.04508200	1.71732400
H	-1.96987600	5.91773300	2.12317600
C	-0.89543100	5.09663600	0.44373200
H	-0.95115600	6.01014800	-0.14131300
C	-0.25136500	3.97612000	-0.08185100
H	0.19697400	4.02806600	-1.06806200
C	1.92661400	1.77102900	-1.06810600
C	2.28036300	1.02084900	-2.19905300
H	1.68343800	0.16665900	-2.49456500
C	3.41421400	1.34468200	-2.94316800
H	3.67003900	0.74519400	-3.81019000
C	4.22210300	2.41590900	-2.56037600
H	5.10640600	2.66724900	-3.13849200
C	3.88934200	3.15997800	-1.42610100
H	4.51345800	3.99445000	-1.11880500
C	2.75306900	2.83977600	-0.68314900

H	2.50537200	3.42350400	0.19719500
C	-1.57101200	-2.34377400	2.51877300
C	-2.89816500	-2.80095900	3.14423600
H	-3.65522700	-2.01294600	3.11546000
H	-2.73656700	-3.06133600	4.19691900
H	-3.29473000	-3.68021100	2.62961500
C	-1.09878600	-1.02969600	3.14866500
H	-0.18295600	-0.64711300	2.66567100
H	-0.86997700	-1.18428200	4.20892500
H	-1.86051300	-0.24996900	3.07107800
C	-0.51455000	-3.44648100	2.71372500
H	-0.82827700	-4.38426300	2.24652200
H	-0.36232600	-3.63070300	3.78342100
H	0.44996900	-3.16389600	2.28159200
H	-0.47506200	-1.89656000	0.23335200
C	3.94082900	-1.71205800	-1.10257700
C	2.73429500	-2.20577300	-1.66486500
C	2.68504600	-2.54833200	-3.02355300
C	3.84180800	-2.38602100	-3.77921700
C	5.03210700	-1.89046700	-3.20518000
C	5.10193700	-1.53897400	-1.85990400
C	2.31795200	-1.77004300	0.39590900
H	1.76658500	-2.92884600	-3.45923000
H	3.83366600	-2.64787200	-4.83296000
H	5.91307000	-1.77593700	-3.82949400
H	6.01437800	-1.14273600	-1.42725700
H	1.88728200	-1.89672600	1.40171800
N	3.65713500	-1.46329800	0.22552800
N	1.74387900	-2.24145000	-0.70166100
C	4.55132400	-0.77914100	1.15880300
H	5.54520000	-1.21852900	1.03043600
H	4.61500700	0.27562800	0.86811100
C	4.11940800	-0.91640400	2.61674800
H	3.98913300	-1.98385700	2.83738300
H	4.96965900	-0.58782500	3.23321000
C	2.25600200	-0.69304800	4.32257200
H	1.39460700	-0.09790200	4.63611100
H	1.92858600	-1.73520700	4.22402500
H	2.99214200	-0.66904500	5.14117900
C	2.86208200	-0.16134300	3.03839400
C	2.62633800	1.17387000	2.65752900
H	1.99398600	1.80926200	3.27524600
H	3.32656400	1.71417200	2.02207500

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Fe	-4.17204600	-0.91061200	0.07113700
P	-2.44376300	2.02830700	0.06396900
P	0.59014000	-0.65368700	0.50106700
O	-3.63720200	2.65944700	0.74116800
C	-2.66512200	0.35028700	-0.56268100
C	-2.11447500	-0.87544200	-0.02108300
C	-2.61355800	-1.95012800	-0.82041600
H	-2.39799500	-2.99637800	-0.66794500
C	-3.47850200	-1.42199100	-1.81783300
H	-4.04165200	-1.99761300	-2.53905400
C	-3.52619500	-0.01102100	-1.65786600
H	-4.13871300	0.66935900	-2.22859800
C	-1.16413900	-1.03774600	1.13439200
H	-1.36365600	-0.25231800	1.87038000
C	-1.31180300	-2.40845700	1.80254900
H	-1.03944900	-3.21700600	1.12068200
H	-2.35138500	-2.56148800	2.10379600
H	-0.67912800	-2.49625300	2.68575700
C	-6.15521100	-0.37504400	0.33154200
H	-6.71137500	0.22119200	-0.37849000
C	-5.36913500	0.12980200	1.40855000
H	-5.17418100	1.17297800	1.61190600
C	-4.75005300	-0.98063000	2.05696100
H	-4.06338000	-0.92393400	2.89025100
C	-5.15671000	-2.17315800	1.38291000
H	-4.83379200	-3.17894800	1.61390600
C	-6.02556400	-1.79793000	0.31398400
H	-6.47064100	-2.46949500	-0.40723900
C	0.70832100	-1.87312900	-0.87204000
C	0.43391200	-1.42322400	-2.17004500
H	0.27157300	-0.36830700	-2.34681600
C	0.39813400	-2.31468500	-3.24169000
H	0.18720800	-1.94539000	-4.24081400
C	0.64735800	-3.67155100	-3.03101500
H	0.62643600	-4.36654400	-3.86550400
C	0.93091800	-4.13125500	-1.74303400
H	1.13192400	-5.18489500	-1.57170300
C	0.95620600	-3.23986800	-0.67051200
H	1.18218500	-3.60850100	0.32344700
C	1.69362500	-1.33787600	1.80162400
C	1.40554600	-1.12257100	3.15930300
H	0.47667800	-0.64117700	3.44880100
C	2.30861000	-1.50631900	4.14939500

H	2.06411700	-1.33823900	5.19430900
C	3.52431900	-2.09831800	3.79937700
H	4.22848400	-2.39700600	4.57030700
C	3.82997300	-2.29377700	2.45216400
H	4.77766000	-2.73796800	2.16338300
C	2.92535100	-1.91387800	1.46008700
H	3.18671400	-2.06055900	0.41922100
C	-1.76394000	3.07916400	-1.31549500
C	-2.63852700	2.99837800	-2.57620000
H	-2.54732200	2.03010700	-3.07266800
H	-2.31521400	3.76701400	-3.28766200
H	-3.69361200	3.18227600	-2.34915600
C	-0.33564700	2.62997200	-1.64187200
H	0.32748300	2.79475100	-0.76638700
H	0.08184700	3.24368500	-2.44886600
H	-0.29268800	1.58878700	-1.96512300
C	-1.77271700	4.52460700	-0.78737100
H	-2.79386200	4.86779600	-0.60738000
H	-1.30543300	5.18753100	-1.52534100
H	-1.21916400	4.61945900	0.14957100
H	-1.29251300	1.87656400	0.88699400
Ni	1.12486400	1.47628300	0.37012500
C	4.48904700	0.31356300	-0.88426600
C	3.74022000	-0.27994400	-1.93434700
C	3.99148000	-1.60655200	-2.30641300
C	5.00509400	-2.28990900	-1.64016700
C	5.75865300	-1.67589300	-0.61782400
C	5.50970700	-0.36574100	-0.21559300
C	2.97675900	1.70992900	-1.68504000
H	3.40116300	-2.07926000	-3.08337700
H	5.22154600	-3.31908500	-1.91012200
H	6.54586400	-2.24049400	-0.12722100
H	6.08073200	0.09778500	0.58211000
N	3.97170800	1.58930400	-0.74272900
N	2.80882400	0.62859800	-2.42051800
C	4.38652200	2.58279600	0.24291600
H	4.69408200	2.03702300	1.13877500
H	5.26840400	3.11440000	-0.13371800
C	3.29361600	3.59140300	0.59146500
H	3.76874000	4.32665300	1.26042800
H	3.02544500	4.16576800	-0.30578900
C	1.08387700	4.18707400	1.64157700
H	0.14930700	3.80807600	2.06511700
H	1.54002900	4.85355800	2.39107200

H	0.83429600	4.81497500	0.77897300
C	2.03094500	3.06274300	1.26325800
C	2.04011500	1.88094000	2.03613900
H	1.34509200	1.78020200	2.86965000
H	2.92853600	1.26025700	2.13280300
H	2.43277600	2.63277800	-1.81023500