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Electronic Supplementary Information

The influence of NHCs on C–Si and C–C reductive elimination: A computational study of the selectivity of Ni-catalyzed C–H activation of arenes with vinylsilanes

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1. Computational details

Geometry optimizations were performed in toluene using the SMD solvation model[1] at the B3LYP[2] level of theory with the LANL2DZ basis set for Ni and the 6-31G(d,p) basis set for the other atoms. Zero-point vibrational energy (ZPVE) and thermal corrections at reaction temperature (120°C and 90 °C for **cat1** and **cat2**, respectively) were obtained by vibrational frequencies at the same theoretical level. The results of frequency calculations were also examined to verify whether each optimized stationary point is an energy minimum or a transition state. The single-point energies and solvation energies in toluene were computed with the Grimme's dispersion corrected functional B3LYP-D3-BJ[3] and a mixed basis set ECP10MDF for Ni and 6-311++G(2d,2p) for the other atoms. Using the wave function got from B3LYP/LANL2DZ/6-31G(d,p), we performed further wave function analysis by Multiwfn 3.4[4] and natural bond orbital (NBO) analysis by GenNBO 5.0.[5] All DFT calculations were performed by using Gaussian 09 software package.[6] The 3D diagrams of molecules were prepared by CYLview.[7]

The percent buried volumes $\%V_{bur}$ of NHC ligands were calculated using the web based Samb*V*ca 2.0 program at https://www.molnac.unisa.it/OMtools/sambvca2.0/index.html.[8] The steric contour plots were generated by the same program, following the procedure reported previously by Liu.[9] The default parameters in Samb*V*ca 2.0 were used as suggested by Cavallo: sphere radius: 3.5 Å, distance from the center of the sphere: 2.1 Å, mesh spacing: 0.1 Å, H atoms omitted, atom radii: Bondi radii scaled by 1.17.

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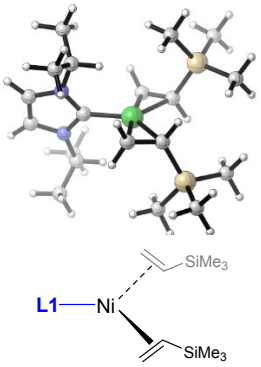
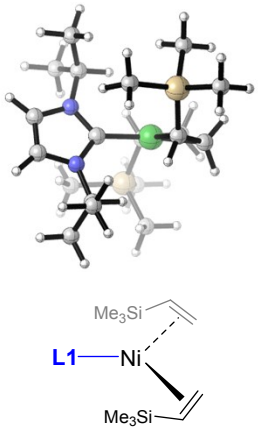
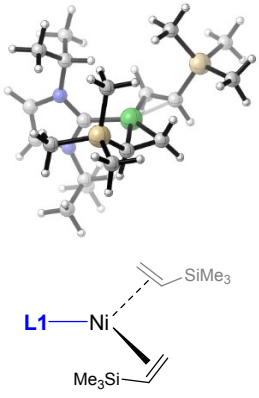
2. Different isomers of cat1 and cat2

For both **cat1** and **cat2**, rotation around the Ni-η^2-alkene bonds will lead to different isomers. We have optimized all the possible isomers, and their geometries and relative free energies are listed below. Finally, the isomer with the lowest energy was used for further calculations.

Table S1. Geometries and relative energies of different isomers of **cat1**.

isomer	geometry	relative free energies (kcal/mol)
cat1		0.0
cat1-b		0.9
cat1-c		1.1

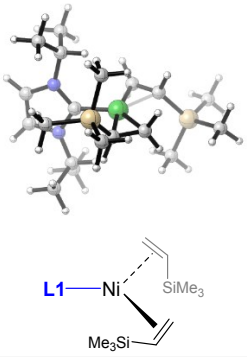
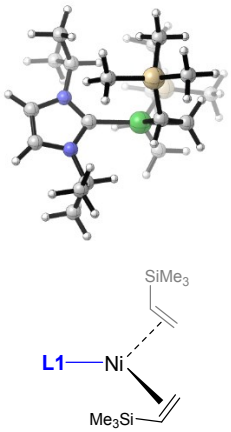
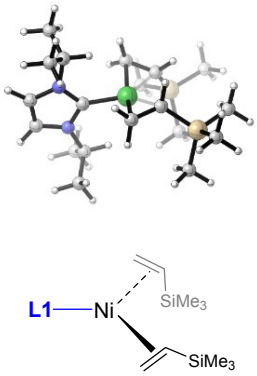
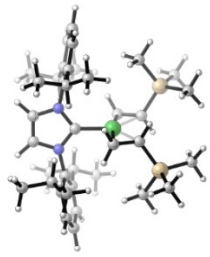
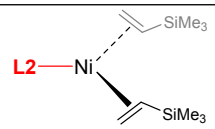
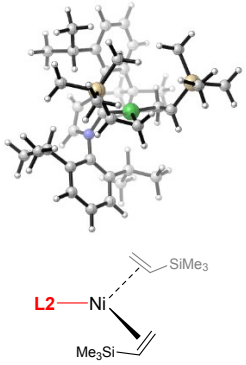
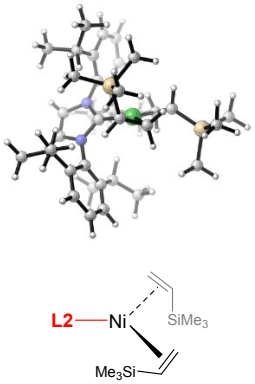
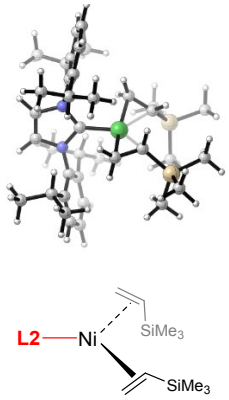
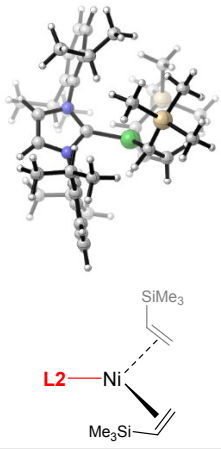
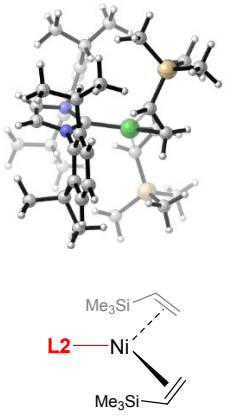
cat1-d		2.4
cat1-e		7.0
cat1-f		8.6

Table S2. Geometries and relative energies of different isomers of **cat2**.

isomer	geometry	relative free energies (kcal/mol)
cat2		0.0

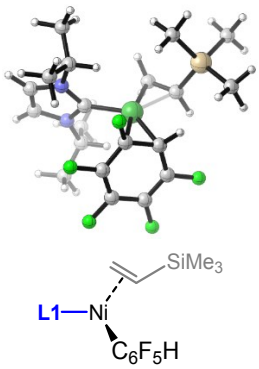
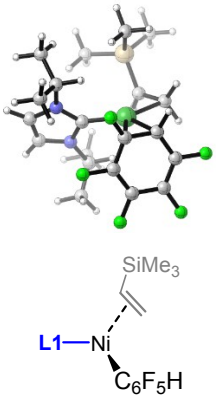
		
cat2-b		6.8
cat2-c		8.7
cat2-d		10.1
cat2-e		13.4

cat2-f		17.2

3. Different isomers of 2

We have optimized all the possible isomers of complex **2**, and their geometries and relative free energies are listed below.

Table S3. Geometries and relative energies of different isomers of **2-cat1**.

isomer	geometry	relative free energies (kcal/mol)
2-L1		0.0
2-L1-b		1.2

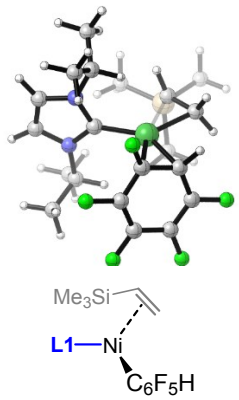
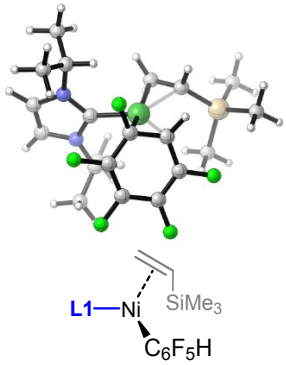
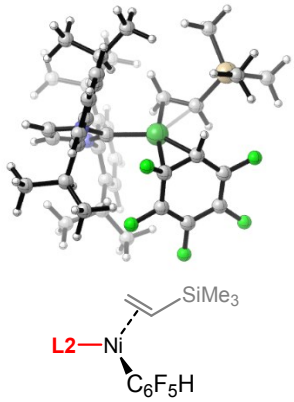
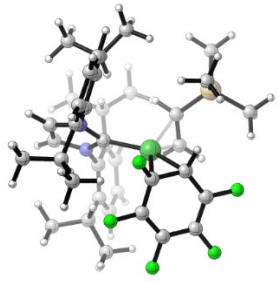
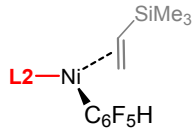
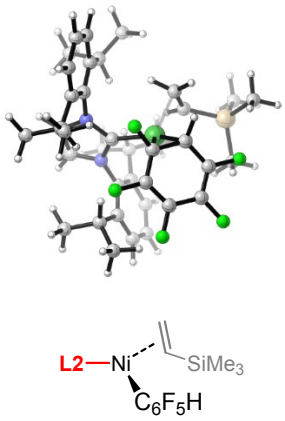
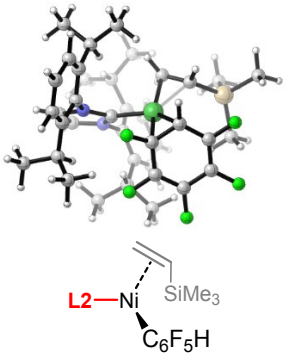
2-L1-c		3.4
2-L1-d		4.1

Table S4. Geometries and relative energies of different isomers of **2-cat2**.

isomer	geometry	relative free energies (kcal/mol)
2-L2		0.0
2-L2-b		-1.1

		
2-L2-c		0.5
2-L2-d		4.6

4. On the endergonicity of ligand exchange for cat1 and cat2

As shown in Fig. 1, the substitution reaction for **cat2 (L2)** is endergonic by 17.9 kal/mol, which is 10.0 kcal/mol higher than that of **cat1 (L1)**. The energy differences should be attributed to the significant ligand-substrate steric repulsion in **2-L2.** To obtain a better understanding of the steric environment, we created the NHC steric contour plots of **2-L1** and **2-L2** respectively using the following procedure:

(A). The Ni atom is placed at the origin of the coordinate system. The negative *z* axis is oriented along the Ni atom and the coordinated C atom of NHC. Thus, the NHC ligand is placed in the half-space along the negative *z* axis. The *x* axis is aligned along the two N atoms on the NHC ligand

(B). Delete the Ni atom, C_6F_5H and $H_2C{=}CHSiMe_3$ moieties.

(C). The van der Waals surface of the ligand was built up. The contour lines are created along the *z* axis.

Finally, the contour line of zero is drawn through all points on the van der Waals surface having the same *z* coordinate as the Ni atom. The positive contour lines (coloured in yellow and red) indicate regions on the ligand van der Waals surface having a positive *z* coordinate, *i.e.* closer to the half-space containing the substrate. The negative contour lines (coloured in

green and blue) indicate regions on the ligand surface with a negative *z* coordinate, *i.e.* more distant from the half-space containing the substrate. As shown in Fig. S1, there is significant steric repulsion between NHC and H_2C=CHSiMe_3 in **2-L2.**

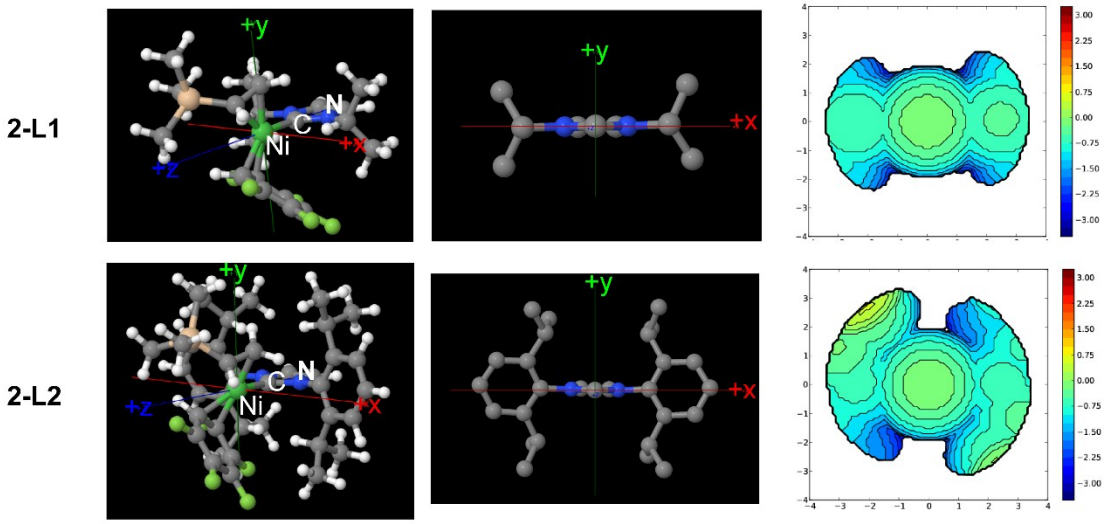


Fig. S1 Steric contour plots of NHC ligands in **2-L1** and **2-L2.**

5. Free energy profiles for hydrogen transfer to 2-site of H_2C=CHSiMe_3

We also considered the hydrogen transfer to 2-site of H_2C=CHSiMe_3, and the corresponding free energy profiles are listed below. As shown in Fig. S2, for **cat1**, the hydrogen transfer to 2-site of H_2C=CHSiMe_3 can occur readily, but the following C(sp^2)–C(sp^3) reductive elimination requires a much higher barrier (33.1 kcal/mol for **TS2-L1-b**). Similar result was observed in the case of **cat2,** as shown in Fig. S3.

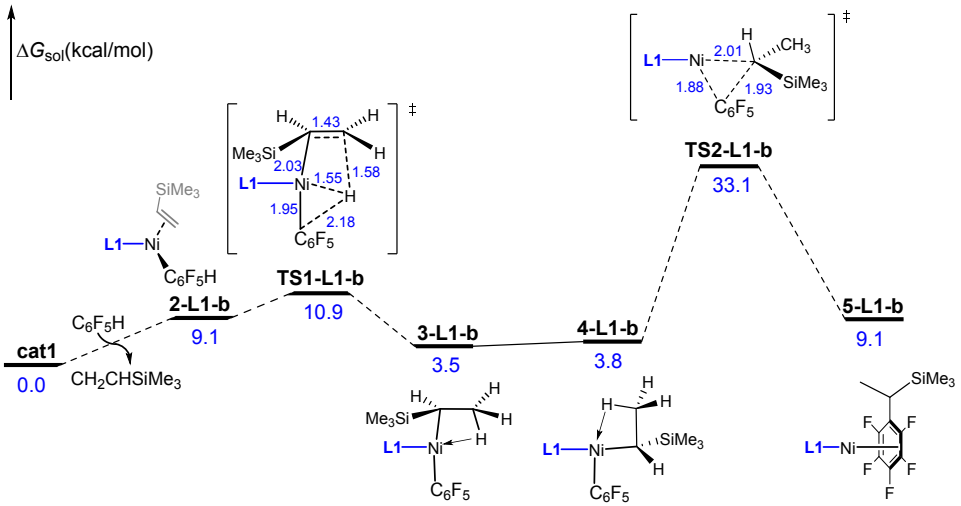


Fig. S2 Free energy profiles for hydrogen transfer to 2-site of H_2C=CHSiMe_3 catalyzed by **cat1**, with bond lengths in Å.

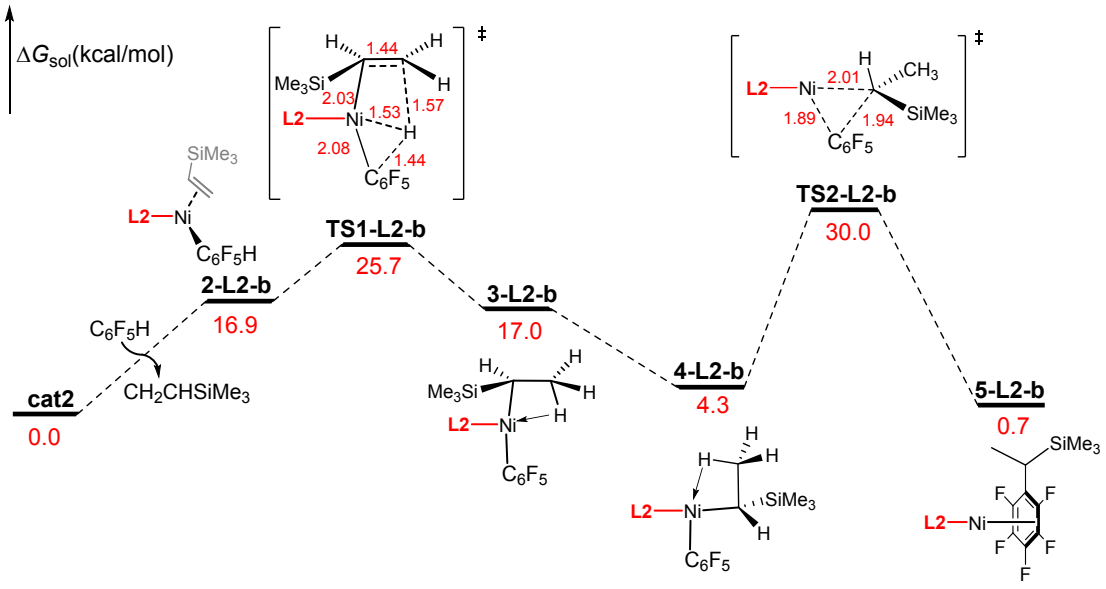


Fig. S3 Free energy profiles for hydrogen transfer to 2-site of H_2C=CH$SiMe_3$ catalyzed by **cat2**, with bond lengths in Å.

6. On the possibility of concerted $SiMe_3$ transfer

Herein, we explored the possibility of concerted $SiMe_3$ transfer; that is, intermediate **3** in Fig. 3 directly undergoes $SiMe_3$ transfer to yield **7** via a concerted transition state. However, we failed to locate the concerted transition state. Then we performed a relaxed potential energy surface (PES) scan by decreasing the values of ∠C(C_6F_5)-Ni-Si. As shown in Fig. S4, the potential energy curve indicates there exists an intermediate during the $SiMe_3$ transfer.

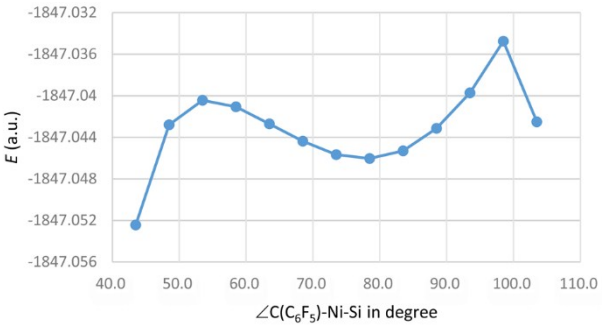


Fig. S4 The potential energy curve for $SiMe_3$ transfer**.**

7.The feasibility of alkene loss from 4-L1

As shown in Fig. 3, the direct C–Si reductive elimination transition state **TS4-L1** is 2.3 kcal/mol higher than **TS3-L1**. To investigate the influence of different density functional methods on the relative energies between the two transition states, we chose the widely-used M06, M062x and ωB97xd functionals to calculate their energies. As shown in Table S5, **TS4-L1** is higher in energy than **TS3-L1** based on the results of various functionals, which should indicate that the alkene loss prior to the C–Si reductive elimination (the gray path in Fig. 3) is less favorable. In addition, the gray path (alkene loss and then C–Si reductive elimination) in Fig. 3 involves two comparably higher-lying transition states **TS4-L1** and **TS5-L1,** and the C–Si reductive elimination in this route (19.8 kcal/mol barrier for **5-L1** to **TS5-L1**) requires a much higher barrier as compared to that in the direct C–Si reductive elimination (6.8 kcal/mol barrier for **5-L1** to **TS5-L1**).

Table S5. The energy differences between **TS4-L1** and **TS3-L1** calculated using different functionals.

density functional method	$\Delta G^{\neq}$(**TS4-L1**) − $\Delta G^{\neq}$(**TS3-L1**) (kcal/mol)
M06	11.4
M062x	3.2
ωB97xd	7.6
B3LYP-D3	2.3

8. Optimized structure of 4 and its influence on the subsequent alkene loss

As shown in Fig. 3, the alkene loss from intermediate **4** requires 9.1 and 10.7 kcal/mol respectively for **L1** and **L2**. Although the energy barrier is similar, it should be noted both **4-L2** and **TS4-L2** are higher in energy due to the steric repulsions between alkene and the bulky **L2** ligand. This stronger steric repulsions are well revealed by the fact that the coordinated alkene in **4-L2** is twisted as compared to **4-L1** (see Fig. S5).

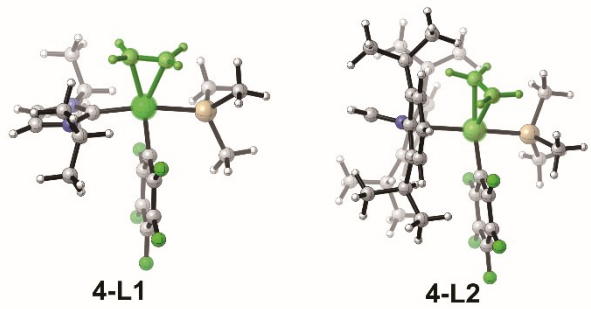


Fig. S5 Optimized structure of **4-L1** and **4-L2.**

9. Optimized structure of transition states

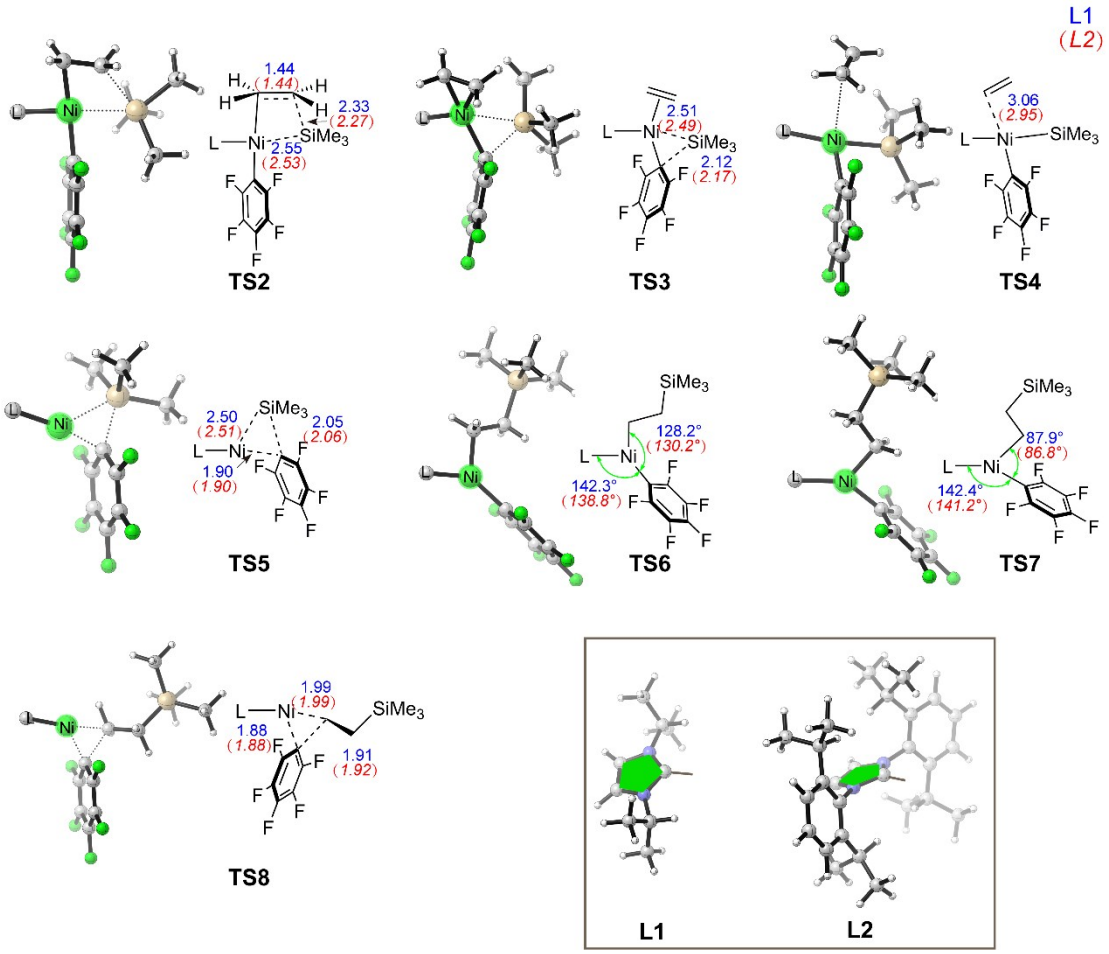


Fig. S6 Optimized structures of transition states, with selected bond lengths in Å and bond angles.

10. On the possibility of triplet state PES

We also considered the impact of the lowest-lying singlet and triplet electronic states during the isomerization from **3** to **9**. As seen from Table S6, for intermediates **3-L1**, **8-L1** and **9-L1,** the triplet electronic states are all higher in energy than their singlet state counterparts. We then tried to optimize the triplet **TS6-L1**, while we failed. We next performed a TDDFT calculation on **TS6-L1** and the TDDFT result reveals that the first triplet is 9.6 kcal/mol higher than the ground singlet. Therefore, based on the results given above, the triplet PES is high-lying and the singlet and triplet surfaces do not cross during the isomerization.

Table S6. The energy differences between singlet and triplet of the intermediates during isomerization from **3** to **9**.

intermediate	*G*(triplet) − *G*(singlet) (kcal/mol)
3-L1	13.2
8-L1	7.8
9-L1	9.3

11. The percent buried volumes %V_{bur} of NHC ligands

During the calculation of percent buried volumes %V_{bur}, the geometries of NHC ligands were taken from the optimized TS3 or TS8 separately. It should be noted that the calculated %V_{bur} values are affected by the way the ligand geometries were obtained; that is, the %V_{bur} for the same NHC ligand derives from TS3 or TS8 will be different. As listed in Table S7, **TS3** with bulky ligand (bigger %V_{bur}) has higher free energy overall. However, for **TS8**, the similar trend cannot be outlined.

Table S7. Calculated %V_{bur} of NHC ligands in various **TS3** and **TS8**.

	%V_{bur} of NHC in **TS3**	$\Delta G^{\neq}$(**TS3**)	%V_{bur} of NHC in **TS8**	$\Delta G^{\neq}$(**TS8**)
L2	31.5	31.1	38.4	25.3
L2′	32.3	23.9	36.0	20.0
L2″	30.4	24.7	33.3	31.5
L1	27.0	25.1	28.3	29.9
L1′	26.2	19.9	27.3	27.7

12. Table of calculated energies and imaginary frequencies.

Table S8. Calculated energies and imaginary frequencies.

stationary point	thermal correction to Gibbs free energy at B3LYP/LANL2DZ/6-31G(d,p) (in a.u.)	single-point energy including solvation energy at B3LYP-D3/ ECP10MDF f/6-311++G(2d,2p) (in a.u.)	imaginary frequencies
cat1	0.449809	-1608.125064	
2-L1	0.351921	-1849.372734	
TS1-L1	0.349242	-1849.356026	656.85*i*
3-L1	0.351785	-1849.380463	
TS2-L1	0.360432	-1849.357039	120.45*i*
4-L1	0.357841	-1849.362121	
TS4-L1	0.348319	-1849.337999	61.82*i*
5-L1	0.306101	-1770.727415	
TS5-L1	0.3049	-1770.694646	119.18*i*
6-L1	0.302628	-1770.71507	
P1	0.097101	-1137.443409	
TS3-L1	0.359109	-1849.352513	66.35*i*
7-L1	0.357736	-1849.378055	
TS6-L1	0.351207	-1849.362396	107.10*i*
8-L1	0.351353	-1849.367997	
TS7-L1	0.351729	-1849.359928	103.95*i*
9-L1	0.351758	-1849.378132	

10-L1	0.350647	-1849.360964	
TS8-L1	0.352413	-1849.338214	329.55*i*
11-L1	0.352024	-1849.373618	
P2	0.144131	-1216.103818	
2-L1-b	0.354984	-1849.373826	
TS1-L1-b	0.351109	-1849.367098	655.71*i*
3-L1-b	0.354509	-1849.38233	
4-L1-b	0.354765	-1849.382109	
TS2-L1-b	0.355124	-1849.335838	298.68*i*
5-L1-b	0.355166	-1849.374092	
cat2	0.764393	-2306.410002	
2-L2	0.671749	-2547.647055	
TS1-L2	0.664717	-2547.636299	997.11*i*
3-L2	0.669464	-2547.661559	
TS2-L2	0.674612	-2547.638928	126.83*i*
4-L2	0.671631	-2547.636678	
TS4-L2	0.668922	-2547.616881	38.27*i*
5-L2	0.61879	-2469.013529	
TS5-L2	0.615494	-2468.985562	107.71*i*
6-L2	0.616243	-2469.005774	
TS3-L2	0.674869	-2547.629572	66.93*i*
7-L2	0.672087	-2547.65262	
TS6-L2	0.666982	-2547.651786	94.10*i*
8-L2	0.662119	-2547.656985	
TS7-L2	0.665816	-2547.647934	79.39*i*
9-L2	0.667614	-2547.660198	
10-L2	0.664249	-2547.649123	
TS8-L2	0.666056	-2547.629428	331.37*i*
11-L2	0.663743	-2547.665185	
2-L2-b	0.667812	-2547.644821	
TS1-L2-b	0.668812	-2547.631725	994.42*i*
3-L2-b	0.673345	-2547.650121	
4-L2-b	0.667854	-2547.664941	
TS2-L2-b	0.669934	-2547.625959	302.43*i*
5-L2-b	0.663342	-2547.666164	

13. Cartesian coordinates of all optimized structures

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cat1-b

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cat1-c

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cat1-d

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cat1-e

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N,3.038633279,-1.1749293835,-0.696435767
C,1.0792669326,-1.774268013,2.2409468716
C,3.2548928795,-0.8128836948,-2.1092459471
C,-3.775119833,-2.3206048303,-1.4276205404
C,-2.6740646122,-4.9114560292,-0.1636566592
C,-2.5980349008,-2.282151216,1.4015263615
C,1.7502527704,2.550408065.9658895121
C,-0.5082179642,4.1171876187,-0.357586282
C,-1.2170378249,1.7542048017,1.4434757422
C,3.4560194699,-1.7678718547,1.3801349625
C,4.052591418,-1.5142316991.1897672494
C,1.2968315264,-0.8074842018,3.4096185048
C,1.0541751599,-3.2357863356,2.7023392728
C,4.0755591033.4748859091,-2.2219568581
C,3.8756699453,-1.9786695174,-2.8847132007
H,-3.6528162965,-1.243189111,-1.58370827
H,-4.7579394963,-2.4728732872,-0.9644908166
H,-3.8042399812,-2.7994032306,-2.4129837807
H,-2.6095643365,-5.4117501347,-1.1370507304
H,-3.6586883907,-5.1423569254.2617651124
H,-1.921559333,-5.3697616871.4898189569
H,-1.8949998556,-2.7145363502,2.1216227923
H,-3.6083759691,-2.4682607576,1.7874817272
H,-2.4480029148,-1.1972773558,1.3888620117
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H,4.1404919875.7882013718,-3.2689845394
H,5.0978813129.3379418307,-1.8518795868
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H,3.2726033799,-2.885904205,-2.7798452107

cat1-f

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C,1.1190081356,-1.0190769639,-1.5323573056
C,-1.9620338681.0536397314.1721732207
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H,-0.8934742911,2.7353107416,-0.1812159733
H,-0.0403247132,2.2293388055,1.3480348997
H,1.1032761409,2.2635726414,-1.5197905656
H,1.6945702964,-0.3739623317,-2.1961642551
H,-0.8007649626,-2.0323105177,-1.4600456385
H,-0.6958589017,-0.6794183981,-2.6833601053
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C,-1.6495751978,-2.4758140767,2.648523043
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H,-5.251438979.2730353069.0409410816
H,-2.6260819521,-2.6692572385,3.1065149091
H,-0.882587276,-2.8537444049,3.3319024913
H,-1.5908160232,-3.0471471686,1.7172672977
H,-1.3630822817.9163970894,3.451304501
H,-0.7713767629,-0.4687692875,4.3864082888
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H,-3.8645868107.5883529325,-3.7768832984
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cat2

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C,-1.0472202395,1.0795002961,-1.7093585513
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H,-0.4597623892.6824520282,-2.5355568034
H,-2.0118781397.5989385248,-1.5739648181
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C,-3.4247535711,-1.6378029424,-0.5414036354
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C,1.9898899253,-0.11163344,-3.9588866568
H,5.4494763716,-1.6495359263.9825809765
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H,-5.5228209848,-1.4324516132,-0.9746280109
C,-5.1359031342,-1.1145567183,1.1096591876
H,-1.9956523734,-1.8932241863,-2.1076781999
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H,-4.4815801428,-3.6918634012,-2.1465965019
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H,-3.3982056935,-1.3963933428,-4.0322683013
H,-3.5938758172,-0.0804575818,-2.8677110916
H,-2.8749246195,-2.8753342302,4.1657975163
H,-1.140226042,-2.7732437924,4.5096643213
H,-1.7049069315,-3.5648537876,3.03080201
H,-1.9460929805.7595754072,3.4719184757
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cat2-b

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C,1.3772361365.9559930144,1.4673147592
C.1284363301,-1.0568036646,-0.1990373525
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H.1310286561,2.624927215,1.8947576952
H,-1.8490476495,2.4764758639.306490474
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C,-2.0317268989,3.1432816908,-4.0320896744
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H,-3.0695592337,2.7896401475,-4.0034709604
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H,1.889397262,-1.9725530221,1.9921410325
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H,4.3085020424,-3.8478255951,2.2008947081
H,4.6871764631,-1.507570712,3.1579157175
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H,2.9731191514,-3.5386780422,-3.8379772467
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H,1.5876017212,-3.7499317671,-2.7568673622
H,2.7728137649.2386141851,-4.0549914005
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cat2-c

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C	1.80037	0.81486	2.14761
C	-1.26039	1.96696	0.69892
C	-0.62053	2.2033	1.93071
C	-0.23275	-0.45094	-0.7294
H	2.41655	1.57836	1.67158
H	1.52117	1.04604	3.17104

H	2.44019	-0.72617	0.83225
H	-1.06029	1.68055	2.78782
H	-1.09212	2.63849	-0.14334
H	-2.19136	1.40972	0.65422
Si	1.50961	-1.87755	2.94374
Si	0.17414	3.83976	2.40089
N	0.63075	-0.72619	-1.7768
N	-1.3986	-1.08393	-1.13326
C	0.02813	-1.44163	4.04349
C	1.30167	-3.59382	2.15814
C	3.01821	-2.01754	4.0969
C	1.27567	3.71056	3.94132
C	1.16721	4.61003	0.98648
C	-1.2266	5.04766	2.84381
C	0.02536	-1.5001	-2.76582
C	-1.24001	-1.73112	-2.3594
H	0.24825	-0.56003	4.65754
H	-0.21386	-2.26011	4.73241
H	-0.86711	-1.21348	3.45782
H	0.58422	-3.61688	1.33351
H	0.97119	-4.32152	2.90961
H	2.26033	-3.95533	1.76983
H	3.93381	-2.26219	3.54503
H	2.87397	-2.80098	4.85222
H	3.20034	-1.07668	4.62967
H	0.78167	3.15405	4.74714
H	1.49291	4.71297	4.33146
H	2.23613	3.22415	3.7426
H	1.98913	3.96186	0.66469
H	1.60184	5.56856	1.29624
H	0.53182	4.81001	0.11712
H	-1.89979	5.21226	1.99414
H	-0.83429	6.02587	3.15006
H	-1.83662	4.66721	3.67233
H	0.54784	-1.79747	-3.65988
H	-2.04343	-2.28029	-2.822
C	1.96053	-0.18602	-1.9806
C	2.08484	1.12753	-2.49294
C	3.08643	-1.01627	-1.77951
C	3.37576	1.62063	-2.72001
C	4.35268	-0.47067	-2.03468
C	4.50093	0.83637	-2.48424
H	3.50137	2.62913	-3.09831
H	5.23591	-1.08084	-1.87912
H	5.49323	1.23936	-2.66712
C	-2.72626	-0.98956	-0.55179
C	-3.14594	-1.94157	0.40273
C	-3.61105	-0.00897	-1.06126
C	-4.45448	-1.84287	0.89481
C	-4.90989	0.03702	-0.53782
C	-5.32705	-0.86007	0.4393
H	-4.79794	-2.55307	1.63867
H	-5.60463	0.78549	-0.90475
H	-6.33694	-0.8027	0.83598
C	2.97452	-2.48248	-1.36137
H	2.00004	-2.62037	-0.88298
C	0.87192	1.96784	-2.88977
H	0.04593	1.6899	-2.23081
C	-2.25451	-3.09874	0.84044
H	-1.22001	-2.75415	0.77651
C	-3.23149	0.94953	-2.18989
H	-2.1413	0.96991	-2.26186
C	3.03785	-3.41051	-2.59351
H	3.99662	-3.30206	-3.11341
H	2.93861	-4.45833	-2.28812
H	2.244	-3.19881	-3.31466
C	4.05764	-2.9107	-0.35401
H	4.10457	-2.24364	0.51074
H	3.849	-3.92284	0.00735
H	5.05281	-2.93778	-0.81093
C	1.08858	3.48161	-2.73411
H	1.77055	3.88158	-3.49311
H	0.13444	4.00583	-2.85728
H	1.4881	3.73883	-1.7505
C	0.45323	1.65508	-4.34292
H	1.25888	1.90862	-5.0418
H	0.20654	0.59937	-4.48405
H	-0.42868	2.24317	-4.62232
C	-3.78392	0.44304	-3.53935
H	-4.8793	0.40801	-3.52477
H	-3.4823	1.11203	-4.35329
H	-3.4219	-0.56012	-3.78141
C	-3.70345	2.39536	-1.94752
H	-3.3956	2.7673	-0.96725
H	-3.27752	3.05755	-2.7096
H	-4.79271	2.48882	-2.01679
C	-2.40875	-4.30011	-0.11703
H	-1.75706	-5.12423	0.19495

H	-3.44072	-4.66967	-0.11379
H	-2.1479	-4.04282	-1.14733
C	-2.50983	-3.56151	2.28429
H	-1.72466	-4.25764	2.59473
H	-2.51773	-2.72735	2.99069
H	-3.4628	-4.09442	2.37839

cat2-d

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C,2.9821952831,-2.4543186088.2643197162
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H,-2.4658462219,1.4106890169,1.4774402501
C,-2.3880074548,3.8129978759,-2.9993810347
H,-2.3399568022,4.0684114358,-4.0642428241
H,-3.363003751,4.1399076508,-2.6205017203
H,-1.6204269823,4.3955141176,-2.4845161749
C,-3.3793350031,1.5651363457,-3.4934781133
H,-3.2729668434.4781047763,-3.4524256249
H,-4.3240757558,1.8341872337,-3.0109342537
H,-3.4693080111,1.855045242,-4.5459311481
C,3.3458748852,3.0127457882,-2.0230576623
H,4.2298104536,3.0929541581,-1.3799518564
H,3.6292395799,3.3505816635,-3.0266388506
H,2.5924329936,3.704390276,-1.6377052794
C,3.9797400227.6349240576,-2.5224078384
H,4.8012819011.6723185233,-1.8007425724
H,3.662393521,-0.4072993803,-2.6131463104
H,4.3940247737.9492912271,-3.4867153975
C,2.9107666586,3.4794185355,2.7274408781
H,3.8551048523,3.7113541309,2.2218809939
H,2.1449547815,4.1447308398,2.3211917108
H,3.0323281665,3.7195846926,3.7899171698
C,3.7216057134,1.1231934109,3.0456524359
H,3.4825459768.0575738009,3.0180812893
H,4.6044414705,1.2894858276,2.4203563355
H,4.0061711152,1.3791183481,4.0720614759
C,-3.0574836511,3.1358374992,2.6111554203
H,-4.0208359537,3.2591527115,2.1033922747
H,-3.1847660925,3.4494610001,3.6537269137
H,-2.3445452811,3.8187738006,2.1409572158
C,-3.68832263.7513761688,3.1076821754
H,-4.5892254572.816243892,2.4907472539
H,-3.375241927,-0.2959050822,3.1365985781
H,-3.978032676,1.0461375196,4.1222032959

C_6F_5H

H,1.7919178078,-1.5592579473,1.1631467796
C.7236664542,-1.7368687082,1.1355795303
C.2043247579,-2.8504126657.487266233
C,-0.1600011699,-0.8565157405,1.7465543528
C,-1.1666641284,-3.0902018322.4430315241
F,1.0236185457,-3.7254768107,-0.1156139689
C,-1.5356619112,-1.0720037614,1.7173236951
F.3001311541.2314443014,2.383086906
C,-2.0356054069,-2.1944832417,1.0619336164
F,-1.6531057618,-4.1679487177,-0.1852939495
F,-2.3749929646,-0.2140620348,2.3108219843
F,-3.3538283768,-2.4137318412,1.0268912969

$CH_2CHSiMe_3$

C,-5.4081334299,-2.5279315618,-1.4602337306
C,-4.5586237453,-3.4107812724,-0.9206179329
H,-4.0450158189,-4.1669584698,-1.5137221413
H,-4.3337590729,-3.4213404984.1446469049
H,-5.5703968615,-2.5955754923,-2.5400469095
Si,-6.3412280739,-1.1878506965,-0.5211941496
C,-5.9085565878,-1.2599116378,1.317505319
C,-5.8656614098.50163574,-1.229353382
C,-8.2000084459,-1.4550377224,-0.7566142806
H,-6.179541779,-2.2225447441,1.7655649302
H,-6.4488802282,-0.4817564331,1.8696752607
H,-4.8390563827,-1.099073182,1.4940189368
H,-4.7984644322.7098895578,-1.0925014755
H,-6.4250118887,1.3088375751,-0.741395294
H,-6.0767647037.5614217009,-2.3035740728
H,-8.4762157181,-1.4490249763,-1.8176382228
H,-8.7804391544,-0.6658333074,-0.2638358196
H,-8.5253477671,-2.4142559796,-0.3382099204

2-L1

Ni,-0.4295098372,-0.0431772176,-0.5456275434
C,-2.1433849755,-0.8573955608,-1.4191669529
C,-1.1948477862,-1.8396793797,-1.1068131817
C,1.1900978545,-0.7968881164.2756580211
H,-0.3683889814,-0.3442723758,2.1897644514
H,1.5816294754,-0.7374511897,-2.2134872037
H,-0.5352046991,-2.2477028237,-1.8721386232
H,-1.3066832354,-2.4767567942,-0.230947301
H,-2.1425977817,-0.4895257767,-2.4482667548
Si,-3.7667393763,-0.6837562849,-0.4807140091
N,1.463059919,-1.0176409526,1.5944530241
N,2.3244893786,-1.2053887221,-0.3688018895
C.5292283469,-0.7071695852,2.6943808855
C,2.4934296301,-1.2088146842,-1.8353199183
C,-3.505513867,-0.8749378853,1.3855639143
C,-4.6029156723.9855079597,-0.8225243473
C,-4.9450052673,-2.0502946278,-1.0723486629
C,2.7347019608,-1.5497428167,1.7670033439
C,3.2767930646,-1.6698936309.5302696319
C,1.0870698422.4114332852,3.5793427156
C.1814222421,-1.9709846422,3.4862826484
C,3.702930443,-0.3697873862,-2.2574075638
C,2.5723773213,-2.6456923248,-2.3623365562
H,-2.9694534178,-1.7970251094,1.6368962319
H,-4.4682929435,-0.9097377805,1.9106051058
H,-2.9389638302,-0.0320561019,1.7970589684
H,-4.1658191569,1.8070136927,-0.24320451
H,-5.6655803798.9411267369,-0.554060278
H,-4.5496390807,1.2610137055,-1.8826416611
H,-5.148963247,-1.9659633339,-2.1465749473
H,-5.9089342834,-2.0061619067,-0.5502021792
H,-4.5194255824,-3.0458942485,-0.8996230549
H,3.1428897918,-1.7887709363,2.7359647412
H,4.2434060341,-2.0362068307.2231805446
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H.3433759466.6980159103,4.3296896896
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H,-0.5926556621,-1.7448337581,4.2262614488
H,1.0494767192,-2.3640426936,4.0270153141
H,3.6300792894.6565343559,-1.8895615501
H,3.7620047537,-0.3345226547,-3.3499378857
H,4.640867933,-0.8014866564,-1.8912234465
H,3.4778771431,-3.151347288,-2.0089595712
H,2.5972367116,-2.6444373872,-3.4565511338
H,1.7073746082,-3.2321950913,-2.0390975253
H,-2.0860264785,1.9859676535,-0.8190616506
C,-1.0405881653,1.841097378,-1.059299378
C,-0.6135979526,2.1867197495,-2.3782844167
C,-0.0508850223,1.8802749394,-0.0273889314
C.6625091718,2.5916069089,-2.6522072812
F,-1.525374088,2.1547009733,-3.3719878927
C,1.2527402593,2.3979243221,-0.3135123078
F,-0.4759343565,2.0642221974,1.2726976096
C,1.6090110493,2.7025462082,-1.5936152942
F,1.0617863484,2.8887149782,-3.9033150122
F,2.1547132954,2.464334632.6838137384
F,2.8803351507,3.027401733,-1.9021980606

2-L1-b

Ni.4304864121.033890229,-0.1229008338
C,1.63780221.3508248576,-1.8032247303
C,2.0585461825,-0.7785964161,-1.097793562
C,-0.9295864863,1.4228657289,-0.442998818
H.369355381,2.4327405062,1.4857084823
H,-1.3190095656,-0.5371620734,-1.9731285227
H,1.7808754079,-1.7835555663,-1.4112583705
H,2.9318168472,-0.739101713,-0.4479884312
H.9692605561.1652839256,-2.6479029436
Si,2.6059029807,1.9603721962,-1.8688116538
N,-1.160102615,2.6352624485.1452890413
N,-1.9186237982,1.3230976829,-1.3828547379
C,-0.4226882622,3.1625801303,1.3125906746
C,-2.1113446635.1573303314,-2.2671704711
C,4.0759668355,1.7453542128,-3.0504776611
C,1.5269284325,3.3496628978,-2.5751797928
C,3.3067164648,2.4089979659,-0.1668990195
C,-2.2602047935,3.2703654671,-0.418381305
C,-2.7370294785,2.4446547557,-1.3813760542
C,-1.3363785238,3.1995173924,2.5426847226
C.195673759,4.5298486791,1.0089446633
C,-3.4699439261,-0.5020311216,-2.0102536925
C,-1.9180693972.5483534613,-3.7352408477
H,4.761185687.9643236086,-2.7002712455
H,4.6545860436,2.673197466,-3.1438081018
H,3.7476552317,1.4628340876,-4.0579568961

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H,2.047586494,4.3144942123,-2.5384515285
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H,4.0050809056,1.6391928504.1834857574
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H,-3.573977641,2.5600395911,-2.0514619381
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H,-0.7553628104,3.4700459965,3.4301438568
H,-1.7910421904,2.2223669359,2.7144985463
H.8623413811,4.4869794561.1439359019
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H,-0.57247136,5.2864118615.8132883257
H,-3.5858558791,-0.7786280855,-0.9592062831
H,-3.5622241309,-1.4106393527,-2.6136257153
H,-4.2976614995.1616716952,-2.2834516126
H,-2.698713356,1.238226089,-4.0742867114
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H,-0.9482911179,1.0304644465,-3.8896940286
H,1.6973196867,-1.343451819,1.7043018494
C.7151457061,-1.4705614207,1.2600590695
C.3537030841,-2.7808434104.8185760145
C,-0.3420328963,-0.5753354002,1.6203364926
C,-0.9467795078,-3.1826296229.7165465637
F,1.342606259,-3.6461965692.5139697933
C,-1.6969508962,-1.0412272775,1.5637307823
F,-0.0895816013.3623611951,2.6069056254
C,-1.9891482066,-2.2839612132,1.0865129194
F,-1.2835702746,-4.4031684355.2577701256
F,-2.6876698189,-0.1825015872,1.8777779764
F,-3.2648748534,-2.6617318556.8747123239

2-L1-c

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C,1.7723099087.6346285195,-1.4859111663
C,2.2396759785,-0.420138128,-0.6974278671
C,-1.1010076211,1.3259804102,-0.4674432182
H.7249042412,2.2261781927,1.0022557229
H,-2.0890116314,-0.6441028877,-1.7226871412
H,2.8318386135,-0.2338819426.1988896259
H,2.3437242669,-1.4257298331,-1.1014255601
H,1.987219379,1.641649204,-1.1199138131
Si,1.5270110748.4859846839,-3.3432328053
N,-1.0463958785,2.5876712157.0559280083
N,-2.2687470826,1.3192704465,-1.1811733754
C.0230090692,3.0633697333.955257851
C,-2.8232783083.1482379363,-1.8917913595
C.5924166378,-1.098530699,-3.790472694
C.6551025875,2.0325193005,-4.0028774786
C,3.2293939617.3888353094,-4.1792068842
C,-2.145970626,3.3452338851,-0.3237784059
C,-2.9150127756,2.5476036849,-1.1042358717
C,-0.530454638,3.3236431043,2.3592387201
C.7333260357,4.2841355724.3637554916
C,-4.1694490593,-0.2674534866,-1.2859530825
C,-2.9448417077.416032204,-3.3952173532
H,1.1552082346,-1.9843974683,-3.4717621553
H.4498515232,-1.1833094386,-4.8749360723
H,-0.393758099,-1.1543899127,-3.3199572775
H,-0.2951956405,2.2264963997,-3.4958634051
H.4523144543,1.9551671137,-5.0779980548
H,1.2853909066,2.9190300622,-3.857952849
H,3.8449767253,1.2683665832,-3.9553303765
H,3.136645533.322746446,-5.2707495693
H,3.7870622877,-0.4932914517,-3.842705697
H,-2.2908782874,4.3671521082,-0.0117231815
H,-3.852644897,2.7458291487,-1.5982115049
H,-1.2581783759,4.1428050277,2.3588751435
H.2838907825,3.6011733274,3.0362799309
H,-1.0138931556,2.4264891861,2.7527491725
H,1.1025733745,4.0763402938,-0.6450733843
H,1.586913149,4.5583499237.9916757635
H.069190308,5.1541535372.3113927648
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H,-4.499401479,-1.2123204053,-1.7280882895
H,-4.9428562245.4813012681,-1.4906743143
H,-3.6652861644,1.215811614,-3.5996943873
H,-3.3004800613,-0.4860216915,-3.9032391135
H,-1.9858880509.6977265849,-3.8349382653
H,1.4685450861,-1.6149451441,1.5623541678
C.5181896148,-1.6833383008,1.0437850151
C.2086967324,-2.9164018073.3932712863
C,-0.5839759544,-0.8718459188,1.4621129635
C,-1.0754611713,-3.3482212287.2157652775
F,1.2318108031,-3.6935980844,-0.0182320046
C,-1.9138911925,-1.3921900243,1.3654279572
F,-0.3815027481.0036171905,2.5098448996

C,-2.1555064936,-2.5698185063.7197691345
F,-1.3576545241,-4.4951053681,-0.4298906226
F,-2.9329949652,-0.6508751014,1.8424806611
F,-3.4123462518,-2.9949959352.4921944569

2-L1-d

Ni.6837430344.2108030046.0434503765
C,2.6508421188.1596912267,-0.6911622482
C,1.8959512189,1.2134746073,-1.224445706
C,-0.8539271262,1.3715355405,-0.3356801149
H.4450371835,2.5926725689,1.4404184215
H,-1.0623897955,-0.6720001189,-1.7813060297
H,1.9658790964,2.2238830938,-0.8227535831
H,1.511064898,1.1703248466,-2.2429601409
H,3.2440387435.4096026344.1942513056
Si,3.3328295382,-1.2575953813,-1.7272181052
N,-1.1829383393,2.5795854087.2072700799
N,-1.8479360047,1.1330389876,-1.2415496145
C,-0.4044678314,3.2552878078,1.264873936
C,-1.909636612,-0.060911472,-2.1072646678
C,4.4788556679,-0.5187021448,-3.0516278809
C,4.3834527857,-2.3929986433,-0.6355324079
C,1.974477647,-2.2284997775,-2.6220052787
C,-2.3551554467,3.0794138815,-0.3464861964
C,-2.7729625796,2.1697346807,-1.2607883628
C,-1.2215644375,3.3561883008,2.5563866528
C.1070326477,4.6140233287.7781749799
C,-3.2106428242,-0.836362799,-1.8805493956
C,-1.7122020536.3220399002,-3.5777391354
H,3.9313571641.136392975,-3.7398254547
H,4.9597306023,-1.2999213041,-3.6537479712
H,5.2749367888.0829215855,-2.5967720469
H,5.1894312109,-1.8309905376,-0.1476667324
H,4.8567437265,-3.1817832108,-1.23318291
H,3.7943269922,-2.8832325792.1442561918
H,1.3315576902,-2.7704448935,-1.9219986111
H,2.409162326,-2.966505607,-3.3075945003
H,1.3404348372,-1.5654154339,-3.2227394791
H,-2.7894432162,4.0199103246,-0.0473582121
H,-3.6351387903,2.1742159083,-1.9084323667
H,-2.0794054075,4.0282049378,2.4401956653
H,-0.5956818934,3.7517843042,3.3626651911
H,-1.5865378507,2.3715451392,2.8557538349
H.689022967,4.5100865198,-0.1428089086
H.7504652694,5.0645228113,1.5405428637
H,-0.715811373,5.311067491.5848148984
H,-3.3334357941,-1.1198919863,-0.8323891905
H,-3.2060048432,-1.7513169499,-2.4812613274
H,-4.0851401418,-0.2489558411,-2.18107265
H,-2.5400829572.9378492285,-3.9462831308
H,-1.6679234547,-0.5806388785,-4.1951159497
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H,1.9912795126,-1.2716257961,1.7799635131
C.9928109946,-1.3691334552,1.3696260961
C.580789145,-2.6534298336.9053684761
C,-0.0451065591,-0.4748488163,1.7851468066
C,-0.7304118992,-3.0402316311.8624682224
F,1.5269950852,-3.5473702809.5447044165
C,-1.4022629219,-0.9268210348,1.8197679474
F.2667641686.4886832005,2.725908903
C,-1.7381392806,-2.1548665671,1.3310409287
F,-1.0981016495,-4.2472991071.3938517894
F,-2.3578977352,-0.0712927033,2.2295466261
F,-3.0281702158,-2.5226646851,1.2057878573

TS1-L1

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C,2.5172502107.9943131745,-1.0839589886
C.0499566742,1.8841269791.2559531977
H,1.0244945385.6059160212,2.1861530234
H,-0.3967105045,1.9559453807,-2.2140202831
H,2.3340910223,1.8034599574,-1.7886781304
H,3.079381479,1.2860167025,-0.198445854
H,2.1725484742,-0.509563546,-2.5394223288
Si,3.459017215,-1.7572236342,-0.7313441499
N.0499488494,2.2880400553,1.557890055
N,-0.5910807559,2.8887480764,-0.4071653826
C.6260238397,1.5018613469,2.6672656556
C,-0.8373070253,2.8926651203,-1.8631630538
C,3.5684636901,-1.5629648778,1.1464320817
C,2.6526712121,-3.4113814433,-1.1674569589
C,5.2057798331,-1.7212060693,-1.4708970143
C,-0.5794634752,3.5184864339,1.7028960537
C,-0.9837356865,3.8967202396.4648127411
C,-0.4629421693,1.0830324947,3.6595514098
C,1.7700370326,2.2662130842,3.3395105963
C,-2.3388430504,2.8684465291,-2.1626711473

C,-0.1220960058,4.0710790905,-2.5303434454
H,3.950264947,-0.5772406444,1.436987604
H,4.2455769211,-2.3112531445,1.5765443415
H,2.5870903165,-1.6988493334,1.6124529773
H,1.6950949783,-3.5487281596,-0.6533235795
H,3.2990988538,-4.2512758895,-0.885355102
H,2.4636615042,-3.493855245,-2.2447477219
H,5.1801895444,-1.8056702804,-2.5639838357
H,5.8183403797,-2.5483774071,-1.0916206067
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H,-1.2806750453.5657587089,3.1507531482
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H,2.2404242517,1.637890529,4.1023456627
H,1.4120899121,3.1763579412,3.8335128457
H,-2.8182444713,2.0112883388,-1.6837873536
H,-2.5005810185,2.788121523,-3.2420683042
H,-2.8344665962,3.7829783498,-1.8187250789
H,-0.5439203902,5.0313696906,-2.2132738776
H,-0.2284084184,4.0052198139,-3.617636255
H.9455018229,4.072729752,-2.2899323919
H.6251058912,-1.1870607416,-0.9027557435
C,-0.7780315147,-0.9791182946,-0.2206100139
C,-1.8484706385,-1.0385407599,-1.1133495158
C,-0.9588155036,-1.7038362848.9573191004
C,-3.0233977463,-1.7392181376,-0.8635589383
F,-1.7670494288,-0.3729201426,-2.2970541653
C,-2.113326547,-2.4217691906,1.2525841061
F.0287545213,-1.718383458,1.8951018995
C,-3.1577428569,-2.4404955747.3321478837
F,-4.0303708007,-1.7473917013,-1.7554149786
F,-2.2364838477,-3.090813627,2.4130830352
F,-4.2816950014,-3.1281816206.5933724844

3-L1

Ni,-0.1525922273,-0.2743469073,-0.56964001
C,-2.1945733219,-0.7728295832,-1.2168871986
C,-1.2868887848,-1.8151771041,-0.6264665891
C,1.3916743193,-1.0948212951.1199681006
H,-0.1264360016,-0.6952410347,2.0902024306
H,1.7144744309,-0.8808512795,-2.3662919541
H,-0.9947444044,-2.6208577172,-1.3017831434
H,-1.5570458402,-2.2042716769.3579613936
H,-2.3029258834,-0.8854247496,-2.3019847507
Si,-3.8786175341,-0.4510131611,-0.370585239
N,1.6757105998,-1.3867614576,1.4187605724
N,2.4926418605,-1.4896147505,-0.5766025509
C.7634406576,-1.1300404978,2.5520254828
C,2.6389020492,-1.3623551084,-2.0413035693
C,-3.5784638597,-0.1296160583,1.4678841176
C,-4.6627880461,1.0773967633,-1.1601515122
C,-4.9892449003,-1.9595446099,-0.6171472104
C,2.9401057288,-1.9525596925,1.5312794626
C,3.4530119776,-2.0180185096.277640455
C,1.3679237953,-0.1061251619,3.5163059062
C.3832234433,-2.4429026972,3.2424810629
C,3.8126973114,-0.4442074765,-2.3920884113
C,2.7478336153,-2.74166498,-2.6966113799
H,-3.1765920797,-1.0091067668,1.9831986636
H,-4.5138975735.1408747345,1.9728118036
H,-2.8754820754.6986340506,1.6163937671
H,-4.0301545043,1.9636730901,-1.0300070334
H,-5.6372526207,1.3035965754,-0.710886048
H,-4.8230192018.9422880903,-2.2364854406
H,-5.1826309664,-2.1442939947,-1.6803941414
H,-5.9610552791,-1.8210127303,-0.1281920193
H,-4.5369780031,-2.8673196003,-0.2016634968
H,3.3619098977,-2.2514102303,2.4773880873
H,4.4038475195,-2.3879652691,-0.0711215472
H,2.2870027976,-0.4813569162,3.9797388941
H.6556043265.1116397811,4.3183948622
H,1.5909967602.8298084757,2.9994220255
H,-0.0330800037,-3.1579264699,2.5264770441
H,-0.368179447,-2.2537298357,4.0154288261
H,1.2474740292,-2.9094720672,3.7279631739
H,3.7161538263.5232160596,-1.8917003326
H,3.8349019523,-0.2684095471,-3.4716682452
H,4.773690382,-0.8865888819,-2.1065595402
H,3.665472176,-3.2607294583,-2.3982728844
H,2.7654286381,-2.6350514617,-3.7857921421
H,1.8947406527,-3.3723413471,-2.4287581988
H,-1.7092435885.2853250406,-1.1410675068
C.4464367456,1.6083652396,-0.7252630501
C.9241139396,2.1522244786,-1.9087230366
C.3868424639,2.5019686606.3339793717

C,1.330586028,3.4763106153,-2.0554460238
F,1.0095191961,1.3700454446,-3.0284915507
C.7756170821,3.8369878227.2560364208
F,-0.086343177,2.084149139,1.5488770409
C,1.2542424421,4.3270547347,-0.9561674243
F,1.7891703323,3.949736161,-3.2311527972
F.6957767806,4.6607073619,1.3198875256
F,1.6373408869,5.6114901762,-1.0650487723

TS2-L1

Ni.6398655391.874763525,-0.5230281849
C,1.7370689465,-0.6632215119,-0.1094796172
Si,-0.7953866149,2.982461481,-0.4293255818
C,-0.9938429988,-0.0070015664.1197700134
N,1.9375903726,-1.7874454263,-0.8503873928
N,2.4957994658,-0.845126547,1.0070968112
C,-2.5898974884,2.4640168764,-0.8148211999
C,-0.5279810946,3.3550663981,1.4138668105
C,-0.7572942684,4.7073499269,-1.2673522128
C,-1.3713415691,-0.2700718697,1.4301023203
C,-1.8139198698,-0.6057284697,-0.8310409313
C,1.3109351909,-2.0474166465,-2.1622801783
C,2.8076861872,-2.6586120786,-0.2054601411
C,2.6249772832.1398884192,2.1015428937
C,3.1589077749,-2.0661831899.9618723537
H,-2.6648525704,1.9321886002,-1.7684925196
H,-3.2096558117,3.3657981956,-0.8904857131
H,-3.0165544227,1.8229372113,-0.0409320718
H,-0.6998398164,2.4867603038,2.0515677717
H,-1.213685019,4.1533100777,1.7276435924
H.4909605606,3.7158255446,1.6002390163
H.1591271556,5.2788731107,-1.0839293607
H,-1.5912879672,5.2968323028,-0.8661356057
H,-0.9021869674,4.6527210325,-2.3533132205
C,-2.4776816222,-1.0367665025,1.7922341227
F,-0.6446421538.2409013682,2.4710302079
C,-2.9266137499,-1.3877175866,-0.5380389535
F,-1.5526620368,-0.4151448834,-2.1621982642
H.6780179745,-1.1765402313,-2.3397271866
C.4239506999,-3.2947749296,-2.1042838848
C,2.3733825395,-2.1381534684,-3.2620768902
H,3.0922072603,-3.6121954594,-0.6204038983
H,1.8771654897.9024478767,1.8703696049
C,2.2816316107,-0.494129293,3.452002674
C,4.0183642392.7771125864,2.0941171326
H,3.8076735193,-2.4069459393,1.7525626747
C,-3.2649350352,-1.6038135813.7953101031
F,-2.7920523992,-1.2444297164,3.0855394075
F,-3.6817988533,-1.9316007246,-1.5121896073
H,1.0157754717,-4.2055004988,-1.9594599482
H,-0.1260947038,-3.4009627142,-3.0441933984
H,-0.3028213204,-3.2243141447,-1.2905097213
H,2.9981403219,-1.2400666804,-3.2856016723
H,1.8893761264,-2.243736234,-4.2379899574
H,3.0272301217,-3.0055902055,-3.1193947646
H,1.2871057299,-0.9442410719,3.4312441976
H,2.2897474952.275961158,4.2297137788
H,3.0109678608,-1.2595884028,3.7391164144
H,4.7984332399.0387979511,2.3103990972
H,4.0755718275,1.5564129638,2.86062062
H,4.2406189635,1.2343518005,1.1252539617
F,-4.3340675947,-2.354230637,1.1140230264
H,2.3518931869.9733889223,-2.369181368
C,2.1762320117,1.5808430675,-1.4829334998
C,1.2139413994,2.6431126374,-1.5564222609
H,3.0605013143,1.728208069,-0.8665916782
H,1.5045937942,3.558127204,-1.0455617059
H.7575402736,2.8349086007,-2.5263690151

4-L1

Ni.5689479047,1.0478545488,-0.5033626852
C,1.7469945948,-0.5086555693,-0.1097173307
Si,-1.1350655655,2.7495121336,-0.3257385125
C,-0.9541718214.0068634962.0562320457
N,1.975093816,-1.587546985,-0.9102889111
N,2.4977723012,-0.746558736,1.0026636284
C,-2.9461515661,2.2610307868.0507393112
C,-0.5788265949,3.7324567414,1.2162373749
C,-1.4329801772,3.9795586056,-1.7679511847
C,-1.2403904023,-0.3360801661,1.3733258891
C,-1.75467111,-0.6304307453,-0.88688868
C,1.3769529601,-1.7817168441,-2.2471466876
C,2.8506193793,-2.4827083207,-0.3072935248
C,2.6133695172.1713710069,2.1559332557
C,3.1792910244,-1.9536779615.8961854379
H,-3.4132509818,1.7222132826,-0.7811901029
H,-3.5214642653,3.1849050669.1978070432
H,-3.0646572232,1.6525585633.9510613137

H,-0.5372698096,3.0810339973,2.0966052013
H,-1.299677999,4.5317857486,1.4338985457
H.4063848712,4.1995089442,1.1045009623
H,-0.5799655654,4.6157753043,-2.0215572856
H,-2.2634498081,4.6449938934,-1.4992427361
H,-1.7351795071,3.4501637416,-2.6805268759
C,-2.2257443581,-1.2449980804,1.7476528818
F,-0.5507379002.2572581185,2.3897709089
C,-2.7558241834,-1.5453415094,-0.5728575952
F,-1.5896168086,-0.3445466236,-2.2117114743
H.7091476135,-0.9284323367,-2.377542798
C.5454533152,-3.0668747927,-2.2880045352
C,2.4545084138,-1.751936351,-3.3353760719
H,3.1527867227,-3.407064687,-0.7730751339
H,1.8790411713.954710557,1.9550431082
C,2.2412834417,-0.5395648126,3.4606104171
C,4.0166045886.784412282,2.2205914708
H,3.8223638769,-2.3309086151,1.6748133057
C,-2.9917422927,-1.8612974007.7621040427
F,-2.4482012495,-1.5355777523,3.0433191866
F,-3.4960433819,-2.1261373373,-1.5359809792
H,1.1746576759,-3.9586913285,-2.1904431034
H.0166020627,-3.1363891526,-3.2432364994
H,-0.1966524194,-3.0807553245,-1.4855903142
H,3.03821739,-0.8272003496,-3.2935281535
H,1.9858956621,-1.815067172,-4.3223406679
H,3.1472703546,-2.5953780009,-3.2409550463
H,1.2483973293,-0.9877488196,3.3952803297
H,2.2335415812.1840476801,4.2815799906
H,2.9667667244,-1.319654224,3.7164400529
H,4.7747425487.0256273257,2.4441348689
H,4.0564151535,1.537818505,3.0135576454
H,4.2894746065,1.2670353336,1.2776854444
F,-3.9461397171,-2.7477274233,1.0947490996
H,2.680075599,1.1422165663,-2.0232014171
C,2.3253998991,1.8298114991,-1.2625014283
C,1.3055736332,2.7274862764,-1.5417788068
H,3.0122250252,2.0170297734,-0.4422065676
H,1.2456577671,3.6561550971,-0.9858947293
H.8472441826,2.7398235464,-2.5253309235

TS3-L1

Ni.5465958023.7434952726,-0.9742570294
C,1.6665241569,-0.7223183438,-0.2292814992
Si,-0.7505619128,2.6308402626.0458543826
C,-1.1385433758.5500015312.1319956131
N,1.5869795219,-2.0469846634,-0.5667035181
N,2.7321791728,-0.6741243702.6259413947
C,-1.5310787148,2.993017425,1.7537965469
C.9192436044,3.5471740512.2012291165
C,-1.9519202482,3.4864086164,-1.1446423794
C,-1.0366125775,-0.0358764007,1.408340586
C,-2.2596869878.1178635769,-0.6000997576
C.5961273255,-2.6000998263,-1.5083930891
C,2.5752867312,-2.7956109536.0603455245
C,3.2434264251.5647436988,1.2393840313
C,3.2982286488,-1.9293439648.8114916301
H,-2.5702867829,2.651021588,1.8149838388
H,-1.5343846629,4.0795244379,1.9125308985
H,-0.9794159616,2.5440216563,2.5849363158
H.6973773348,4.6243338948.2112743662
H,1.63538284,3.361229939,-0.6004022849
H,1.3974439774,3.3157346167,1.1586519587
H,-1.6618963446,3.447724091,-2.1954484818
H,-2.0241178461,4.5421809206,-0.8520943147
H,-2.9575787108,3.0626486582,-1.0586966891
C,-1.9269379815,-0.9662336944,1.9179918216
F,-0.0052103368.3128952987,2.2106737771
C,-3.1777767887,-0.8190063841,-0.1291282431
F,-2.5019591831.5988189802,-1.8393715587
H,-0.000903316,-1.734222113,-1.8073672758
C,-0.3112559757,-3.6198148171,-0.8139724574
C,1.2843553699,-3.1822105309,-2.7473662681
H,2.6784399426,-3.8608549321,-0.0721999959
H,2.5225324874,1.3271761577.9386918246
C,3.258788683.4591165662,2.7670548889
C,4.6186841411.9265589246.6682056124
H,4.1478081897,-2.100690723,1.4533284308
C,-3.0140178247,-1.3646529901,1.1384036191
F,-1.7560928394,-1.4990519532,3.139670932
F,-4.2145627373,-1.2060982878,-0.890774245
H.2430505688,-4.5156682025,-0.5127946899
H,-1.1084711909,-3.936892631,-1.4937345456
H,-0.7728222141,-3.1898750365.0791020195
H,1.9323228163,-2.4402938215,-3.2232045616
H.5325757847,-3.4991264217,-3.4770764053
H,1.8941071892,-4.0576169515,-2.4972865601
H,2.2712255604.1937543099,3.1513900647

H,3.5521287848,1.4199824894,3.2019622895
H,3.9776918197,-0.2915902549,3.1135867472
H,5.3763967692.1849812395.9448809215
H,4.9442997512,1.8960387903,1.0591652491
H,4.5862283019.9913696771,-0.4234174107
F,-3.8883926752,-2.2626154514,1.6092032067
H,1.5160002823.0315785001,-3.235384046
C,1.5271640363.9787978972,-2.6994432329
C.3971675427,1.8173135666,-2.6951823931
H,2.5234759064,1.3912953291,-2.5435907871
H.5273221109,2.8920047752,-2.5978926768
H,-0.5056893901,1.5167459809,-3.2232782118

TS4-L1

Ni,-0.890491232.8202903379.4336427434
C,-2.1642393457,-0.7558124398.3746693392
Si.0058730717,2.8925504965.1504166451
C.8302910532.3348047889,-0.0613486197
N,-2.0889251163,-1.9667765376.9976138767
N,-3.2279736214,-0.8847827413,-0.4696250453
C,1.2415597034,3.3064754412,-1.2368583621
C,-1.6012215673,3.8488601001,-0.2980397838
C.7357580673,3.6550073162,1.7399490951
C,1.1666915831.0161746732,-1.3789247852
C,1.8086866731.0191370847.8828712251
C,-1.0490780007,-2.3204806031,1.9859832511
C,-3.0767745208,-2.8294763186.5473862979
C,-3.6792221723.1843374677,-1.3837682512
C,-3.7986564437,-2.1448309722,-0.3778375538
H,2.2498519604,2.9464412788,-1.0046037698
H,1.3058061328,4.3945206771,-1.3697613391
H.9467388869,2.8717051266,-2.1976886252
H,-1.8526055127,3.7113382862,-1.356383686
H,-1.452784822,4.9255490365,-0.1333627596
H,-2.4705787906,3.5478234038.2967361764
H,-0.0023617063,3.7197245064,2.5465518071
H,1.1014645474,4.6724040389,1.5456377003
H,1.5795772228,3.0660445396,2.1155589426
C,2.3730981235,-0.5706221137,-1.7458822755
F.289085673.2860112101,-2.3824220422
C,3.030434565,-0.5670528985.5640394227
F,1.5794101284.2728273798,2.2024523396
H,-0.4973541108,-1.3908753264,2.1439315603
C,-0.0954337629,-3.3740724604,1.4136584199
C,-1.6810170041,-2.7620452183,3.3091921356
H,-3.1870910819,-3.8387001374.9113513033
H,-3.0055363983,1.021150012,-1.1740009307
C,-3.4916589233,-0.2347133671,-2.8443257698
C,-5.1146070258.6060691845,-1.0604543864
H,-4.653685487,-2.4482486096,-0.9608605206
C,3.3173112866,-0.8651675829,-0.7648799227
F,2.6407997421,-0.8618535057,-3.0325784931
F,3.9317876356,-0.8574320559,1.5211400713
H,-0.6067908281,-4.3279605081,1.2427016859
H.7238275119,-3.5552047862,2.1163800487
H.3342605777,-3.0390886936.4656208841
H,-2.3738499114,-2.0062776293,3.6921363653
H,-0.898796522,-2.9175821475,4.0583445617
H,-2.2304809751,-3.7039211256,3.2034675382
H,-2.4503495554,-0.5090928218,-3.0362348621
H,-3.7527953184.5974847031,-3.5057631111
H,-4.1313806683,-1.0838671754,-3.1085669447
H,-5.8289648515,-0.2005855131,-1.2585861529
H,-5.4007466732,1.4611933012,-1.680522426
H,-5.2096831816.8986227512,-0.010064987
F,4.4887523548,-1.4353305034,-1.0972519693
H,-0.8298444946,1.6346969111,3.4364700379
C,-1.877332469,1.3995207552,3.2729483488
C,-2.7804447847,2.3398663192,2.9848852343
H,-2.1659168778.3600326752,3.396091295
H,-3.8318523245,2.0980733907,2.845255489
H,-2.507825219,3.3872135189,2.8879400935

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Ni,-0.2615264079,-0.4853566542,-0.1717029962
C,1.6396325625,-0.4236602846.0561488362
Si,-0.7540339198,1.6509039822.3146568934
C,-2.1114725888,-0.8592971372,-0.4369931321
N,2.5944620973,-0.2396244423,-0.9018974543
N,2.3476802294,-0.7108898412,1.1877319951
C,-2.1649860717,2.4043381528,-0.7174705413
C,-1.2552572739,1.762503466,2.1500304363
C.7262131063,2.8305807732.0621552107
C,-2.9270742225,-1.3632527024.572105195
C,-2.6954450477,-0.8410168761,-1.701267193
C,2.2869689071.0438592375,-2.3209000394
C,3.8657667461,-0.4109825459,-0.3791459618
C,1.7199857764,-1.0279152484,2.4893903115

C,3.7104308937,-0.7075809719.9384236621
H,-2.0210478514,2.2419316538,-1.7908433946
H,-2.2158924075,3.4882894366,-0.5468669206
H,-3.1356620377,1.9773059782,-0.4461036745
H,-2.0365402115,1.0403571913,2.404877224
H,-1.6372750994,2.7684263264,2.3723859194
H,-0.4065714819,1.5805052535,2.818997539
H,1.6195561701,2.51594752.6116611085
H.461771028,3.8396618007.4078986252
H.9948979136,2.9137141979,-0.9972306279
C,-4.2281774249,-1.815641968.3682538649
F,-2.4612976367,-1.4273759993,1.8520034206
C,-3.9889332607,-1.2809052368,-1.9662465534
F,-1.9916647485,-0.3631276743,-2.7650032716
H,1.2206607025.2883041315,-2.3193082755
C,2.5099183573,-1.2040813901,-3.1808436456
C,3.0817033932,1.2507599173,-2.8240210134
H,4.7620724806,-0.3070565282,-0.9697577868
H.6588554273,-0.8098295672,2.335324691
C,1.8791207855,-2.5155213152,2.8170170884
C,2.2667373981,-0.1201974809,3.5937844764
H,4.447011256,-0.9083490423,1.6999873283
C,-4.7616428157,-1.7729997871,-0.9170203093
F,-4.9740087102,-2.2963179809,1.3809557469
F,-4.5049739849,-1.244554759,-3.2093101709
H,3.5633622816,-1.5052503698,-3.1860991262
H,2.2131014021,-1.0020452256,-4.2147801529
H,1.9133165475,-2.0449974272,-2.8143958254
H,2.944063611,2.1168968235,-2.1709063906
H,2.7404507496,1.521215316,-3.827721243
H,4.1534697017,1.0336498832,-2.8891389415
H,1.4626118142,-3.1385130083,2.019592896
H,1.3485313117,-2.7509482777,3.7448029131
H,2.9316176863,-2.7876563811,2.9537615819
H,3.3193507701,-0.3331117368,3.8107646071
H,1.7013683479,-0.2804047399,4.5166321029
H,2.180523192.9351672136,3.3192758341
F,-6.0108114436,-2.2100726553,-1.1451758663

TS5-L1

Ni.3453867841.1319413636,-0.2207297175
C,2.1499724721,-0.1304248836.2695211005
Si,-0.8662701764.8321179592,-2.2932236273
C,-1.5406590015.2718513718,-0.4353201847
N,2.8367283615,-1.3178522842.2981178335
N,3.0385799039.7675749228.8018819718
C,-2.5928895603,1.0389511066,-3.0683376097
C,-0.0219763035,2.5235043463,-2.4207960495
C.0158214309,-0.4653632394,-3.3607358148
C,-1.9433952353,1.2314561538.5153289271
C,-2.0785723656,-1.016781884,-0.2406486074
C,2.2610176303,-2.5979625111,-0.1544210467
C,4.1048087382,-1.1594355798.8364637821
C,2.7317251404,2.1964209617.995439571
C,4.2322825213.1549308496,1.1539436102
H,-3.1508931337.0954238505,-3.0739452739
H,-2.5047022856,1.3753522776,-4.1095362202
H,-3.1980497661,1.7786496053,-2.5319586183
H,-0.4465396157,3.2421100862,-1.7150637604
H,-0.1625214953,2.9255843395,-3.4336726239
H,1.0526196408,2.4555593893,-2.2304783971
H,1.096773247,-0.4668980801,-3.1968345016
H,-0.1686251662,-0.2464390092,-4.4220729928
H,-0.359578556,-1.4728080287,-3.1620525923
C,-2.8033802809.9459919436,1.5713402567
F,-1.5450247793,2.5213834991.3966874963
C,-2.9416442177,-1.3360386218.8003521576
F,-1.8024150129,-2.0061319307,-1.1252244353
H,1.2914538144,-2.3131657412,-0.5767421418
C,2.0275974701,-3.5388046178,1.0309886951
C,3.1205153499,-3.231949615,-1.2512349338
H,4.803861297,-1.9737089425.9439393212
H,1.7412866508,2.3158646831.54419789
C,2.6420023399,2.5365979703,2.4860960711
C,3.7359987192,3.0780556132.2478579041
H,5.0620126889.6903995427,1.5876933588
C,-3.2976723136,-0.3473572933,1.7161561626
F,-3.142598157,1.8910245151,2.4643669864
F,-3.4146221447,-2.5845172573.9538982743
H,2.9698093121,-3.823490548,1.5127537961
H,1.5345544347,-4.455794095.692375673
H,1.3878150721,-3.063947357,1.7811862088
H,3.2773414287,-2.5338590635,-2.0792001782
H,2.6207317028,-4.1222625492,-1.64576049
H,4.1009734186,-3.54338424,-0.8735191917
H,1.8978877203,1.9062574906,2.9825979428
H,2.3456104976,3.582511614,2.615776857
H,3.6043773056,2.3961552503,2.9910493888

H,4.7425276447,3.0014324464.6744882179
H,3.4295979064,4.1269647597.3100488248
H,3.7913794101,2.7997780419,-0.8090839348
F,-4.111023487,-0.6434435813,2.7371526639

6-L1

Ni,3.0085310781,-0.4973867022,2.9394614383
C,2.9263005354,-0.2958057132,4.861643489
Si,-0.1391395843.2826145053.3311551943
C,1.7550990702.2969706429.5850275967
N,2.7946325274.8494582871,5.5926084537
N,2.9619556179,-1.2871296593,5.7985204042
C,-0.5229732347,-0.839216289,-1.1397650487
C,-0.9442410368,-0.3875344265,1.9024133531
C,-0.7991381211,2.0188436778,-0.0101258598
C,2.4015815281,-0.8630757944,1.1323656429
C,2.5890902939,1.3426058169.2453827272
C,2.7318795946,2.1973801902,4.9925091235
C,2.7490528845.577124899,6.949473251
C,3.0987398394,-2.7195146961,5.4618991403
C,2.8547873874,-0.7726864206,7.0789290219
H,-0.0812469958,-0.4510115419,-2.0648148983
H,-1.604955859,-0.9228687606,-1.2990048494
H,-0.1279274715,-1.8478457682,-0.9805422634
H,-0.5818614579,-1.3927260704,2.1372591029
H,-2.0339981051,-0.4386281416,1.7878165155
H,-0.7304935399.2546089216,2.7644545259
H,-0.5522330684,2.7236319301.7908152647
H,-1.8932960439,1.9780516342,-0.0852845613
H,-0.4177806481,2.4340225525,-0.9474807955
C,3.8321325551,-0.966752252,1.2659441932
F,1.6951668665,-2.0515491325,1.0726724264
C,3.9962935564,1.2881696636.3533400682
F,2.0930154241,2.5143479266,-0.2201718465
H,2.7748402845,2.0080884372,3.9152610895
C,3.9494455378,3.0303256696,5.4017806086
C,1.4047203608,2.8816576216,5.3280927606
H,2.6478724249,1.3440332938,7.7009658355
H,3.2117289211,-2.7221351195,4.3732127479
C,4.3614092711,-3.3070572701,6.0968644849
C,1.8307436743,-3.4911855159,5.8350395466
H,2.8628225517,-1.3902755832,7.9630738301
C,4.6048605081.1497517424.8290703042
F,4.4566628625,-2.1883230735,1.2460602942
F,4.7332512887,2.3614095354.0078679814
H,3.959192395,3.2318055909,6.4787641547
H,3.9320367027,3.9934636335,4.882373819
H,4.8793248602,2.5171217352,5.1383650121
H.5565188881,2.2615128692,5.0223857532
H,1.3375470094,3.8380644603,4.8004016649
H,1.3125315307,3.0865362143,6.4003440435
H,5.2477290003,-2.7348215724,5.8065560608
H,4.4972512981,-4.3398458608,5.7616533803
H,4.3004917476,-3.3190063846,7.1910158023
H,1.6643622054,-3.5016042614,6.9181138956
H,1.9181601653,-4.5300071982,5.5015939669
H.950889685,-3.0522836799,5.3549390898
F,5.9436211843.0674319369.8613826734

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Ni.0438453842.3592639569,-0.8758576915
C,1.9426990188.1990151773,-0.3975024793
Si,-2.7888905073,1.8613841307.1925827031
C,-1.7721952611.2325780104.1331539515
N,2.7291098256,-0.9148102319,-0.4794056837
N,2.7813894701,1.1604758008.0862269239
C,-3.6464341869,1.9196483335,1.879946069
C,-1.6856429956,3.3839050159.0070475162
C,-4.1173850494,1.9151360864,-1.150702595
C,-0.6128587359.0909142671.9789298565
C,-2.4424934019,-1.002200712,-0.1688336594
C,2.2631711964,-2.2236521144,-0.9775952966
C,4.0258875603,-0.6501996557,-0.0563349606
C,2.372441409,2.5525285528.3539672949
C,4.0584762217.6572991209.3009087805
H,-4.2910757267,1.0455783883,2.0292406601
H,-4.2783653763,2.8121871077,1.9679240794
H,-2.9220492852,1.9421079997,2.7013515785
H,-2.3052462571,4.2888790483.0477380115
H,-1.1520680124,3.3963207287,-0.9492439829
H,-0.9501231318,3.4494912639.813230871
H,-3.7192527731,1.7512136831,-2.1565031012
H,-4.59072059,2.9053066474,-1.1432331552
H,-4.9016199147,1.1723202312,-0.9807691125
C,-0.287299191,-1.1756327256,1.573111128
F,-0.2691627799,1.1740483075,1.7887210696
C,-2.0855255042,-2.2135684192.3491197378
F,-3.5330840407,-0.967538221,-0.9732378975

H,1.1938077545,-2.076514332,-1.1543495336
C,2.4536636131,-3.3137839105.0814624411
C,2.9475615606,-2.574678263,-2.3025596589
H,4.8009849924,-1.3997536928,-0.0413203978
H,1.3190501734,2.5805861721.065996807
C,2.4885063229,2.8777807969,1.845560386
C,3.1598808351,3.5289559643,-0.5246692325
H,4.8671188201,1.2577319342.6861719498
C,-0.9734576118,-2.3002710251,1.2337873132
F.7967040535,-1.2525162609,2.3732044579
F,-2.7460347704,-3.3472115483.0353568744
H,3.5156901983,-3.5139048633.2622272324
H,1.9958035049,-4.2474505449,-0.2595624233
H,1.9910981386,-3.0308563798,1.0289257994
H,2.8099336289,-1.7796136264,-3.0414370682
H,2.5245301046,-3.4988722071,-2.7085390467
H,4.0234889722,-2.7309926466,-2.1674695516
H,1.9161957576,2.162181793,2.4396788402
H,2.0942068595,3.8806534512,2.0389453895
H,3.5309322363,2.8606762707,2.1827450381
H,4.2260525479,3.5314488425,-0.2721055833
H,2.7833600134,4.5466709195,-0.3807312408
H,3.061395314,3.2746881409,-1.5844878718
F,-0.5831118954,-3.5158077315,1.6620224496
H.9456082037,-0.2699705546,-3.2287107885
C.4432436133.6277195391,-2.8772955589
C,-0.9299610491.6451943216,-2.6892775203
H,1.0037279806,1.5510536103,-3.0012625648
H,-1.4685483514,1.5875418876,-2.6647485021
H,-1.5376008861,-0.2361358358,-2.8780360518

P1

Si,-1.3847165048,3.2434209245.5708116354
C,-0.6367136458,1.4759685534.4333199841
C,-3.0279888666,3.2363207697,-0.3537914168
C,-1.6668255201,3.7179805228,2.3711139038
C,-0.1608535958,4.4398642957,-0.2205100768
C,-0.3377815269.6431695935,1.5128337053
C,-0.3531440546.9388481714,-0.8247014157
H,-2.8995861432,2.9716048916,-1.4077616056
H,-3.4954937165,4.2273629361,-0.3124766344
H,-3.7321684869,2.5222387664.0878173361
H,-2.3676659969,3.0474440233,2.8770290457
H,-2.0926413522,4.7285110866,2.4067713008
H,-0.739364335,3.7309833326,2.9511243912
H.8048265676,4.4247593488.2971822887
H,-0.5431609877,5.466543291,-0.1733222495
H.0195110691,4.1989927145,-1.2725857715
C.2037125765,-0.632255107,1.3658782854
F,-0.5663764518,1.0481377955,2.7789106686
C.186884997,-0.3278052465,-1.0192476025
F,-0.6061388945,1.6651006334,-1.9369693384
C.4673463144,-1.1197277474.0904758431
F.471563194,-1.3901533832,2.4387647556
F.4375837859,-0.7891952899,-2.2523752672
F.9867837549,-2.3409849869,-0.0696685456

TS6-L1

Ni.2663802121.2694587267.131521547
C,-1.0448904695,-1.9289392598,-0.660251428
C.2640716608,-1.6366510021.0540493454
C,2.1020282729.2315258208.4866691103
H.9202726972.5862661509,2.6832185838
H,1.8673363334,-0.1495898271,-1.9899755582
H,1.1312324677,-2.0707500805,-0.4513998997
H.262234651,-1.9700968715,1.0994364428
H,-1.0326544092,-1.5346271288,-1.6858041679
Si,-1.4800907808,-3.7937200773,-0.7715625355
N,2.7051968595.4128017458,1.694989965
N,3.1270038063.1352798567,-0.406055661
C,1.975836347.6088862827,2.9679367564
C,2.9454073328,-0.0159406335,-1.8656165259
C,-1.6234682057,-4.5217749574.9693250469
C,-3.1378002223,-3.9558909518,-1.6696476972
C,-0.1410671464,-4.7193570649,-1.7397384697
C,4.0859859739.4347858773,1.5558988778
C,4.3508595301.2626208487.2354550559
C,2.2922991287,1.9842580658,3.5622306652
C,2.2627879386,-0.5376262699,3.9408312435
C,3.3733944938,1.2600352514,-2.5963000046
C,3.6726702803,-1.2608825487,-2.379477812
H,-0.6664345789,-4.4960169299,1.5028045127
H,-1.9485178799,-5.5687055571.9350514711
H,-2.3540872487,-3.9731788319,1.5757342811
H,-3.9373285179,-3.4298057708,-1.134646212
H,-3.4421392967,-5.0054624291,-1.7638130385
H,-3.0896531999,-3.5359072708,-2.6813761329
H,-0.0085796745,-4.301811668,-2.7450299164

H,-0.4016344039,-5.7781901082,-1.8580454962
H.8299562113,-4.6788757841,-1.2328368218
H,4.7551216932.5715048305,2.3900901964
H,5.2915227804.2260242146,-0.2901482233
H,3.3418539468,2.0656204913,3.8658936076
H,1.6749154051,2.1528344225,4.4496964842
H,2.0776191256,2.7797440464,2.8423958251
H,2.0243058853,-1.5063164094,3.4916429163
H,1.6518867477,-0.4202111273,4.8411841341
H,3.3132077841,-0.5529053524,4.2519368806
H,2.8229470267,2.1282634447,-2.2222011757
H,3.1673940675,1.1612620571,-3.6666611403
H,4.4455243734,1.4513810335,-2.4767693771
H,4.7601965602,-1.1626889607,-2.2898551873
H,3.4413638453,-1.4115022663,-3.4382382819
H,3.3631861819,-2.1561198361,-1.831849917
H,-1.8860478315,-1.4400375381,-0.1506780709
C,-1.3062224014,1.5277916354,-0.0231093856
C,-1.7324846213,2.0777468206,-1.2232865558
C,-2.010603637,1.9546238984,1.0931351888
C,-2.7811093047,2.9861775107,-1.3370420722
F,-1.1143748116,1.7290743897,-2.3892382834
C,-3.0673996451,2.8599987698,1.051948056
F,-1.681251245,1.4767364024,2.3313185866
C,-3.4527787794,3.3789693044,-0.1816958687
F,-3.1603546871,3.4934618096,-2.5273181651
F,-3.7230539162,3.2440271582,2.1659358837
F,-4.4688547065,4.2547996467,-0.2575305822

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Ni.8169444635.1295052427,-0.1283918079
C,-0.8131667388,2.3429377475.7180061388
C.4558977027,1.5857902647,1.0850265804
C,2.3068180782.9477987089,-1.067923039
H,3.1342529365.4791169639,1.2535900575
H.3470000155.9482169838,-2.6384750287
H.3793943714,1.0979466433,2.0608613451
H,1.3353813471,2.2373480404,1.0771029634
H,-1.6787160196,1.668778264.724035322
Si,-1.221369921,3.80897519,1.8782665124
N,3.5798116818,1.1503033038,-0.6237372313
N,2.3346670783,1.3533142541,-2.3699720378
C,4.0420891742.8016680064.7371225631
C,1.1655004842,1.2985901118,-3.2744086314
C,-1.2834635115,3.2263496807,3.6786379271
C.0912458003,5.1657148715,1.7052051731
C,-2.9094264458,4.5147421805,1.3825100928
C,4.3825204991,1.6698065199,-1.6265430015
C,3.5973644861,1.7974414431,-2.7287081041
C,4.6189973176,2.0280706693,1.4485882894
C,5.0254108913,-0.3708894582.6861406313
C.8239428044,2.6917175089,-3.8082160625
C,1.3943141485.2776941858,-4.3928382997
H,-1.9963615203,2.4038530723,3.8117712159
H,-1.5917557255,4.0387452295,4.3479357319
H,-0.3063794816,2.871158666,4.0255472468
H,1.0879079042,4.8116667483,1.9936642487
H,-0.1431978815,6.0264841752,2.3433753703
H.1577162164,5.5348265559.6744692751
H,-2.9140782086,4.8574636111.3406546273
H,-3.1883423172,5.3702255805,2.0097871972
H,-3.7023266795,3.7639530677,1.4826007931
H,5.4259579182,1.9007126395,-1.4819958951
H,3.8331618044,2.1619507348,-3.7158284139
H,5.5472120257,2.3731450154.9797032938
H,4.848196505,1.7769979404,2.4887524521
H,3.9047344088,2.8568893765,1.4481033875
H,4.5744210139,-1.2363357462.1912390476
H,5.3044284416,-0.6660625792,1.7022978138
H,5.9430081561,-0.1057458026.1495141055
H.6787093547,3.4030132284,-2.9898443777
H,-0.1014342588,2.6464021392,-4.3903257898
H,1.6105665887,3.0793577919,-4.4649438127
H,2.2136685153.5793130674,-5.0546277097
H.4894315028.1852815356,-5.0012164259
H,1.630203297,-0.7087077898,-3.9819182487
H,-0.75443604,2.7499680125,-0.3012598214
C,-0.5723388983,-1.0419586207.5587329019
C,-1.6178616411,-1.4271381082,-0.2721770683
C,-0.5897317486,-1.6287361982,1.8187887299
C,-2.6217545991,-2.3199475444.093488275
F,-1.699676192,-0.9149103461,-1.5369306051
C,-1.566864975,-2.5245014016,2.2464570873
F.3860586358,-1.3327287305,2.723265857
C,-2.5922751117,-2.8725924969,1.3708682917
F,-3.6136125096,-2.6572886604,-0.7538904936
F,-1.5370375829,-3.0664078835,3.4796568291
F,-3.5447903311,-3.7392059464,1.755095581

TS7-L1

Ni.1191662108,-0.2494174767.0032312194
C.7386747107,2.3732466786.1164633837
C,-0.4576432662,1.5043767123.4745745882
C,1.9918507672,-0.9247498501,-0.4732143253
H,1.8634343554,-0.8695177702,2.0275641396
H.8242830864,-0.4649187187,-2.6408615869
H,-1.3650635707,1.8015967294,-0.0581327089
H,-0.6690055974,1.4790490921,1.5494231089
H.9117609472,2.3743287619,-0.9687895517
Si.5696175663,4.2030021477.6662579824
N,2.9710087687,-1.3449199384.3782771767
N,2.5101814447,-1.1542222325,-1.7134764707
C,2.8486306188,-1.3110499169,1.8516938067
C,1.7849641318,-0.8705910226,-2.9713565545
C,-0.9649632768,4.9843628564,-0.1174058898
C.4406200981,4.2956014063,2.5521176965
C,2.1142631435,5.1377241024.0888506818
C,4.0705702938,-1.8210188296,-0.312999967
C,3.7791253475,-1.70052327,-1.6365493823
C,3.9233805431,-0.4103002905,2.465924322
C,2.8657158787,-2.730011022,2.4259889586
C,2.524837621.1842678899,-3.7975875886
C,1.5330590644,-2.1626556825,-3.7532282583
H,-0.9424552343,4.9124034476,-1.2114400993
H,-1.0382767617,6.0485030774.1382391785
H,-1.8873104592,4.5020728279.2249891141
H,-0.4613705608,3.7955234222,2.9222807068
H.399669616,5.3371558713,2.8929341034
H,1.3017843548,3.8250719166,3.0417254677
H,3.0287076626,4.721607002.5282443525
H,2.0690397238,6.1968305433.3707050695
H,2.2245649864,5.094724069,-1.001374156
H,4.9537091312,-2.2012740332.1756109677
H,4.3641973048,-1.9572311446,-2.5054146853
H,4.9284291422,-0.8247234503,2.3296238761
H,3.7507571229,-0.3075670496,3.5415840909
H,3.9019448074.5888460275,2.0204574517
H,2.0813332133,-3.3437462033,1.9728442892
H,2.6906243714,-2.695498262,3.5056272593
H,3.8303208346,-3.2223134442,2.2592880472
H,2.6948226822,1.0941392394,-3.2143299416
H,1.9310925542.4485524104,-4.6779847489
H,3.494868503,-0.1846885738,-4.148697302
H,2.4679363196,-2.6120149193,-4.10590318
H.9141244934,-1.9497416769,-4.6301771702
H,1.0072531483,-2.8973279227,-3.1361055998
H,1.6605701036,1.9944018888.5807181093
C,-1.6499817317,-0.8307182411.2819993609
C,-2.5000560871,-1.0752442861,-0.7917303244
C,-2.1655007972,-1.1567184521,1.5323317405
C,-3.7731944044,-1.6232027524,-0.6568869691
F,-2.0969236874,-0.7774206446,-2.0587697184
C,-3.4306764066,-1.7069672614,1.7224724331
F,-1.4221488697,-0.9432354917,2.652556818
C,-4.2411789607,-1.9423428966.6150194716
F,-4.557428706,-1.8469843377,-1.7289274282
F,-3.8818854372,-2.0169228392,2.9531241643
F,-5.4656028586,-2.4747952165.7728634705

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Ni,-0.4262458829.1952435275.3794039528
C,-2.2115057541,1.1992615593,1.2347212192
C,-0.9229166918,1.9327192757.9661823332
C,-0.4018330284,-1.7115707605,-0.1336114698
H,-1.1608915301,-0.4277150001,-2.1415382224
H.4221826449,-1.596354393,2.2294581703
H,-0.4067036913,2.3130540323,1.8478491438
H,-0.9339097613,2.668898231.158877226
H,-2.3022206907.9111771761,2.2887283784
Si,-3.8274142028,2.0302070843.6370109842
N,-0.7127690452,-2.2526614477,-1.3449341451
N,-0.0166851417,-2.7779568459.6221233196
C,-1.1844282465,-1.4601764735,-2.4993665766
C.4336330849,-2.6693466328,2.0255683481
C,-4.0358794112,3.6552948299,1.5765366633
C,-3.7222481342,2.3497654168,-1.2222458687
C,-5.2874206659.8809231138.9985062243
C,-0.5269673469,-3.6279486791,-1.3441412122
C,-0.0868987097,-3.9591101754,-0.1029276219
C,-2.6207671839,-1.8434636464,-2.8663520498
C,-0.2191171863,-1.5838415933,-3.6806460617
C,-0.5440333465,-3.3774364224,2.9673840677
C,1.8711119744,-3.1742617151,2.1752580638
H,-4.0969984558,3.4897288589,2.6586556916
H,-4.9515467637,4.1760531454,1.2714576681
H,-3.1938186095,4.3325345534,1.3950988341

H,-2.8667856072,2.981778195,-1.4849275927
H,-4.6256654091,2.857560864,-1.5812599078
H,-3.6288518841,1.4145058296,-1.7869969294
H,-5.1969886159,-0.0710581995.4614753384
H,-6.2369487499,1.3367885682.6927225795
H,-5.3663372734.6493413673,2.0673542476
H,-0.7155541774,-4.2461512235,-2.2074242191
H.1793061223,-4.918400357.3114555663
H,-2.6809269408,-2.8752430482,-3.2301935001
H,-2.9913510783,-1.1892629649,-3.6616635408
H,-3.2890740477,-1.7478899215,-2.0047632838
H.7905969947,-1.2818727421,-3.3920104459
H,-0.5475558103,-0.929503763,-4.4939927123
H,-0.1816082121,-2.6068815751,-4.0709912128
H,-1.5592979975,-2.9861822637,2.8485396106
H,-0.2385839153,-3.2212341743,4.0067693303
H,-0.5698982095,-4.4578719163,2.7868108554
H,1.9444128025,-4.2529073618,1.9968254637
H,2.2271818061,-2.9801755549,3.1913954359
H,2.5398112917,-2.6629289956,1.477358117
H,-2.222326256.18595181.6777146007
C,1.382223234.6813985214.0536202638
C,2.3600771803.6376175149,1.0393752286
C,1.8259967797,1.1038396003,-1.193087604
C,3.692599702.980280258.823604402
F,2.0336983576.2379687596,2.3040982593
C,3.1448985593,1.4581529002,-1.4661899625
F.9468457284,1.1857747922,-2.2349686171
C,4.0880949565,1.3972410316,-0.4441830828
F,4.6020857183.9165034097,1.8157275773
F,3.5223559073,1.8592805631,-2.695943416
F,5.3695228198,1.732814057,-0.6800949096

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Ni.7739575623.4358601473,-0.2655718125
C,-0.6202974293,2.4804154571,1.2972279819
C.3219355894,1.2791442998,1.3663746122
C,1.693740387,-0.1086866916,-1.9519275928
H,2.1910317266,-1.8962463599,-0.264063946
H.4500463092,2.0052242096,-2.4471019728
H.0887916908.6237608284,2.2116383595
H,1.390106503,1.5968081312,1.4722859912
H,-1.6552726781,2.1301768479,1.1810957111
Si,-0.5830555656,3.648705293,2.806970751
N,2.4676325209,-1.2093893749,-2.1701992706
N,1.650409898.5158171351,-3.1630014822
C,2.7782689893,-2.2127295458,-1.129464041
C.8931991934,1.7600348714,-3.4163220324
C,-0.9503154535,2.6847936742,4.3957477293
C,1.1190534202,4.4717387617,2.9529443239
C,-1.9015462328,4.9912414579,2.5716232612
C,2.8960136773,-1.2695476449,-3.4861878977
C,2.3792577962,-0.1797240814,-4.1136601918
C,4.2665948823,-2.1811280142,-0.7720239273
C,2.3028095391,-3.6031672251,-1.5577485503
C,1.833264141,2.8905291692,-3.8427421721
C,-0.2372421714,1.5150067202,-4.4184579875
H,-1.9056969125,2.1503431531,4.3316426316
H,-1.0081968314,3.3557663112,5.2614700631
H,-0.1732770114,1.9422717597,4.6109596268
H,1.9109004091,3.7401889443,3.1521283973
H,1.1390473961,5.2014906734,3.7715348251
H,1.3887048414,5.0066669017,2.0339088044
H,-1.7354251519,5.5630821979,1.6505869294
H,-1.9040998226,5.7062606662,3.4033961654
H,-2.9075125678,4.5591627776,2.5094880493
H,3.5197084207,-2.0627561192,-3.8666447224
H,2.4709719472.1453920293,-5.1378586766
H,4.8917799443,-2.4797271857,-1.6208316715
H,4.465994993,-2.8750427544.0505278187
H,4.5738686116,-1.1797312247,-0.4548059864
H,1.2420540395,-3.5898065732,-1.8242888587
H,2.43752407,-4.3073721923,-0.731334826
H,2.8707981119,-3.9835745085,-2.4139791692
H,2.6280817039,3.0418959891,-3.1055673503
H,1.2711752493,3.82484691,-3.9360412166
H,2.2993899236,2.685567203,-4.8127938083
H.1474215502,1.23597109,-5.4056960932
H,-0.8285635305,2.4281822814,-4.5377179372
H,-0.9037922098.7246488151,-4.0644615101
H,-0.4116681753,3.0941830133.4075911137
C,-0.7796909725,-0.6057965345,-0.1622063863
C,-1.9323663497,-0.2812722204,-0.8684854876
C,-0.8457571312,-1.779680755.5799983525
C,-3.0842626237,-1.0639863377,-0.8577271181
F,-1.9688320795.8502206158,-1.6262729695
C,-1.972572521,-2.5970870981.6223979931
F.2315507735,-2.185234702,1.3089581153

C,-3.1046677233,-2.2327899502,-0.1015174649
F,-4.1746549265,-0.7082993318,-1.5632854016
F,-1.9853937519,-3.7295679975,1.350781319
F,-4.2046771783,-3.0061090933,-0.0755208445

TS8-L1

Ni,-0.0267048228,-1.35824691,-0.8765142237
C,-3.0013760193,-1.0278963509,-0.0117044867
C,-1.9143126553,-0.7437057501,-1.042778722
H,-2.2373896052,-0.027149476,-1.7984147887
H,-1.6627415551,-1.6811767253,-1.6242924578
H,-3.2849065594,-0.0957829937.4957031598
C,-5.3048982828,-0.7153716988,-2.0946039259
C,-4.2373852469,-3.5359896771,-1.3963634759
C,-5.851731279,-1.93583192.6949182684
H,-5.4957677108.3061499227,-1.7441181909
H,-6.2567383599,-1.1167383051,-2.462888382
H,-4.6287733314,-0.6469053343,-2.954810521
H,-3.5354412338,-3.5140565712,-2.2381455694
H,-5.1557180005,-4.0184738218,-1.7523884268
H,-3.8056694698,-4.1857433254,-0.6253468287
H,-5.4719009322,-2.5566760068,1.5151691655
H,-6.7935144809,-2.3828973804.3545740674
H,-6.0899328889,-0.9507854455,1.1134549707
H,-2.6258586973,-1.6955016449.7724340154
C,-0.5415205957.3549478901,-0.3017189356
C,-0.5557057773.6095305069,1.0822480352
C,-0.2942278464,1.493123352,-1.0912822051
C,-0.3394193369,1.8651220774,1.6354085851
F,-0.7315250307,-0.4217623483,1.9498189908
C,-0.0751382249,2.7619837179,-0.5757179027
F,-0.2611485741,1.3547059203,-2.4438374748
C,-0.1051140453,2.9576908097.8040962346
F,-0.3338781162,2.0358931066,2.970954622
F.1660635539,3.806435969,-1.3904219605
F.0964810125,4.1809081163,1.3251886708
C,1.7214475203,-2.1094020165,-0.7504813491
N,2.8321518792,-1.798655944,-1.4846945088
N,2.1681350349,-3.0393457095.1468140397
C,3.9393191775,-2.5108829235,-1.0498840969
C,3.521050826,-3.2926895823,-0.0205280018
H,4.9146184361,-2.4121431152,-1.4995584547
H,4.0666363176,-3.9955609389.5889240414
Si,-4.5970391712,-1.8044609806,-0.7175788069
C,2.8374405392,-0.8074058351,-2.5789743263
H,1.8023531549,-0.4576315699,-2.62687311
C,1.310481929,-3.6510945891,1.1808167455
H.3107025077,-3.2665407461.955765264
C,3.2066350265,-1.4678442333,-3.9095801852
H,3.1195789293,-0.7399404849,-4.7222639453
H,4.2370488851,-1.8408515767,-3.9058187729
H,2.5382781134,-2.3061986705,-4.1290694465
C,3.7410773726.3793598044,-2.2329726256
H,4.7931190368.0827544498,-2.1558373128
H,3.6673124538,1.1430945778,-3.0135619528
H,3.4409793124.8325611491,-1.2833086814
C,1.3017353259,-5.1762630494,1.0516004542
H,2.2828091588,-5.6103768747,1.2743491504
H.5833479377,-5.6045379765,1.757535114
H,1.0127265988,-5.4822725947.0412462041
C,1.7171374953,-3.1717640113,2.5770013024
H,1.0390767371,-3.5889959854,3.328269586
H,2.7346427373,-3.4883762335,2.8317354053
H,1.6655254507,-2.0812259232,2.6413986126

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C,1.7671157868,-0.0445107049.5110435434
C.9181738114.2092469173,-0.7575724214
H,1.1555701065,-0.5420210645,-1.5179028788
H,1.1664425249,1.1865954302,-1.1819896631
H,1.4826893333,-1.0129770762.9418129374
Si,3.6528654498,-0.0317160654.24656661
C,4.1475094947,-1.4069824224,-0.9576854358
C,4.1995589777,1.6412358219,-0.4517957925
C,4.4936257428,-0.3238277178,1.9176853735
H,3.815089983,-2.3901965076,-0.603625383
H,5.2364721516,-1.4545672793,-1.0793316323
H,3.7174605399,-1.2556328096,-1.9547517727
H,3.770650086,1.834459781,-1.4421493773
H,5.2901619675,1.6876710835,-0.5586769084
H,3.9013429792,2.4696028931.2020546362
H,4.2575724595.473371574,2.6326247434
H,5.5849800505,-0.3579481693,1.8147353775
H,4.1777772339,-1.2721831173,2.368194664
H,1.5168298701.7097358258,1.2697217298
C,-0.5696375836.1657832523,-0.4906557299
C,-1.3026354309,1.30411587,-0.2285262586
C,-1.2679944122,-1.0847076307,-0.4360315827

C,-2.6649094107,1.2710563417.1434831492
F,-0.7320582932,2.5270600152,-0.334091734
C,-2.6566845094,-1.1582184099,-0.0587247982
F,-0.4940324001,-2.2121379844,-0.2633874293
C,-3.3192670487.0666761616.2551225946
F,-3.319905138,2.4282518355.3581023018
F,-3.1624006668,-2.2940887392.5217745633
F,-4.5943001951.0282479823.6771551529
Ni,-2.4528484327,-1.2490578435,-1.9701285054
C,-2.9983577899,-1.6479024247,-3.7799694753
H,-3.2633117789.8192503775,-3.5152504372
H,-2.3326875213,-3.7882435041,-2.6953025788
N,-3.4521024056,-0.7956585413,-4.7447930809
N,-3.0246780106,-2.87399985,-4.3795137223
C,-3.6053876467.6594544918,-4.5423561355
C,-2.612510633,-4.1196985321,-3.700285169
C,-3.752977568,-1.4740494059,-5.913785297
C,-3.4821675508,-2.7869013927,-5.6825881171
C,-5.0765332291,1.0692217297,-4.6461048394
C,-2.6987776266,1.4387277474,-5.4980502998
C,-3.7861857794,-5.0964270114,-3.5961951069
C,-1.3887372902,-4.7315673672,-4.386023776
H,-4.1281481927,-0.9839411254,-6.7982720181
H,-3.5783913345,-3.6436543851,-6.3306661765
H,-5.471790339.9106603383,-5.6555732307
H,-5.1843969875,2.1321623537,-4.4089880055
H,-5.6893708816.4984510235,-3.9418357005
H,-1.6568122102,1.1212717427,-5.3925562134
H,-2.7543582932,2.5085627878,-5.2739922086
H,-2.9972990639,1.3015389341,-6.5433420367
H,-4.643592225,-4.6257037462,-3.1058176065
H,-3.4905509388,-5.9676745388,-3.0034735815
H,-4.1049089722,-5.4563568357,-4.5808217772
H,-1.6179740291,-5.0638084374,-5.4047859863
H,-1.0440829887,-5.6034625934,-3.8214117238
H,-0.5668809413,-4.010674578,-4.4353910032

P2

C,-2.0128836139,1.2454597437,3.3849758666
C,-1.5159801298.1810674459,2.3799007071
H,-0.4419869201.0182143536,2.5096910882
H,-1.6666260782.533543858,1.3554720837
H,-1.8729783511.8685359338,4.4070996595
Si,-1.1707220876,2.9521500175,3.2583623539
C.6967329113,2.769858084,3.5116143314
C,-1.5080575321,3.7186680778,1.5613029712
C,-1.8949568866,4.0573425664,4.6124078351
H.9310878232,2.2665598528,4.4569969359
H,1.186751541,3.7505925607,3.5339194315
H,1.1670629146,2.1943921921,2.7058736396
H,-1.1002872374,3.1106468712.7455207484
H,-1.0518532458,4.7126425121,1.4806851636
H,-2.5825601552,3.837119015,1.3779305375
H,-2.9778823209,4.1829368344,4.4959660939
H,-1.4466832903,5.057743444,4.5936964114
H,-1.7189872141,3.6392118954,5.6105091457
H,-3.0955879113,1.3819838617,3.2605156656
C,-2.2197768856,-1.1494647507,2.5323862502
C,-3.3802333095,-1.456050245,1.8207763935
C,-1.7661996529,-2.1216841977,3.4248437955
C,-4.0530695353,-2.6653146636,1.9706867973
F,-3.881527031,-0.5619584563.9471618007
C,-2.4152237507,-3.3403594179,3.5987684872
F,-0.6565593386,-1.8897533156,4.1521256794
C,-3.5673298768,-3.6124379497,2.86698685
F,-5.1614661561,-2.9215561461,1.2619275469
F,-1.9417395287,-4.2486764263,4.4631893347
F,-4.2042255705,-4.7791683713,3.0242167149

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Ni.4627735055,-0.1894697071.2319430071
C,2.0116108027,-1.1804922747,-0.8970124853
C,1.2716753643,-0.2926503223,-1.6678580249
C,-0.87939777,1.2026722674,-0.2531130004
H.4160181763,-0.6340746918,-2.2403246967
H,1.6865710266.6636360428,-1.9773513174
H,1.6261844603,-2.2027328146,-0.8620684714
Si,3.8861619277,-1.0593671287,-0.6373349922
N,-1.0529558351,2.4628638004.2875287791
N,-1.8441468166,1.1677521645,-1.2451250742
C,4.4924096125,-0.5723751182,1.0903380963
C,4.5756951685,-2.7767937978,-1.0407603438
C,4.6042793889.1885691662,-1.869376421
C,-2.0751209316,3.1648403813,-0.3482897878
C,-2.5764137156,2.3517071955,-1.2998425846
H,4.0915284227.39201274,1.4235231741
H,5.5859104279,-0.4799289643,1.0794778053
H,4.2411217426,-1.3273418968,1.8419384393

H,4.1750380545,-3.5355675264,-0.3591175474
H,5.6689446917,-2.7996445006,-0.9545963246
H,4.3189945252,-3.0819527844,-2.0621201969
H,4.3591908908,-0.0762250893,-2.9041441155
H,5.6979857777.2187498555,-1.7882825387
H,4.2418845181,1.2064663109,-1.6920203747
H,-2.3373444502,4.1705686946,-0.065680878
H,-3.3761917493,2.4944093889,-2.0073554094
H,2.080001049,-0.7233152904,2.133923701
C,1.161520304,-1.2304424636,1.8610066225
C,1.1833645346,-2.6558097404,1.8503927137
C,-0.0822000285,-0.5644839426,2.1183491306
C.0549278111,-3.4000111164,2.0278233237
F,2.372494846,-3.2802384235,1.6894760978
C,-1.2444003826,-1.3778892106,2.3456076164
F,-0.0351795785.5833046045,2.8936238133
C,-1.1820338612,-2.7384337869,2.2777908882
F.0663073436,-4.7457829206,1.9821942916
F,-2.4210592164,-0.7676394375,2.6109191963
F,-2.2850821332,-3.4977127611,2.4164412047
C,-0.319413075,3.1122062988,1.3580694257
C,-0.9546549733,3.2773869154,2.609575577
C.9439469157,3.6775335781,1.0761811233
C,-0.2693972041,4.0008347637,3.5937811956
C,1.5864969761,4.3789578472,2.1050145718
C.9899542226,4.5385751931,3.3520246209
H,-0.7292935298,4.1392613391,4.566870824
H,2.5608243522,4.8194574987,1.9243509432
H,1.5049155945,5.090850816,4.1333568341
C,-2.1155322727.1274143644,-2.2193468417
C,-2.9774578241,-0.9358456778,-1.8718841054
C,-1.6080094249.2843800057,-3.5311430603
C,-3.2678473163,-1.8858122515,-2.8607769293
C,-1.941804786,-0.6914595024,-4.4796308792
C,-2.7529916559,-1.7715427066,-4.148224896
H,-3.9156605164,-2.721978367,-2.6220318432
H,-1.5613478108,-0.6023297036,-5.4919272309
H,-2.9942136102,-2.5201836815,-4.8977481334
C,-0.7566846368,1.480904189,-3.9588546076
C.4524717167,1.0847512337,-4.8278350318
C,-1.6096397573,2.523522473,-4.7126630768
H.1465161678.7536134767,-5.8260638332
H,1.1095502875,1.9502710086,-4.9665106872
H,1.0417218086.2837430274,-4.3744537778
H,-0.997179093,3.3885535196,-4.9910223373
H,-2.0244480046,2.0972771915,-5.6330921537
H,-2.4459571247,2.8879770877,-4.1098883596
H,-0.3695553697,1.9583565704,-3.0538786547
C,-3.6518223171,-1.0266284985,-0.5059155578
C,-3.9128220851,-2.4699090422,-0.04666777
C,-4.9780711055,-0.2362446172,-0.5022885848
H,-4.716719428,-2.9430864473,-0.62170255
H,-3.0217204475,-3.0976560719,-0.1341972605
H,-4.2209884634,-2.4731132826,1.0018393495
H,-5.4532848988,-0.2986273989.4831276045
H,-4.8275671404.8228570641,-0.7310439087
H,-5.6787035921,-0.6437583482,-1.2403647234
H,-2.992280565,-0.5631064123.2301461454
C,1.5691050412,3.6206477926,-0.3168291141
C,1.0760816838,4.7999840096,-1.1822224749
C,3.1056218748,3.5954849024,-0.3002152799
H,1.3770880399,5.7588177603,-0.7443683564
H,1.5056867724,4.7423313418,-2.1890888385
H,-0.013021207,4.8066473849,-1.2848040233
H,3.4835750551,3.4200973977,-1.312829601
H,3.5327926505,4.5472449414.0338645638
H,3.4944289855,2.8057113194.3497659864
H,1.236647052,2.6942090517,-0.792280617
C,-2.3510031118,2.736485716,2.9198575962
C,-2.436568798,2.0280107051,4.2852192114
C,-3.4040936666,3.8627689503,2.8639545308
H,-2.3254752518,2.7311066765,5.1181951952
H,-3.418520835,1.5548919455,4.3932143948
H,-1.6737258142,1.2554479056,4.3819254655
H,-4.4049308997,3.4583211702,3.0531867358
H,-3.2025659531,4.6236689076,3.6266647742
H,-3.4278042386,4.3682660319,1.8944152485
H,-2.603016096,1.9942866454,2.1581434861

2-L2-b

Ni.0684549404.5488946813,-0.1555580841
C,1.6740903612,1.7588051469.8597517393
C.4431077501,1.9587013173,1.4337128481
C.5034913153,-1.3460058961.3514016074
H.0795071995,1.3499481132,2.2584030302
H,-0.1321694652,2.8583299458,1.2315817655
H,2.2732167515.9363232361,1.2498792366

Si,2.5938785958,3.0642129241,-0.1637701441
N,1.0617311577,-2.3757532162,-0.3790626585
N.2242185613,-1.952335514,1.5601072195
C,1.7255684812,4.7335325151.0090160454
C,4.3285049551,3.1950755084.5897062275
C,2.7519528752,2.6386575592,-2.007930455
C,1.1187450696,-3.5595924887.3530976725
C.5893189434,-3.2962764168,1.5665895251
H.6991594149,4.7076702049,-0.3696118632
H,2.2633599647,5.5029248428,-0.5590061568
H,1.6884391769,5.0634047826,1.0536271812
H,4.2839654925,3.4564577171,1.6534996688
H,4.9170941198,3.9714118316.0857624223
H,4.8867263747,2.2559843998.503734391
H,2.7258960147,1.5628672646,-2.2053241343
H,3.6962272386,3.0271615089,-2.4090307374
H,1.9468062052,3.0951351216,-2.5950658086
H,1.5330710084,-4.4657147532,-0.0560349505
H.4409893714,-3.9262122797,2.428144897
H,-0.0620696722,2.2478305061,-2.0177733768
C,-0.8652574721,1.8292269038,-1.4167893398
C,-1.8852314111,2.7348913679,-0.9991289535
C,-1.2151638388.436981713,-1.6167383978
C,-3.1610458385,2.3309388584,-0.7401971977
F,-1.5753604789,4.0486064573,-0.8806771184
C,-2.5819236278.0598917566,-1.3665887431
F,-0.6480381176,-0.2054335933,-2.7207007601
C,-3.5057449447.9618602918,-0.929643447
F,-4.1136797501,3.1822600674,-0.3075000555
F,-2.9379573797,-1.2370665858,-1.5256652294
F,-4.7591086982.5790064481,-0.6135368518
C,-0.2971970551,-1.3332209193,2.7618032208
C.6202622499,-0.9107362632,3.7509409925
C,-1.6950235375,-1.2634673419,2.9533525989
C.0996464434,-0.3672375599,4.9330245485
C,-2.156158955,-0.7043020204,4.1527444292
C,-1.2724921141,-0.2560962367,5.1305153439
H.7793698654,-0.028500111,5.7079626155
H,-3.223254727,-0.623850351,4.3270304436
H,-1.655829244.1731338062,6.0520583768
C,1.630416577,-2.3198418531,-1.7126131012
C,2.9817009515,-1.926961991,-1.8507869259
C.8621588584,-2.7755623346,-2.807186585
C,3.5296941843,-1.9278738364,-3.1402301703
C,1.4682329141,-2.7625092399,-4.0705494823
C,2.7798926159,-2.3324572085,-4.2405545315
H,4.5598716406,-1.6205686591,-3.2839603222
H.9027874801,-3.0941058728,-4.9347163231
H,3.2246860518,-2.3254394073,-5.2319068612
C,2.1325878274,-1.0693927224,3.6001243348
H,2.3483727627,-1.2260920616,2.5390429936
C,-2.6871602513,-1.8218119926,1.9360202049
H,-2.2422009126,-1.7245379904.9425619637
C,3.8668972535,-1.6011031517,-0.6471441624
H,3.2225663476,-1.2120002739.1467850486
C,-0.5523011152,-3.3347556085,-2.6508019026
H,-0.9845835005,-2.9035711064,-1.7447180164
C,2.9200516604.1742214424,4.0532592943
H,3.9770904347.0617367901,3.7877848014
H,2.5491887491,1.0886015019,3.5824327971
H,2.8761036611.3129178648,5.1387747469
C,2.6328996651,-2.3121073728,4.3661817548
H,2.45181422,-2.2075146728,5.4418735787
H,2.1353303446,-3.2274403394,4.0330282259
H,3.7107909187,-2.4442979438,4.2195717165
C,-2.9477178562,-3.3227132363,2.1871365394
H,-3.3799133125,-3.4830890305,3.1818280421
H,-3.6554951689,-3.7120379831,1.4468037468
H,-2.0340734056,-3.9195987412,2.1171292165
C,-4.0262263588,-1.067721524,1.9158759179
H,-3.8876059889.0146623404,1.8495242128
H,-4.6131348317,-1.3823112806,1.0495299644
H,-4.6271817849,-1.277126722,2.8080912721
C,4.5515614252,-2.8789828035,-0.1144919604
H,3.8279511698,-3.6406167048.1870037027
H,5.2017783283,-3.3180957536,-0.8798255785
H,5.1724716215,-2.6456643018.758176653
C,4.9386151739,-0.5365329325,-0.9342040892
H,5.7231343948,-0.9139300554,-1.5991554164
H,4.5163992755.3621551261,-1.3904861423
H,5.4301903856,-0.2471207888.0008279367
C,-0.5139732309,-4.869424208,-2.4847120658
H,-1.5286328982,-5.2642337368,-2.3600069774
H,-0.0758099347,-5.346994146,-3.3687347944
H.0704874175,-5.1810819774,-1.6150098103
C,-1.4914762487,-2.9754553882,-3.815948625
H,-1.215668791,-3.4933492294,-4.7414027133
H,-2.5131204672,-3.2839149222,-3.5712937054

H,-1.499937463,-1.9020033812,-4.007056217

2-L2-c

Ni,-0.2028271316,-0.3351991087,-0.61732977
C,-1.870160523,-1.9446907918,-0.0235495547
C,-1.9471708648,-1.4094472555,-1.2808831491
C,-0.8351158848,1.327208149.3249138266
H,-2.4589956042,-0.4751800362,-1.4918203671
H,-1.693068717,-2.0000660511,-2.1578711772
H,-2.3019843258,-1.3535138759.7846984193
Si,-1.4485448647,-3.7528304098.3448003822
N,-1.5686765818,2.3712384768,-0.2057297911
N,-0.6848333794,1.7067918163,1.6439177001
C.0710005262,-3.9203113907,1.457894348
C,-2.9520470226,-4.5053232225,1.2263002236
C,-1.1978679452,-4.708731746,-1.2672308676
C,-1.8590524992,3.3412634624.7507386345
C,-1.3050314374,2.926015307,1.9090809585
H.9899873695,-3.6993138432.9064367683
H.1581533646,-4.9434704886,1.8439710084
H.0275251384,-3.2447712665,2.3195096386
H,-3.1699023984,-4.0178467984,2.1824283254
H,-2.784412482,-5.5695508199,1.4338688576
H,-3.8530881252,-4.4308858142.6058556271
H,-2.1004886333,-4.6972257978,-1.888978683
H,-0.9715396931,-5.7589456174,-1.0445718575
H,-0.3658789538,-4.3200195934,-1.8599791409
H,-2.4265017419,4.2259039333.5146798406
H,-1.2881306199,3.3755910701,2.8879219783
H.4549895269,-1.6823062554,-2.7052378637
C,1.0413744177,-1.2942630949,-1.8758863983
C,2.0618274726,-2.1564582823,-1.368033639
C,1.2844091521.1336945786,-1.8025337965
C,3.2387462931,-1.6917976439,-0.8620443606
F,1.8775162929,-3.4960888057,-1.4561034441
C,2.5701522562.5862164723,-1.3423676082
F.7635646444.9029836542,-2.841284155
C,3.4997250395,-0.2911077432,-0.8718826835
F,4.181955262,-2.5171808406,-0.3648656951
F,2.8262825298,1.9145051629,-1.336063262
F,4.6717842904.132581697,-0.358873992
C,-2.0566704369,2.5169143032,-1.5641599676
C,-1.2616663265,3.2059082587,-2.5098817964
C,-3.3643949759,2.067343098,-1.8635451752
C,-1.7888342234,3.3670895125,-3.7979102821
C,-3.8358748391,2.2599669344,-3.1690587898
C,-3.0538334004,2.8919109475,-4.1300568724
H,-1.1998954856,3.8758223265,-4.5528230482
H,-4.8302262032,1.9160920269,-3.4330487386
H,-3.4365447787,3.0275467539,-5.1379928058
C,-0.0159716663.9863339246,2.7086489804
C,-0.7961390724.1900423893,3.5766700454
C,1.3643401939,1.2035619038,2.9245233898
C,-0.1433490269,-0.4456813821,4.6415846942
C,1.9626621546.5363143757,4.0016184825
C,1.2228198569,-0.2863342153,4.8460630281
H,-0.7141803321,-1.0686018616,5.3223162474
H,3.0225743978.6677165854,4.1875745728
H,1.7109325415,-0.7924994506,5.6742801706
C.0893122202,3.8299121578,-2.1543707114
H.5548784181,3.204795886,-1.3887765575
C,-4.293209619,1.4616289693,-0.8079873877
H,-3.6688222125,1.0294560362,-0.0192115877
C,2.1812327796,2.1813539772,2.0809007368
H,1.7889128951,2.1546689491,1.0602099823
C,-2.3122115579.0601527165,3.4395410556
H,-2.5805756038.326600991,2.4125561288
C,-5.1991133453.3397002504,-1.3480403317
H,-4.6387548373,-0.4251980758,-1.8923285649
H,-5.7128559508,-0.1524470053,-0.5152823259
H,-5.975046199.7278251853,-2.0165806739
C,-5.173866385,2.5557629785,-0.1658588166
H,-4.5790457714,3.3414513129.3069130197
H,-5.8142873475,3.0286161209,-0.9190149299
H,-5.8241533395,2.1222538102.6025127679
C,-0.0973509474,5.2488993313,-1.5726771266
H.8765125337,5.6831591444,-1.3200993946
H,-0.5781025787,5.9094230175,-2.3037010901
H,-0.7055649236,5.2557998368,-0.6648729931
C,1.0732059155,3.9058495592,-3.334757763
H,2.0556495439,4.2186567842,-2.9666973493
H,1.1941314861,2.9411998529,-3.8288185473
H.7625739645,4.6457072327,-4.0812771069
C,2.0329875909,3.6259667437,2.6080092663
H,2.6346519461,4.3114756592,2.0004986688
H,1.0000154342,3.9804759636,2.5785421714
H,2.3857671356,3.6992360024,3.6434419594
C,3.6757994134,1.8295655873,2.013350964

H,4.1901932285,2.0641962641,2.9524544503
H,3.8454031346.7749777028,1.7906770299
H,4.1573330815,2.4159714451,1.2259682928
C,-3.0401847601,1.0404831197,4.3840441867
H,-2.805786621.8190940369,5.4314478158
H,-2.7633178378,2.0811640893,4.1945752198
H,-4.1257709284.956258638,4.2588526069
C,-2.8184916094,-1.3697937503,3.6963277635
H,-2.2537656613,-2.1084131489,3.1234043184
H,-2.7489439574,-1.6441164207,4.7542843701
H,-3.873351222,-1.4509920986,3.4128818671

2-L2-d

Ni.3003417812,-0.5289143559,-0.5347776016
C,2.223926841,-1.4386550769,-0.1206025637
C,1.1808100248,-2.02613433.5834425284
C,-1.4651000716,-0.8007819779.3554473875
H.6929215655,-2.9316985801.2328821827
H,1.0327707616,-1.7995977242,1.6324134095
H,2.4804832116,-1.9031532414,-1.0745391066
Si,3.6653395151,-0.5326046069.7234228645
N,-2.6349423818,-1.3490760496,-0.1375325927
N,-1.7822504202,-0.5576172229,1.6788106413
C,3.8254899615,-1.1866562988,2.4969136856
C,5.2272107116,-0.9988984259,-0.2421143337
C,3.5573735669,1.3531158484.8473829796
C,-3.6186316271,-1.437771078.8453037953
C,-3.0910672462,-0.9298504608,1.9774208075
H,2.9738534024,-0.8957481503,3.1219663285
H,4.7269567272,-0.7792825654,2.9722204735
H,3.907824167,-2.2791309129,2.5246899389
H,5.3778362022,-2.0849585025,-0.2665064037
H,6.1214211776,-0.5532975641.2103472183
H,5.1714191223,-0.6468294653,-1.2779571327
H,3.7288029432,1.8598719435,-0.1050142289
H,4.3275636071,1.7093997684,1.5435393932
H,2.5900588974,1.6821891405,1.2417289539
H,-4.5893827034,-1.8576319372.6405192358
H,-3.5121749082,-0.7970520071,2.9600383931
H,1.203965363,-0.6716904065,-2.8966011488
C,1.0947049836.2196250702,-2.2841394061
C,2.1615000477,1.1613148072,-2.3167803752
C,-0.2314034132.6989484665,-2.0047325353
C,1.9747552819,2.4817030867,-2.0321394087
F,3.3982451931.7282913862,-2.6485683918
C,-0.3927523244,2.0976530957,-1.7179381587
F,-1.2722977041.1607795031,-2.7495067078
C.6722678383,2.9489943779,-1.7026831994
F,3.0031637409,3.3522538131,-1.9931874925
F,-1.6326857826,2.5640164075,-1.4487462458
F.5311964301,4.2408315423,-1.3509063413
C,-2.9493782115,-1.8275185853,-1.4718735119
C,-2.5272115698,-3.1153159147,-1.8605465439
C,-3.793262203,-1.0380381919,-2.288458126
C,-2.9308156,-3.5845094622,-3.1191437838
C,-4.1754823464,-1.5646743181,-3.5273550502
C,-3.7450283252,-2.8204446692,-3.9464316809
H,-2.6162006691,-4.5715547868,-3.4441513678
H,-4.8182993443,-0.980402988,-4.1778299104
H,-4.0520445578,-3.2052437636,-4.9150854276
C,-0.9262971698,-0.0423920666,2.7291152367
C,-0.7115355065,1.3511209772,2.8228766907
C,-0.4391618786,-0.944638083,3.7050228535
C.0722299554,1.8179494045,3.8864279649
C.329975436,-0.4165079833,4.7515764691
C.5953568456.9461946229,4.8368473899
H.2641413353,2.8810436608,3.9802838108
H.7206810098,-1.0825344789,5.5141922176
H,1.1979355651,1.3321301428,5.6544154633
C,-4.3101516968.3393480892,-1.8721939044
H,-3.6999324546.6883856392,-1.0355712095
C,-1.716403745,-4.0375594979,-0.9554540826
H,-1.3933535069,-3.4587688083,-0.087708516
C,-0.769136792,-2.4400187255,3.7084847909
H,-1.1527752523,-2.7058038042,2.7191311955
C,-1.3758070491,2.3405392533,1.8693938612
H,-1.5077251465,1.8451589325.9060945725
C,-2.584882476,-5.1996638759,-0.4338525752
H,-2.9423672421,-5.8329801178,-1.2536424963
H,-2.0080234624,-5.8334438928.2494152355
H,-3.4624622463,-4.8333697636.1092372168
C,-0.4513514116,-4.5703091801,-1.652928577
H.1677489518,-3.7512873273,-2.0324459584
H.1523431919,-5.1598249713,-0.9538626385
H,-0.695730556,-5.222638939,-2.4980804544
C,-5.7770684031.2651574703,-1.3993689746
H,-6.1258157067,1.2541653295,-1.0811592697
H,-6.4325649458,-0.0750882014,-2.2092829168

H,-5.9117854575,-0.4197066384,-0.5570553375
C,-4.1842074075,1.3901605151,-2.99180058
H,-4.433474699,2.3815820551,-2.5986119385
H,-3.169956428,1.4268465077,-3.3903316093
H,-4.8747113637,1.1910363818,-3.818633576
C,-2.7784536021,2.7249989585,2.3869527352
H,-2.7144383455,3.2206995352,3.3626535392
H,-3.2641035498,3.4163818683,1.689132491
H,-3.4286203197,1.851792865,2.4962214778
C,-0.54785634,3.6114583081,1.6206996461
H.4872789638,3.3824365724,1.3518702846
H,-0.9863038101,4.1806463853.7971124857
H,-0.5300052289,4.2702804939,2.4963261191
C,-1.8719929534,-2.7534208071,4.7424467785
H,-1.5287039969,-2.5270014452,5.7580374453
H,-2.7843982957,-2.1768563979,4.5668281365
H,-2.1371024615,-3.8161750574,4.7084804024
C.4510756328,-3.338609799,3.986599291
H.1726194759,-4.389950215,3.8550034364
H,1.2859037061,-3.12735374,3.3139500164
H.8129637317,-3.2300454885,5.0144398915

TS1-L2

Ni.7090217255.55963093,-0.2519701033
C,2.2743515872,-0.4023501586,-1.2388876364
C,2.5963510282.9027528008,-0.7521361752
H,2.6704332017,1.7312448973,-1.4511607542
H,3.2231849228,1.0053117141.1309059209
H,2.0024182412,-0.4348374068,-2.3004371734
Si,3.1526450959,-1.9768877508,-0.6560282695
C,3.3497188,-2.0044016062,1.222081007
C,2.1665301893,-3.4879807845,-1.2298248537
C,4.8615139372,-2.0236424174,-1.4757087707
H,3.9048781303,-1.1343018962,1.5904949082
H,3.8981462507,-2.8991997918,1.5415288914
H,2.3768145991,-2.0108711014,1.7230434896
H,1.1757008883,-3.5347670637,-0.7639374473
H,2.6886060531,-4.419937606,-0.9815260378
H,2.0178331987,-3.4784180005,-2.3165745562
H,4.7850348835,-1.9625466461,-2.5679068766
H,5.394344112,-2.9519748739,-1.2351565563
H,5.488055672,-1.18733729,-1.1443495294
H.7167315089,-0.8738525988,-0.7381215114
C,-0.6743443434,-0.9241587796,-0.2749703234
C,-1.5863237277,-1.1121049371,-1.3112392185
C,-0.9037309915,-1.7057886202.8556801029
C,-2.672457977,-1.977242962,-1.2333763901
F,-1.4375873937,-0.4198526023,-2.4681846571
C,-1.9752761645,-2.5816283424.9857067743
F,-0.0530071868,-1.6198419391,1.9118154659
C,-2.874303274,-2.7147982322,-0.0698650721
F,-3.543226334,-2.0883908073,-2.2533334935
F,-2.1647118996,-3.2840218193,2.1174692318
F,-3.9185439243,-3.5510167424.03045951
C.1014413723,2.2319186306.4705938227
N,-0.4895402111,3.2682680718,-0.2194286551
N.2404249942,2.7430536666,1.7423879549
C,-0.6898941089,4.3806847717.5969469817
C,-0.2350367795,4.0512807602,1.8253402913
H,-1.1359610883,5.2885369478.2253737852
H,-0.2096781529,4.6114299804,2.7454311855
C,-0.8971837334,3.2812055825,-1.6098301335
C,-0.0023344265,3.7871788981,-2.5778245689
C,-2.2148379226,2.8870954176,-1.9373953939
C,-0.4515237538,3.867048457,-3.9029249873
C,-2.606644124,2.9877564319,-3.2781204723
C,-1.7374275526,3.4694027086,-4.2523185687
H.2139331361,4.2511665891,-4.669291048
H,-3.6073323111,2.6839852974,-3.5650303598
H,-2.066391775,3.5378364968,-5.2856622417
C.7734138566,2.0608989197,2.9034970807
C,2.1468882374,2.1947857304,3.204873384
C,-0.1188046912,1.3628324374,3.7485361442
C,2.622447169,1.5629154606,4.3613475936
C.4139969402.7539428998,4.8920315217
C,1.7692881748.8444278482,5.1931544799
H,3.6741278794,1.6389365462,4.6165510684
H,-0.2417705994.2018053896,5.5565853112
H,2.1602758657.3602132919,6.0837974174
C,-1.6245280904,1.3110336651,3.4915008076
C,-2.2651417252,-0.0349488026,3.8742688246
C,-2.3463622349,2.4557700961,4.2349646451
H,-2.3194278183,-0.1678897355,4.9608163028
H,-3.2935633919,-0.0752808097,3.4991612651
H,-1.717197709,-0.8828963798,3.4601501259
H,-3.4229736701,2.4234923259,4.0322449533
H,-2.2070059238,2.3662426778,5.318384285
H,-1.9807153501,3.4407235836,3.9313376325

H,-1.7852254876,1.4585087244,2.4194727231
C,3.0913689777,3.0496449357,2.3612844501
C,4.5066178875,2.4575511314,2.2395696868
C,3.178600036,4.4838410895,2.925605741
H,5.0606915199,2.519300536,3.182513594
H,4.4888235128,1.4080028087,1.9319402927
H,5.0811680592,3.017386081,1.4937941961
H,3.8418499565,5.1002920028,2.3080985591
H,2.2010813637,4.9733882968,2.95501262
H,3.5802108639,4.478047098,3.9455266985
H,2.6735323833,3.1106206827,1.3524652614
C,-3.2153525542,2.4082240595,-0.8857140259
C,-4.007331956,3.5909386504,-0.2882064077
C,-4.2046005187,1.3578657474,-1.4217181329
H,-4.5751325927,4.1108076319,-1.0684818451
H,-4.7214819472,3.2304836413.4609503831
H,-3.3584395806,4.3231355283.1994216682
H,-4.7416230982.8949598734,-0.587023191
H,-4.961309954,1.8077682417,-2.0743513928
H,-3.7043165127.5689218171,-1.9857712947
H,-2.6445506536,1.9409666582,-0.0770472256
C,1.3931242809,4.2950509355,-2.2227460075
C,2.4629625129,3.8689460643,-3.2447458603
C,1.3968041581,5.8295931642,-2.0649850261
H,2.3480470337,4.3913028565,-4.2007242009
H,3.4616925931,4.1118195356,-2.8657852583
H,2.430111748,2.7941579895,-3.4471686758
H,2.396501038,6.1855028453,-1.7908787866
H,1.1113933697,6.3209970331,-3.0021726562
H.700246845,6.1618557724,-1.2892298997
H,1.6700758049,3.861168579,-1.2585000684

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Ni,-1.9488999907,-3.7612712081,2.8197047784
C,-0.2152969147,-4.9963389295,2.2129375731
C,-0.0691610665,-3.5411456408,2.5572955635
H.3114887273,-2.907578899,1.7587815193
H.40813195,-3.3203752194,3.5127250369
H,-0.2427974321,-5.1561846067,1.128657016
Si.9594157361,-6.2524803801,3.0551385713
C.7830437661,-6.1035664011,4.928782104
C.4709492824,-7.9904268676,2.4920935134
C,2.727271803,-5.8721221696,2.5050729432
H,1.1102379098,-5.1262324726,5.3005911544
H,1.3808669548,-6.8670256333,5.4410227444
H,-0.2601111079,-6.2348271421,5.2381248539
H,-0.5496453436,-8.2431739223,2.8033521097
H,1.138900487,-8.7497219907,2.9164708289
H.5167950755,-8.0880300712,1.4008300369
H,2.8305176387,-5.9424416007,1.4157233374
H,3.4444861848,-6.573722563,2.9476244135
H,3.0311997266,-4.8611765944,2.7992228336
H,-1.2424829553,-5.3885921026,2.5647320457
C,-3.5645499304,-4.8748412267,3.1630339632
C,-4.5275195827,-5.2417258271,2.2360017362
C,-3.7063894464,-5.4864669148,4.4003489637
C,-5.5891213184,-6.1017519084,2.5077574671
F,-4.4655132152,-4.7570592337.9619971813
C,-4.7395726059,-6.3554981331,4.7388332689
F,-2.7765729647,-5.2508790313,5.3785376821
C,-5.7004036492,-6.6593693992,3.7780623596
F,-6.5128497479,-6.392956504,1.5687184227
F,-4.8291143198,-6.9009052135,5.968915754
F,-6.7160882566,-7.4907729434,4.0703111564
C,-2.3714521667,-1.9366735325,3.041436801
N,-2.1391725115,-1.1261527689,4.1275044032
N,-2.9064800911,-1.0839363873,2.105043921
C,-2.5031328411.1931363268,3.857803277
C,-1.5943675928,-1.5115549404,5.4152469197
C,-2.9745313446.2206480868,2.5929107691
C,-3.3636310072,-1.402165649.7653456188
H,-2.3968906666.9750952535,4.5909211783
C,-2.4700739542,-2.0182485921,6.4039068747
C,-0.2249915241,-1.2733568507,5.6706465985
H,-3.3491971917,1.0333743265,1.9931660232
C,-4.7387797412,-1.6578895847.5568544611
C,-2.4405309832,-1.3375936778,-0.2999152452
C,-1.9183065989,-2.3406980833,7.6498930192
C,-3.976121574,-2.1482323064,6.1718733966
C.267332175,-1.6127558033,6.9381534931
C.7009600621,-0.5981726876,4.6586069136
C,-5.1608546748,-1.882324172,-0.7591222408
C,-5.7622580247,-1.6537573863,1.6929484598
C,-2.9206848477,-1.5775222298,-1.5942687024
C,-0.9789958736,-0.9456033073,-0.1008325896
H,-2.5578073391,-2.7452709447,8.4261192276
C,-0.5651007506,-2.1492532033,7.9144044855
H,-4.1242167386,-2.4181648464,5.1217339222

C,-4.6881715582,-0.8013575665,6.425621692
C,-4.6482482163,-3.2373414924,7.0252181735
H,1.3154228724,-1.4466500849,7.1646200792
H.2550942084,-0.7127099108,3.666565187
C,2.110364657,-1.2155780741,4.6054270716
C.8178711799.9127612131,4.9538543774
H,-6.2070896155,-2.0914013192,-0.9532926115
C,-4.2647367149,-1.8506848463,-1.8233683407
H,-5.2363889841,-1.934559553,2.6106147884
C,-6.364415406,-0.2466329747,1.898659464
C,-6.9068576104,-2.6634759947,1.4884118599
H,-2.2333029988,-1.53946936,-2.4332269404
H,-0.7451948611,-1.0546110738.9605387008
C,-0.7567631983.5337450747,-0.4778855304
C,-0.0072607034,-1.8494174337,-0.8798710243
H,-0.1617543783,-2.4090477826,8.889254504
H,-4.5557266248,-0.4829489882,7.4661616552
H,-5.7637882058,-0.9010137237,6.2407533377
H,-4.3148489462,-0.0026028445,5.7797893962
H,-4.1358082261,-4.1972371148,6.9469333381
H,-5.6812164757,-3.3760497533,6.688975061
H,-4.6954102833,-2.9570963556,8.0838019503
H,2.6844326061,-1.0065506003,5.5144581175
H,2.6705541852,-0.7863792649,3.7675371458
H,2.0825330686,-2.2997530511,4.4685776698
H,-0.1546048699,1.4125630026,4.9423541153
H,1.4535843609,1.4013008438,4.2067751766
H,1.2665461947,1.082867718,5.9390737963
H,-4.6175534759,-2.033254647,-2.8346660224
H,-5.6064345016.5027181009,2.1401898924
H,-7.0893373536,-0.2598574223,2.7205578795
H,-6.8896718732.0869366384.9960917542
H,-7.6096867327,-2.3291695054.7168065306
H,-7.4802030837,-2.7640656274,2.4162061254
H,-6.5406439934,-3.6505442768,1.204092014
H,-0.9741298415.7096869636,-1.5375639419
H.2841343745.8253001357,-0.2966096699
H,-1.3976161696,1.2011428936.1072333821
H,-0.1743950638,-2.9075843083,-0.6575117037
H,1.028045391,-1.6055653147,-0.6172923187
H,-0.1021027562,-1.7168437692,-1.9629354096

TS2-L2

Ni	0.05669	0.02043	1.30966
Si	-1.29678	-0.55511	3.37435
C	-1.40224	-1.02377	0.55037
C	-3.17424	-0.64289	3.00622
C	-0.78475	-2.2929	3.97123
C	-1.35552	0.54761	4.95084
C	-1.22519	-2.39925	0.44368
C	-2.61381	-0.5658	0.04421
H	-3.54345	0.23496	2.46832
H	-3.69969	-0.69309	3.96829
H	-3.44395	-1.53256	2.43089
H	-0.70777	-3.01449	3.15335
H	-1.54189	-2.65715	4.67799
H	0.17688	-2.28788	4.49807
H	-0.42556	0.5687	5.52833
H	-2.14155	0.15215	5.60731
H	-1.62972	1.58458	4.71306
C	-2.176	-3.2784	-0.06963
F	-0.06245	-2.9628	0.88533
C	-3.59685	-1.39525	-0.49126
F	-2.9255	0.75551	0.11919
C	-3.37631	-2.76831	-0.55557
F	-1.94281	-4.60331	-0.1234
F	-4.75932	-0.88762	-0.94404
F	-4.30758	-3.58545	-1.07148
H	2.10457	1.59869	1.78606
C	1.79149	0.60747	2.09607
C	0.93242	0.46352	3.19671
H	2.47199	-0.19854	1.84275
H	1.10194	-0.36646	3.87797
H	0.58066	1.36964	3.676
C	0.88664	0.63318	-0.40936
N	2.02648	0.18715	-1.04918
N	0.57865	1.78972	-1.09666
C	2.41815	1.05748	-2.06558
C	1.52115	2.06368	-2.08654
H	3.28742	0.86577	-2.67238
H	1.4523	2.94526	-2.70204
C	2.7991	-1.01452	-0.78863
C	4.05257	-0.89352	-0.14494
C	2.33427	-2.2478	-1.30113
C	4.78986	-2.06597	0.069
C	3.11293	-3.38472	-1.04902
C	4.31874	-3.3014	-0.35835
H	5.75086	-2.00575	0.57032

H	2.7763	-4.35063	-1.40584
H	4.90155	-4.19982	-0.17444
C	-0.57594	2.66426	-0.97259
C	-0.55148	3.71478	-0.03341
C	-1.62774	2.52089	-1.90868
C	-1.64588	4.58898	0.0013
C	-2.68565	3.43388	-1.83636
C	-2.70702	4.44931	-0.8854
H	-1.65408	5.40078	0.72242
H	-3.51239	3.34174	-2.53276
H	-3.54461	5.13932	-0.84578
C	-1.63018	1.45786	-3.00794
C	-3.02637	0.8623	-3.27476
C	-1.07729	2.02522	-4.33558
H	-3.66716	1.56911	-3.81554
H	-2.93136	-0.02772	-3.90722
H	-3.54118	0.5805	-2.35682
H	-1.09508	1.25167	-5.11248
H	-1.69588	2.8623	-4.6809
H	-0.04828	2.38333	-4.24656
H	-0.97632	0.63997	-2.68613
C	0.64294	3.98523	0.87304
C	0.24033	4.14934	2.3498
C	1.4326	5.21639	0.38118
H	-0.35009	5.05862	2.51243
H	-0.35489	3.29823	2.69433
H	1.13426	4.22536	2.98024
H	2.31548	5.38214	1.01032
H	1.77273	5.0862	-0.65265
H	0.81757	6.12326	0.41793
H	1.31153	3.12505	0.80939
C	1.09424	-2.35355	-2.18966
C	1.42505	-1.912	-3.63422
C	0.47756	-3.76178	-2.23198
H	2.20613	-2.55207	-4.06235
H	0.53442	-2.0005	-4.26669
H	1.76872	-0.87527	-3.68685
H	-0.48334	-3.72313	-2.75723
H	1.11338	-4.4659	-2.78135
H	0.29813	-4.16478	-1.23271
H	0.33428	-1.67229	-1.79302
C	4.68016	0.44834	0.24199
C	5.29288	0.45944	1.65741
C	5.76445	0.85089	-0.78299
H	6.16641	-0.19802	1.72724
H	5.63032	1.47253	1.90463
H	4.57371	0.14899	2.41944
H	6.18382	1.83205	-0.53092
H	6.58488	0.12406	-0.7868
H	5.3698	0.90599	-1.80305
H	3.89965	1.21422	0.21646

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Ni,-0.0106623254,-0.0360130812,1.3616471432
Si,1.3209525952.1512324497,3.3012257366
C,1.7677791088,-0.4582717077.6957011439
C,2.8857379694,1.2391497141,3.1891776753
C.315816609,1.0516939591,4.6691052467
C,1.8928380307,-1.500989917,4.0623785167
C,2.6930598343.4357514105.164139585
C,2.1728090521,-1.7900258604.6428891299
H,3.7229733649.7175928462,2.7156441517
H,3.1986884431,1.5052786851,4.2073431569
H,2.7197371927,2.1705676541,2.6402752478
H.0574676477,2.0766047443,4.3774833317
H.9457378006,1.1257469526,5.5658376943
H,-0.6085291635.5479193765,4.9699407918
H,1.0685173074,-2.1955070147,4.2553320969
H,2.3920069745,-1.3061812961,5.0207773778
H,2.6124725278,-2.0179919672,3.4203735942
C,3.929599666.0628709779,-0.3549359685
F,2.4245155803,1.7676468704.1667895794
C,3.3956675426,-2.2193164086.1339483954
F,1.3523378393,-2.7676644918,1.1180812779
C,4.2848460027,-1.2821180519,-0.3808002786
F,4.7827992721.9846778273,-0.8463724188
F,3.7151148447,-3.5283572892.1086717772
F,5.4680489787,-1.667177403,-0.8886155955
H,-2.6412884678.2359562012,1.5493922984
C,-1.9054102803.173958187,2.3373524596
C,-1.3122314388,-1.0252255614,2.6688164561
H,-1.8668553305,1.0160400704,3.0202733288
H,-0.8971181303,-1.2007769063,3.653442002
H,-1.5050016943,-1.9236375504,2.0875030453
C,-1.05991115.2667870767,-0.4746198604
N,-1.9363351679,-0.5961856088,-1.0985434227
N,-1.2516307687,1.4440228529,-1.1627356272
C,-2.651078809.0346620968,-2.115984199

C,-2.1464402852,-2.0034105163,-0.8138382795
C,-2.227418617,1.3158541102,-2.1499377756
C,-0.5472932264,2.7039030234,-1.0066624198
H,-3.3793414757,-0.4883410117,-2.7135891451
C,-1.2118737864,-2.9485770366,-1.3014133344
C,-3.3364061259,-2.3977870151,-0.1597457465
H,-2.5213269124,2.1445591034,-2.7724657033
C.5181707696,2.9938260933,-1.8905352707
C,-1.0233856623,3.6475635758,-0.0720553548
C,-1.4545031368,-4.2997062128,-1.0257070767
C,-0.0201882599,-2.5462517902,-2.171743677
C,-3.5256050244,-3.7664713687.0806517012
C,-4.4565862158,-1.4285050242.2220487996
C,1.1387034317,4.243103367,-1.7680764772
C.968856878,2.0367070346,-2.9938211038
C,-0.3577663632,4.8782337584.0100493698
C,-2.2723006669,3.41483374.772487535
H,-0.7490831438,-5.0477669749,-1.3674827388
C,-2.5897492513,-4.7071212158,-0.3307225123
H.3719734051,-1.6016705543,-1.783045862
C,-0.4675213941,-2.3116405364,-3.6317999854
C,1.1300845214,-3.5662311321,-2.1560726681
H,-4.4255740895,-4.0963489681.5893929237
H,-4.0705322141,-0.4081694403.1451179202
C,-4.965782533,-1.6264632475,1.6619820841
C,-5.634307323,-1.5485770035,-0.7684162095
H,1.9670677079,4.4919742432,-2.4226447601
C.7163289146,5.1724040191,-0.8225403623
H.6637993616,1.0255216727,-2.708143364
C.2835106067,2.3785176022,-4.3346450084
C,2.493931407,2.021908816,-3.2031085385
H,-0.6979536845,5.6218580174.7237129029
H,-2.4957501179,2.3468426307.755026926
C,-3.4803938007,4.1514326441.1572501197
C,-2.0851727846,3.8229435745,2.2438018686
H,-2.7526349641,-5.762060541,-0.1283346099
H,-0.8777136539,-3.2316382851,-4.0643391857
H.387365678,-2.0057463957,-4.2455278826
H,-1.2303847377,-1.5332818524,-3.7157955468
H,1.4324772265,-3.8341272727,-1.1423162553
H,2.0003548441,-3.1455984522,-2.6698466275
H.8647861404,-4.4878763351,-2.6866154839
H,-5.4833084089,-2.5839572768,1.7826378845
H,-5.6840251216,-0.8388123697,1.9154815994
H,-4.1534775917,-1.58891042,2.391840914
H,-5.3226832811,-1.3725516782,-1.8024991128
H,-6.4164476832,-0.8205360956,-0.5253442502
H,-6.0831809115,-2.5470967492,-0.7256099215
H,1.2182419332,6.1327881321,-0.7438831043
H,-0.8069586135,2.3365248059,-4.2728413508
H.5994304176,1.6746774099,-5.1131127005
H.560304252,3.3868171669,-4.6631045053
H,2.8432032454,2.9359902808,-3.6961838857
H,2.7709034421,1.185932165,-3.8545590022
H,3.0412427268,1.9200454745,-2.2661304825
H,-3.3135153243,5.2342244745.135412286
H,-4.38727002,3.9640816719.7437806788
H,-3.6727577406,3.8247091182,-0.869955922
H,-1.1981358563,3.3539919708,2.6794301148
H,-2.95733205,3.5202096153,2.8336075678
H,-1.9810863149,4.9069736228,2.3598481374

TS3-L2

Ni.11413587,-0.0794967976,1.3903721627
Si.598650719,2.0038142715,2.6611495973
C,1.5902835148,1.1951954921.9143700226
C.8378125377,3.8170220634,2.0971283213
C,-1.2175395139,2.0501834196,3.2418850559
C,1.8018316678,1.8844952439,4.1249241754
C,1.4497307131,1.9803875135,-0.2398917556
C,2.9120644816.7854952877,1.1582185586
H,1.8736513683,4.039513351,1.8185828151
H.5778857863,4.4719896961,2.9390626428
H.1942380754,4.0948708454,1.2579449978
H,-1.897881381,2.2094470046,2.4006239413
H,-1.3270763736,2.9150485653,3.9117462868
H,-1.5385594884,1.1587712052,3.7832948972
H,1.8705747233.9061329065,4.6026647672
H,1.4693869003,2.6056955718,4.8832341596
H,2.8118746289,2.1834954613,3.8257694024
C,2.4847757938,2.3310615549,-1.0911632973
F.2238026992,2.4561890478,-0.543274916
C,3.9889701289,1.1307728617.3456280338
F,3.2127912468.0147649849,2.2257259889
C,3.7760928976,1.8997602934,-0.7914604121
F,2.2666200685,3.0661259758,-2.1966100949
F,5.2254199653.6785239618.6173459171
F,4.795434213,2.1929837282,-1.6104578224

H,-0.191550115,-2.531383519,1.9729314355
C,-0.535810954,-1.6413252547,2.4852739933
C.3601070935,-0.8935564269,3.2605572273
H,-1.6049902846,-1.5975901646,2.6805619946
H,-0.0052602018,-0.3200897948,4.1062357013
H,1.3998377317,-1.2031206962,3.335554875
C,-0.7564406168,-0.6069183848,-0.3795483701
N,-0.4547804143,-1.7475407289,-1.1049346698
N,-1.7979232744,-0.058980526,-1.1113578049
C,-1.2709752424,-1.8854714563,-2.2263519
C.4398881603,-2.8326782678,-0.7448127937
C,-2.1169284066,-0.8363707111,-2.2242123453
C,-2.6142300715,1.0970508414,-0.7896919947
H,-1.1723911275,-2.7155659441,-2.9058592812
C,1.8096638912,-2.7629488567,-1.0897710163
C,-0.1265987024,-3.9955750151,-0.1671970018
H,-2.9192786167,-0.575823569,-2.8926898632
C,-2.5229081514,2.2614550954,-1.5904366314
C,-3.5804719486.9745171445.2379029715
C,2.6173223064,-3.8602111707,-0.7601341773
C,2.4011699185,-1.5848561032,-1.866181842
C.7309286762,-5.0636883328.1286226262
C,-1.6275641534,-4.1642759819.0840944232
C,-3.3511957728,3.3427327457,-1.2580979091
C,-1.635565111,2.3740168165,-2.8333054416
C,-4.3733250772,2.0929171045.5270317856
C,-3.8649108983,-0.3547927154.9374884412
H,3.674970976,-3.8346781567,-0.9939284126
C,2.0903564036,-4.9945003323,-0.1500947125
H,1.9530143011,-0.6680559887,-1.46992167
C,2.0464393448,-1.6769392031,-3.3665996462
C,3.9282135329,-1.4630002838,-1.7294157905
H.3244163616,-5.9632629257.5791883576
H,-2.0896184242,-3.1736916741.0581479944
C,-1.9588227799,-4.7910189867,1.4524592887
C,-2.2726243051,-5.017748693,-1.0297451243
H,-3.2909699488,4.2542570225,-1.8432029589
C,-4.2494609699,3.2730207799,-0.1996044454
H,-0.8542808881,1.6127012058,-2.7628139239
C,-2.4567702552,2.1089861405,-4.1149362719
C,-0.9416148279,3.7435233457,-2.9773082761
H,-5.1101716448,2.0335987426,1.3206716122
H,-2.9372416383,-0.9296481943.956438321
C,-4.9083284141,-1.156845965.1290652099
C,-4.3379123366,-0.2097363458,2.3928731945
H,2.7396206047,-5.831131758.092841485
H,2.449176221,-2.598341185,-3.8029461034
H,2.4818544518,-0.8311591032,-3.9106703447
H.9686563027,-1.6630283869,-3.5433907548
H,4.2607422756,-1.4609407245,-0.6879134518
H,4.2701019906,-0.5321645547,-2.1919917776
H,4.4469326848,-2.2780030496,-2.2465589727
H,-1.66499127,-5.8448327159,1.5019989679
H,-3.0406180768,-4.7545385157,1.6224602255
H,-1.4721077958,-4.2668065703,2.2780683019
H,-2.1181929408,-4.5903572252,-2.0241005121
H,-3.3530773642,-5.10355295,-0.8680578902
H,-1.853985058,-6.0305474095,-1.0357322063
H,-4.8723813082,4.1295878409.0431115765
H,-2.9495833926,1.1333588377,-4.1139057029
H,-1.8084307918,2.1518358329,-4.9974998855
H,-3.2373934367,2.8682008623,-4.2382149961
H,-1.6545967428,4.531431151,-3.2441415712
H,-0.2014588908,3.698259714,-3.78315863
H,-0.4251142623,4.0444660827,-2.0661011931
H,-5.8606690021,-0.6162452921.0782149799
H,-5.0992695498,-2.1264148118.6034069813
H,-4.5771178839,-1.3464310319,-0.8962638359
H,-3.6579001523.4085443546,2.9845261178
H,-4.3931142814,-1.197226411,2.8638863267
H,-5.3397296977.2288168937,2.4608952423

TS4-L2

Ni.2459445181,-0.010085354,1.0852670938
Si,1.5104143212.2289792642,3.0102569508
C,1.8049994953,-0.9513257718.7090685786
C,3.3814042381.5956542448,2.9764090114
C.761619113,1.8286421893,3.7543655755
C,1.3247030019,-1.1726538493,4.2971129221
C,2.880939842,-0.3618151982.0391596668
C,1.9179248153,-2.3346914779.8663372345
H,3.9802742979,-0.3010467029,2.7833561632
H,3.6841545565.9840148452,3.95801003
H,3.649482933,1.3459950415,2.22698926
H,1.126930685,2.7068930947,3.211185061
H,1.0801417055,1.9300907809,4.8014958867
H,-0.3311652448,1.8424663025,3.7374353241
H.3523616584,-1.1472667334,4.7993508665

H,2.0954122393,-1.0627427032,5.0714846093
H,1.4430627089,-2.1639872062,3.8492338089
C,3.9734127593,-1.0654792748,-0.4521400252
F,2.9068096791.9881269525,-0.1198467916
C,2.9974233056,-3.0814024238.4028209009
F.9333208202,-3.0302084172,1.4983645078
C,4.0350210444,-2.4453361656,-0.2716739529
F,4.9728410795,-0.4309758055,-1.0949327785
F,3.0275598292,-4.4180619108.5645937309
F,5.0783381918,-3.1498036623,-0.7430391331
H,-2.9294610228.6205020046,3.0076354838
C,-2.2705622022,-0.1066601533,3.4752376428
C,-1.8286316132,-1.1853138081,2.82156829
H,-1.9929720447.0917337755,4.5071736556
H,-1.1848146599,-1.9163813794,3.2981509273
H,-2.1253641649,-1.4030838175,1.8018150893
C,-1.0218481157.4210253924,-0.5209344565
N,-1.9556633509,-0.3211712378,-1.2134714248
N,-1.0022833594,1.6088591862,-1.2180277094
C,-2.4817362502.3854525331,-2.2904917668
C,-2.4352229333,-1.6609122033,-0.9266220188
C,-1.8895853575,1.600004699,-2.2877778992
C,-0.1723416248,2.7654364102,-0.941487896
H,-3.2181701707,-0.041881466,-2.9506374656
C,-1.6630861175,-2.7744120372,-1.3332268094
C,-3.7215795143,-1.806124273,-0.3558382858
H,-2.0148044353,2.4477250567,-2.9401676206
C.948030332,3.0081436256,-1.7686711507
C,-0.5686412098,3.659992761.0795666778
C,-2.1885362992,-4.0485904563,-1.0846981574
C,-0.3393457285,-2.6244866445,-2.084168337
C,-4.1965912197,-3.1081264204,-0.1439615911
C,-4.6310327427,-0.6241909821,-0.0143268081
C,1.7178911401,4.146193977,-1.4933706974
C,1.2877389653,2.1476872673,-2.9875534788
C.243837561,4.7774106314.3086188151
C,-1.8797189887,3.485273029.8500593861
H,-1.6161177306,-4.9243485047,-1.3667730547
C,-3.4365138448,-4.2177425572,-0.4918521171
H.1934576561,-1.7731631432,-1.6509595536
C,-0.5834730072,-2.3230955625,-3.5792683577
C.5773182734,-3.8524786082,-1.9622120091
H,-5.176568083,-3.2512636116.2993284366
H,-4.0210336041.283528402.0016726359
C,-5.3021927686,-0.755217376,1.3663438493
C,-5.7196076826,-0.4390016751,-1.093193197
H,2.5916174555,4.3556565294,-2.1012799351
C,1.3817862211,5.012431618,-0.4591750411
H.7990438988,1.176601584,-2.8634884402
C.7330437535,2.8031145579,-4.2722060704
C,2.7933112032,1.8864698877,-3.176321125
H,-0.0207289195,5.4798945785,1.0908851527
H,-2.0357983285,2.4130029583,1.0058202413
C,-3.0708763225,4.0197827636.0240572277
C,-1.8863752418,4.155009428,2.2334638417
H,-3.8198401129,-5.2182212154,-0.3118381063
H,-1.133966579,-3.1419954401,-4.0569308954
H.3727948917,-2.2133040879,-4.1030193731
H,-1.1513459798,-1.4016960832,-3.7324526825
H.7180042297,-4.1644858697,-0.9249022823
H,1.5605704777,-3.6183753188,-2.3820423519
H.1885282414,-4.7087334234,-2.5250398291
H,-6.0570259818,-1.5487420668,1.3784836264
H,-5.8179400776.1784765138,1.6170558384
H,-4.5813505914,-0.9679734828,2.1587743628
H,-5.2965258764,-0.280780929,-2.0892032436
H,-6.3492143383.4259994319,-0.8562904521
H,-6.3686839478,-1.3201656263,-1.1463412513
H,1.9981134774,5.8847545637,-0.2602643194
H,-0.3414370898,2.9976784122,-4.2175725301
H.9123884498,2.1580692981,-5.1396182778
H,1.2294755583,3.7618691037,-4.4606771842
H,3.3347547564,2.8005927725,-3.4436218165
H,2.9400588143,1.1795145968,-4.0004945513
H,3.2566735583,1.4678759128,-2.2832957448
H,-2.9538708937,5.0914054635,-0.1741009861
H,-4.0087540837,3.8817477532.5741932333
H,-3.1727698081,3.5097324705,-0.9372567382
H,-1.023223704,3.8671378074,2.8378820068
H,-2.7906502429,3.8636343437,2.7786405952
H,-1.9010265426,5.2480033022,2.1585265728

5-L2

Ni,-0.45035026.2323245167.4493319545
Si,-0.3087756338,-0.0240000491,-1.7863005423
C,1.4206518313,-0.1188662498.5138199515
C,1.1604035489.8729771361,-2.6029853903
C,-0.172086233,-1.8705996613,-2.2319636872

C,-1.8425129158.6651593559,-2.6848523306
C,1.9712046295,-1.3850975105.6986133834
C,2.3410825304.9247603925.601542134
H,1.2303557552,1.9186477838,-2.2848893294
H,1.0382039261.8668011046,-3.6948707583
H,2.1150128343.3896332956,-2.3718492407
H.7776557316,-2.297324514,-1.8970732288
H,-0.2309312559,-1.9961507134,-3.3221454243
H,-0.9707319893,-2.469328281,-1.7827009499
H,-2.7854388544.304894459,-2.2664118841
H,-1.816239859.379553338,-3.7457262922
H,-1.8535176905,1.7583121455,-2.6453893022
C,3.3203885582,-1.6206596026.9521818637
F,1.1753401506,-2.4887009198.6413147795
C,3.6979650278.7512903346.8566940817
F,1.9232907656,2.2120104048.4455763079
C,4.1927114028,-0.5389256963,1.0285988818
F,3.7936602325,-2.8688667575,1.1275371402
F,4.5369498955,1.8010403067.939920044
F,5.4971287752,-0.7368130611,1.2787864322
C,-2.3073762576.6205306708.8055852948
N,-3.3053046223,-0.2682146126,1.1272483903
N,-2.8388828013,1.8399326709,1.1544008452
C,-4.4097529057.3809052232,1.6699853424
C,-3.2392778642,-1.712829774,1.0199414718
C,-4.1160877839,1.702585989,1.6892028906
C,-2.1775926152,3.1296153881,1.0876445471
H,-5.2885852658,-0.1530732809,1.9928129361
C,-3.9509091292,-2.3499884201,-0.0190390253
C,-2.5301818752,-2.4392249832,2.0040304823
H,-4.684442274,2.5492718646,2.0372165025
C,-2.5838259474,4.0518437557.0982451114
C,-1.215401836,3.4557449749,2.0715770476
C,-3.9147868424,-3.7504516033,-0.0679129251
C,-4.7783320122,-1.5878832686,-1.0520490221
C,-2.5223252979,-3.8350243675,1.8973050312
C,-1.8526130751,-1.7608254646,3.1932749399
C,-1.9913759031,5.3220556976.112020069
C,-3.647179752,3.7389771892,-0.9536655109
C,-0.6515005069,4.7364284604,2.0264672156
C,-0.827275704,2.4960172811,3.1957873203
H,-4.4513212757,-4.2682465373,-0.8563665092
C,-3.2035897688,-4.4865329442.8727286286
H,-4.5009395154,-0.5317005436,-0.9933822927
C,-6.2843528698,-1.6904789371,-0.7340330704
C,-4.5071595577,-2.0555079593,-2.4939405517
H,-1.9786622038,-4.4221452474,2.6291189474
H,-1.5746347567,-0.7487233198,2.8829797625
C,-0.560953711,-2.4601769354,3.6496225724
C,-2.8382982034,-1.6373261799,4.3744040338
H,-2.2836675868,6.0524776808,-0.6352001521
C,-1.0344474216,5.6623598178,1.0608033608
H,-3.7634608728,2.6525609008,-1.0031149699
C,-5.0133560605,4.3460243899,-0.5699090113
C,-3.2470511854,4.222806099,-2.3607002009
H.0958755875,5.0160456474,2.760536171
H,-0.9529397912,1.4743609161,2.8224702916
C,-1.7657057767,2.6698492916,4.4082325926
C.6412407861,2.6293274287,3.6330910554
H,-3.1829561626,-5.5710384906.8122553623
H,-6.6263883955,-2.7306604537,-0.7765197694
H,-6.8709893335,-1.1157414582,-1.4594189231
H,-6.5182974823,-1.306498885.2640580549
H,-3.4401026522,-2.043141268,-2.7324235837
H,-5.0190699049,-1.3965469648,-3.2037402937
H,-4.8783756232,-3.0707586962,-2.670681923
H,-0.7613744353,-3.4226642479,4.1332888217
H,-0.0460007915,-1.836081509,4.3882829946
H.1217032291,-2.634007183,2.8144924064
H,-3.7377721353,-1.0767332813,4.101696637
H,-2.3659207448,-1.1220638171,5.2183941673
H,-3.1542356121,-2.6277553086,4.7216268407
H,-0.5851704131,6.6514142575,1.0494938238
H,-5.3769879415,3.9771963883.3936152571
H,-5.7678037833,4.1001153163,-1.3257089742
H,-4.9504262311,5.4380655971,-0.5037760036
H,-3.2938772733,5.3139405653,-2.4455896105
H,-3.9344420435,3.8123220275,-3.1079546267
H,-2.2332157598,3.9131395044,-2.6279258756
H,-1.6902243146,3.6853835673,4.8136942562
H,-1.496260387,1.9698040985,5.2071025911
H,-2.8130660274,2.4907923213,4.146642932
H,1.3165952913,2.6159562114,2.7744419507
H.90713411,1.796681316,4.2932316819
H.8212744483,3.551632926,4.1959815192

TS5-L2

Ni.3673355796,-0.0999726599,-0.5545113344

Si,1.0628184652,-0.5801175529,-2.9216883595
C,2.1417219116,-0.3553253061,-1.1786384529
C,2.5611124952,-0.4398511981,-4.0873265142
C.3567472355,-2.3171566327,-3.1751218848
C,-0.1292148439.7764676496,-3.5065632828
C,2.6855021514,-1.4809503518,-0.5273278371
C,2.8664284285.8403600884,-0.9927835386
H,3.01978517.5542137779,-4.0407606367
H,2.2437733933,-0.6072506211,-5.1249967433
H,3.3372183098,-1.177952642,-3.8558076554
H,1.1292329562,-3.0823730588,-3.051673939
H,-0.0280581408,-2.3979788001,-4.2008079644
H,-0.4570329073,-2.5514363864,-2.4848644072
H,-1.1425718747.6307862827,-3.1261293894
H,-0.167117796.7729326733,-4.6056088077
H.2169870628,1.7633298342,-3.186376811
C,3.8278758406,-1.4283360528.2635708763
F,2.1169967055,-2.6996477186,-0.6808170473
C,4.0103617519.9277896545,-0.2116786472
F,2.4731463171,1.9680253352,-1.6302904841
C,4.4880309169,-0.2136204828.4307584876
F,4.2816292017,-2.5258657904.8938482134
F,4.6334161709,2.105393747,-0.0242356301
F,5.5753149898,-0.1403370596,1.2084729222
C,-1.1969291623.1763171878.4620237937
N,-2.0451686776,-0.7631530143,1.0120971682
N,-1.6521049239,1.3576392817,1.0140037928
C,-2.9802329536,-0.1836300046,1.8658055733
C,-2.0202634048,-2.1796788067.7345698451
C,-2.7329534129,1.1474562795,1.8678935462
C,-1.1301994156,2.6770733189.7383581982
H,-3.7254844406,-0.7667580484,2.3827697022
C,-2.919847651,-2.6933687792,-0.2230924261
C,-1.1456605154,-3.0111458807,1.4702050577
H,-3.2163222127,1.9555717274,2.3926902862
C,-1.8137226666,3.4904408318,-0.190631407
C,-0.0011866297,3.1371240842,1.4551123336
C,-2.9162353589,-4.0776242132,-0.4445369544
C,-3.9042391155,-1.8116630162,-0.9888634104
C,-1.1839920697,-4.3854264833,1.2056845156
C,-0.2252406468,-2.4571810476,2.5561110402
C,-1.3380755808,4.7937481749,-0.3906423402
C,-3.0529568331,3.0152510412,-0.9470667961
C.4322463885,4.4454103241,1.2093550629
C.7105122577,2.2647050039,2.4879892605
H,-3.5975154311,-4.5018112213,-1.1761388002
C,-2.0568381909,-4.9157084751.2582132479
H,-3.6695072579,-0.7683205923,-0.7629242653
C,-5.3522361777,-2.0697172962,-0.5270188618
C,-3.7805306974,-1.9825487656,-2.5134730231
H,-0.5218574661,-5.0516858485,1.7483137772
H,-0.011138437,-1.4155238169,2.2998322229
C,1.1269837597,-3.1844139043,2.6450733785
C,-0.9294831815,-2.4764594538,3.9288529474
H,-1.8443438751,5.4440329765,-1.0969370435
C,-0.2284466353,5.268004478.299859557
H,-3.1013576456,1.9261404121,-0.8603099815
C,-4.3380058006,3.594771137,-0.3213674792
C,-2.9993617836,3.3469402146,-2.4494790786
H,1.2988408182,4.8297810876,1.7361461618
H.6423395437,1.2298590463,2.1368536355
C.0151434893,2.3494511792,3.8629862848
C,2.2044475531,2.5926621658,2.6461926394
H,-2.068297241,-5.9860322515.0712307302
H,-5.6612617146,-3.1005829057,-0.7341586845
H,-6.0471363251,-1.4026341087,-1.0497345988
H,-5.4701581831,-1.8996266015.5483462598
H,-2.7600049762,-1.7861892067,-2.8547972135
H,-4.4494591845,-1.2828374709,-3.0272442351
H,-4.0542324536,-2.9927496317,-2.8368959615
H,1.0244902216,-4.2037106484,3.0340556109
H,1.7896789856,-2.6477541363,3.3330269114
H,1.6234641333,-3.2412714761,1.6737078556
H,-1.8588460112,-1.8991149071,3.9195008843
H,-0.2794155184,-2.049073244,4.7008743464
H,-1.1753758273,-3.5020482928,4.2282102658
H.1256723963,6.2810305036.1291975055
H,-4.443405959,3.3125507481.7307704766
H,-5.2241619758,3.2322363277,-0.8547857987
H,-4.3415134569,4.6895987434,-0.3731048471
H,-3.0761314283,4.4233520575,-2.6374448404
H,-3.8393315524,2.8698877736,-2.966717618
H,-2.0741982686,2.9894162445,-2.9099363418
H.0460522404,3.3743625533,4.250994997
H.5214310141,1.702087687,4.5881780753
H,-1.0322973356,2.0389944759,3.8152266666
H,2.7256655153,2.6450407533,1.6867395467
H,2.6896455565,1.818345963,3.2502577845

H,2.3630462993,3.5445480379,3.1655749288

6-L2

Ni,-0.6336216423,-0.5062504996,-0.0045745282
Si,3.1770421697,-0.252734799,-1.9851172806
C,2.1753898515,-0.1928006125,-0.3564907234
C,4.650562826,-1.4038831811,-1.713286384
C,2.0974442429,-0.914563708,-3.3857878165
C,3.7834771076,1.472785744,-2.4588470839
C,1.2025085074,-1.2028529049,-0.0456900901
C,2.3891315624.7496551099.6279352547
H,5.3051402796,-1.0420294928,-0.9122308748
H,5.2560330989,-1.4863114187,-2.624365785
H,4.321150078,-2.4132880312,-1.4425910689
H,1.8065361303,-1.9548519639,-3.2198305888
H,2.6451938961,-0.8630149815,-4.3350201873
H,1.1817479563,-0.325039823,-3.5044344445
H,2.9593902789,2.1921641264,-2.5214224767
H,4.2594302429,1.4343967933,-3.4468721815
H,4.5160579646,1.8683814626,-1.7503248377
C.5574483007,-1.3061040695,1.2418337805
F,1.2633548685,-2.3685712498,-0.7921306014
C,1.7716356054.7052992645,1.8972596001
F,3.2387937979,1.788676818.4361594198
C.8971923334,-0.3085586145,2.2040683577
F.1724972143,-2.5278758726,1.7452677584
F,2.0080540996,1.6895715809,2.7886572501
F.3529274619,-0.3771535279,3.4312883018
C,-2.4954965856,-0.0367194804,-0.1778017446
N,-3.5670669088,-0.8910236926,-0.2173195256
N,-3.073444318,1.2028081516,-0.285784331
C,-4.767634395,-0.2040039416,-0.3517141052
C,-3.4898953883,-2.3301553163,-0.1017128988
C,-4.4573065224,1.1160428917,-0.3950989122
C,-2.3573525221,2.4592650605,-0.2772309719
H,-5.716681897,-0.7134274667,-0.4055612634
C,-3.2689100569,-3.0968832362,-1.2640249063
C,-3.67942092,-2.9171375045,1.1671092302
H,-5.0810701654,1.9896295601,-0.498585208
C,-2.0264488389,3.058371536,-1.5091826432
C,-2.0519955537,3.0598400615.9654069542
C,-3.2451940464,-4.490596278,-1.1261191419
C,-3.0450446624,-2.4735831059,-2.6384732977
C,-3.6511704994,-4.3152031966,1.2443792973
C,-3.9145468014,-2.0960432929,2.4329931643
C,-1.3669536745,4.2946823831,-1.474036672
C,-2.3322663423,2.4081521602,-2.8559337443
C,-1.3898989089,4.2929996866.938572878
C,-2.4641705881,2.4315099056,2.2952986039
H,-3.0713911467,-5.1078664484,-2.0022556683
C,-3.4363759392,-5.0960456491.1122906942
H,-3.141752088,-1.3890836809,-2.5391860636
C,-4.1028453025,-2.9354970529,-3.6577954981
C,-1.619289823,-2.7568829623,-3.1481993068
H,-3.7926791059,-4.7971697936,2.2068514933
H,-3.789731353,-1.0400265534,2.1786801852
C,-2.8843786311,-2.4215921998,3.5307435608
C,-5.3515753274,-2.2769766582,2.9596944161
H,-1.0949940016,4.779508899,-2.4068341011
C,-1.0503303915,4.9060000195,-0.2657299016
H,-2.8864868222,1.4845545919,-2.6699076435
C,-3.2219193816,3.2992520138,-3.7421473695
C,-1.0320796267,2.0215868658,-3.5861065769
H,-1.1346746885,4.7816788652,1.8726386925
H,-2.5406121197,1.3514252378,2.1404875989
C,-3.8522002353,2.9469008889,2.7299188591
C,-1.4426055542,2.6526873802,3.4238257902
H,-3.4156116988,-6.1790889657.1960630563
H,-4.0515754638,-4.0151962137,-3.8362492158
H,-3.9475560998,-2.4355523397,-4.6205416461
H,-5.1179217136,-2.7020673951,-3.3184300799
H,-0.8693561536,-2.4221728646,-2.4256500619
H,-1.4422183602,-2.2345513221,-4.0953235299
H,-1.4605679463,-3.8268178457,-3.3243120209
H,-2.9890331461,-3.4499150546,3.8940160637
H,-3.027958385,-1.7559376888,4.3896388287
H,-1.8607792293,-2.295194465,3.169432417
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H,-5.5169133109,-1.6524170335,3.8448065569
H,-5.5443611047,-3.3167823718,3.2468447229
H,-0.536152722,5.8630394172,-0.2599122868
H,-4.1651389442,3.5496973591,-3.2447975075
H,-3.4634785168,2.7823582087,-4.6776093754
H,-2.7255178191,4.2395076035,-4.0054451846
H,-0.4334834509,2.9041994001,-3.8379460874
H,-1.2566826959,1.4934211974,-4.5197742378
H,-0.4153901866,1.3662896055,-2.9632900701
H,-3.8329511569,4.0309375814,2.8916117562

H,-4.1623747697,2.4725042251,3.6679071122
H,-4.6201799017,2.7347714814,1.9799110105
H,-0.4287587677,2.3716919509,3.1286616212
H,-1.7173909439,2.0450381993,4.292378664
H,-1.4192851549,3.6957701584,3.7589472368

7-L2

Ni,-0.1517437506.7664706491,-0.50820325
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C,-0.1477370595,1.7757345724,1.1817641441
C.3217368085,-1.1251019397,-0.0641605326
Si,1.0315811827,3.8949883563,-0.5162828919
C,-1.6924391651,3.2582270284.0226644045
C,-1.1924290123,1.5494344882,2.1458926179
F,1.120606622,1.7572405076,1.7705865638
N,1.5458328063,-1.6706327744.2540797903
N,-0.4732718125,-2.2436685307,-0.2328898318
C.8650265617,5.4957313017.4817392561
C,2.7590139071,3.186590302,-0.257193285
C.8473029585,4.3040140691,-2.3548423498
C,-2.6849619817,2.9925910613.9168643813
F,-1.9660883311,4.1462230557,-0.9723437387
C,-2.4218461989,2.1170183664,2.0066376384
F,-0.9407913604.7164146251,3.181332655
C,1.5117650928,-3.0644296922.2549009567
C,2.7771528754,-0.9723342529.5636581937
C.2457386254,-3.4231725489,-0.0472385091
C,-1.8910991751,-2.2763650022,-0.5347658669
H,-0.1091394143,5.9720848128.3239957948
H,1.6365246273,6.2208883475.1944161922
H.9735652632,5.3082805431,1.5563193365
H,3.494384426,3.8541360195,-0.7250278819
H,2.8751183602,2.1988113681,-0.7113744577
H,3.0133383275,3.0933438715.8008495924
H.9759516604,3.4247486613,-2.9952649061
H,1.6248432864,5.0247645727,-2.6386711199
H,-0.121039987,4.7545090253,-2.5884851627
F,-3.9185115909,3.5278460252.8034898761
F,-3.4307588094,1.8438557688,2.8583760782
H,2.3852732721,-3.6572922555.4709221897
C,3.7034399449,-0.7424755885,-0.476488961
C,3.0631115558,-0.6571362935,1.9117422095
H,-0.2129090699,-4.3935007061,-0.1432416994
C,-2.3037365819,-2.5512364721,-1.8581837453
C,-2.8186588451,-2.1409798508.5263298904
C,4.9267702062,-0.1463286234,-0.1412626317
C,3.443477252,-1.1743908712,-1.9180978123
C,4.3006343798,-0.061508837,2.1857338102
C,2.1111235629,-1.0043987608,3.0562752278
C,-3.6813910942,-2.5879659946,-2.1179628049
C,-1.3303172663,-2.8996139448,-2.9838539706
C,-4.180936744,-2.1806818478.2032744396
C,-2.3816747387,-2.0527259015,1.9887261557
H,5.6579782392.0456428214,-0.9199808122
C,5.2217205719.1961312577,1.1740054959
H,2.3699574515,-1.350528988,-2.0244387588
C,4.169065707,-2.4993487068,-2.2303569725
C,3.8388129803,-0.102711654,-2.9496408864
H,4.5485913033.2022901642,3.2082229553
H,1.0971605165,-1.0272713494,2.6490315876
C,2.1154311014.0270615036,4.197430459
C,2.4333343951,-2.4029455945,3.6254900592
H,-4.0279970378,-2.7880233503,-3.1268251168
C,-4.6109930872,-2.3851828398,-1.1050741128
H,-0.3261353783,-2.6019384464,-2.6691263214
C,-1.3033409101,-4.4256558493,-3.2155745103
C,-1.6424584632,-2.1761803289,-4.3066086078
H,-4.9186354819,-2.0610837578.9884330484
H,-1.4601155311,-1.466295703,2.031934993
C,-2.0770732024,-3.4586894392,2.552456347
C,-3.4081764018,-1.3639160308,2.9018410462
H,6.1750921492.6588325651,1.4140649966
H,5.2548600815,-2.3835197038,-2.137688503
H,3.9532063388,-2.8252770933,-3.254222594
H,3.861538904,-3.3013433252,-1.5524098902
H,3.4002709257.8712026567,-2.7139815841
H,3.4945325189,-0.3969519392,-3.947329786
H,4.9246981024.0270867534,-3.0094381236
H,3.0560128337.0134181179,4.7593903958
H,1.3162782137,-0.2085233753,4.9079824531
H,1.946594199,1.0380288941,3.8244554582
H,2.3674201558,-3.1864516163,2.8655037427
H,1.7317540116,-2.6589565941,4.4275251928
H,3.4456136889,-2.4289271208,4.0457507216
H,-5.6739445063,-2.4091255264,-1.3288726853
H,-1.0316733007,-4.9733744227,-2.308034406
H,-0.5758466774,-4.6831065758,-3.9936067997
H,-2.2844467336,-4.7896487806,-3.5402825775

H,-2.5793280813,-2.527169658,-4.7517558378
H,-0.8479931344,-2.3719458566,-5.0352723779
H,-1.7178262087,-1.093890691,-4.1749343612
H,-2.9702820127,-4.0931382203,2.5153451503
H,-1.7622123542,-3.3849126307,3.5995819243
H,-1.2799335703,-3.9668173597,2.0047182625
H,-3.7522076775,-0.4101508563,2.4999896286
H,-2.9566723865,-1.1667658726,3.8786628336
H,-4.2852678204,-1.9977737234,3.0750681645
H,1.0383168416,1.0585891739,-2.8534118084
C.1272747666.5153660522,-2.6155405072
H.1555279567,-0.5501202372,-2.7984021035
C,-1.0529031618,1.1826644143,-2.407207936
H,-1.1283694439,2.2573188362,-2.5127329088
H,-1.9977229613.6470873825,-2.3445742103

TS6-L2

Ni.3015409545,-0.1796872068.3091834969
C,-0.1809900423,-0.7925786189,2.7815491938
C,-1.0562494305,-0.6681122928,1.5480058798
H,-1.8968065621.0154799456,1.6810881327
H,-1.4129185549,-1.6287601082,1.1586523338
H.1126892996.1966238939,3.1575843228
Si,-0.9293262065,-1.782241586,4.2456452575
C,-1.1576791057,-3.58879582,3.7318730235
C.2934597903,-1.6803306761,5.6875040384
C,-2.5896698093,-1.0488597392,4.7837084453
H,-1.8483881942,-3.6937913522,2.8874509603
H,-1.5588700704,-4.1887562258,4.5576100819
H,-0.2044286177,-4.0395760165,3.4310716091
H,1.272026504,-2.0917710955,5.413652543
H,-0.0665459335,-2.2417112057,6.5583782215
H.4515812749,-0.6441752057,6.0093120679
H,-2.4901026559.001620834,5.0812593721
H,-2.9921865092,-1.593851843,5.6463406247
H,-3.3415760926,-1.0968472608,3.9880819938
H.7543755487,-1.3209159072,2.5396631949
C,2.2958462852,-0.5996580438.3085320339
C,3.276210398.2950910651.7108618159
C,2.7780894354,-1.8527023774,-0.0405244216
C,4.6375367786.0059465711.7497392568
F,2.9293528997,1.5591761799,1.099133966
C,4.1225611326,-2.213223606,-0.0234318434
F,1.9071702792,-2.8351968398,-0.427315581
C,5.061694383,-1.2669178551.3778877196
F,5.5492050159.9206013917,1.138075826
F,4.5349077562,-3.4481024398,-0.3746115408
F,6.3682165979,-1.5803356732.4060086267
C,-0.9720346199.5851004852,-0.8196806811
N,-1.8023953483,-0.0139438864,-1.7332333133
N,-1.1945107825,1.9268573701,-0.9992203539
C,-2.5133946031.9368237427,-2.4632789661
C,-1.9366014935,-1.4348255922,-1.9814762408
C,-2.1339841539,2.15088053,-2.0030076242
C,-0.550240894,3.0183085067,-0.2970079963
H,-3.2098618003.6577483466,-3.2367430755
C,-1.0091433812,-2.0661491737,-2.839722006
C,-3.0365243055,-2.1184648766,-1.420285121
H,-2.4355468298,3.1458161148,-2.2874768217
C.6607195384,3.5341968178,-0.8101475139
C,-1.2021921043,3.5846497538.8181626158
C,-1.1897125634,-3.4320767074,-3.0899411913
C.1116601219,-1.2996324308,-3.5392632792
C,-3.1693386781,-3.4824302455,-1.7128586046
C,-4.0941844897,-1.4196797613,-0.5675454387
C,1.2187859655,4.6387346398,-0.1554841091
C,1.3340161973,2.9582878559,-2.0542039794
C,-0.5976735051,4.6907424287,1.4302505807
C,-2.5407413016,3.0711131658,1.342477885
H,-0.4896644214,-3.9524089785,-3.7342700704
C,-2.2531475982,-4.1352152564,-2.5311212638
H.3568684586,-0.4299656904,-2.9230317659
C,-0.3654016802,-0.7845025453,-4.9139093034
C,1.4046997441,-2.1166149218,-3.6966078342
H,-4.0024092202,-4.0387891614,-1.2955621897
H,-3.6764778073,-0.4668508815,-0.2299288692
C,-4.4805036749,-2.219471274.6890509792
C,-5.3530581918,-1.1089370041,-1.4032412799
H,2.153071329,5.0558113501,-0.5153043356
C.5994565022,5.2123589518.9515239698
H,1.0373492331,1.9081790425,-2.1339677215
C.8546875842,3.6862769276,-3.3275972639
C,2.8701464547,2.9881899737,-1.9767848095
H,-1.0745535169,5.1510714552,2.2899729239
H,-2.7299933731,2.0966168742.884721828
C,-3.6928657253,4.0084776045.9290644269
C,-2.5353479825,2.863149925,2.8675973201

H,-2.3711303931,-5.1947119252,-2.7406942591
H,-0.6291348649,-1.6185359686,-5.5743885533
H.4276939444,-0.2078226436,-5.403236272
H,-1.2431790029,-0.1366309646,-4.827168381
H,1.7167821827,-2.5566753784,-2.7472463551
H,2.2107326879,-1.4658510651,-4.0527463861
H,1.2980267036,-2.9223328679,-4.4318282951
H,-5.0300651012,-3.1343594467.4428274816
H,-5.1324613734,-1.6162921749,1.3304307491
H,-3.6007691314,-2.5031809185,1.2731015261
H,-5.1240172714,-0.4821887103,-2.2706661744
H,-6.0972149296,-0.5813397047,-0.7959495756
H,-5.8154584758,-2.0307936922,-1.7735254346
H,1.0526087386,6.069997196,1.4409821015
H,-0.2291909574,3.6172625341,-3.4601388973
H,1.3272642679,3.2539046586,-4.2168273444
H,1.1199618852,4.7492574655,-3.2913167953
H,3.2671224625,4.0027106325,-2.094300827
H,3.2943348125,2.384059629,-2.7858766951
H,3.2292296696,2.5906438449,-1.0256463299
H,-3.5608676842,5.0091796128,1.3554954793
H,-4.6530459495,3.6175234469,1.2844220182
H,-3.7571517491,4.1170352562,-0.1584371112
H,-1.6990690207,2.2329104356,3.1838397795
H,-3.4656964239,2.3794196146,3.1845981097
H,-2.4621756586,3.8117017728,3.4103952832

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Ni.4121948523,-0.4655197695,-0.1844940284
C.8496744661,-0.8292461747,2.6478982067
C.3228253011.1767211733,1.6335597812
H.9285066789,1.0877671622,1.582432773
H,-0.7169023651.4478001218,1.8357306512
H,1.8466320033,-1.1817818745,2.3593395096
Si,1.0348197628,-0.1716265865,4.4341497202
C,-0.6357745908.3507262525,5.1621044824
C,1.7615825575,-1.5601834152,5.5001693298
C,2.2117872731,1.3127500827,4.4516011256
H,-1.088728764,1.1712983199,4.5946425182
H,-0.5235827454.6948969447,6.1976186192
H,-1.3523993873,-0.4792668549,5.1703178122
H,1.0958083768,-2.4308652302,5.5369202726
H,1.9255843884,-1.2293932529,6.53309446
H,2.7266971277,-1.9028002331,5.1087364691
H,3.1756252144,1.0658683401,3.9903678965
H,2.4147909553,1.6470793109,5.4763395804
H,1.7986530997,2.1684311616,3.905374867
H.2141450619,-1.7247983758,2.6750785333
C,2.3571384003,-0.5736755436,-0.235420339
C,3.1775020634.535899364,-0.3994883533
C,3.0358115423,-1.7850068641,-0.1756996681
C,4.5659561922.4752456257,-0.4924958806
F,2.6278915167,1.7824523371,-0.4832155959
C,4.4192825706,-1.9148573709,-0.2644851419
F,2.3339521351,-2.9465361265,-0.0160199591
C,5.1913790169,-0.766555067,-0.4197240809
F,5.3132585541,1.5851053324,-0.6514390936
F,5.0230170964,-3.1177411242,-0.1982273717
F,6.5293648481,-0.856654259,-0.509063075
C,-1.4754403208,-0.4036772867,-0.6445569699
N,-2.3230742172,-1.4624802913,-0.841649861
N,-2.1890082262.6710696494,-1.1094348343
C,-3.5197311042,-1.0574914021,-1.4227007108
C,-2.0458848935,-2.8448599312,-0.5120357131
C,-3.4357232477.2851899286,-1.5900100707
C,-1.7370576646,2.0469986397,-1.1513195032
H,-4.307634157,-1.7545615158,-1.6580668978
C,-1.2942459911,-3.6258067137,-1.4160694982
C,-2.5945763186,-3.3752185791.6744708814
H,-4.135421966.9936230184,-2.0033263647
C,-0.9217226831,2.4672201332,-2.2236426057
C,-2.1903986357,2.935325166,-0.1534882185
C,-1.0959199539,-4.973945424,-1.0933792966
C,-0.7450208817,-3.0648562656,-2.7257464431
C,-2.3677359589,-4.7316137337.9419548007
C,-3.4379111223,-2.5432404981,1.6377596469
C,-0.5633729181,3.820352271,-2.2715789935
C,-0.4578550174,1.5242767068,-3.3306138465
C,-1.8022653996,4.277355741,-0.2545031327
C,-3.0964764173,2.4968550077.9943433372
H,-0.5188170782,-5.6022577048,-1.7633130649
C,-1.6262373352,-5.5231679412.0704742534
H,-0.6833954859,-1.9771117601,-2.6230858367
C,-1.7055215912,-3.3643866477,-3.894361228
C.6737507968,-3.5676592182,-3.0454927689
H,-2.7760871156,-5.1717034506,1.8459793997
H,-3.2893374843,-1.4876694586,1.3925341214

C,-3.0148157776,-2.7299448274,3.1054423076
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C,-0.9980728407,4.717805683,-1.3009402295
H,-0.5946010203.4984024847,-2.9771714856
C,-1.3172671246,1.697135371,-4.5988994504
C,1.0370129725,1.6935817995,-3.6575280064
H,-2.1348834131,4.9853044537.4979897426
H,-3.0998200976,1.4034158314,1.0228011361
C,-4.5485512968,2.961083384.7639976113
C,-2.5867039254,2.9844055757,2.3625755922
H,-1.4592456588,-6.5720398091.299201706
H,-1.8176782082,-4.4444736579,-4.0426108648
H,-1.3212495174,-2.9358003726,-4.8267949804
H,-2.7024062439,-2.9467343101,-3.7193731159
H,1.3484280313,-3.4289409702,-2.1967227083
H,1.0798712193,-3.0169140771,-3.9009759046
H.6833715518,-4.6293457803,-3.3153240781
H,-3.2325865193,-3.7388387873,3.4717244593
H,-3.5619714723,-2.0290487539,3.7452512237
H,-1.94443396,-2.5479629264,3.2390675633
H,-5.2794173568,-2.6666487195.4441703766
H,-5.5403167708,-2.2358782314,2.1408193837
H,-5.1509419432,-3.9054641968,1.69912559
H,-0.7073604451,5.7629692924,-1.3596155437
H,-2.3775990249,1.5065894363,-4.4021105597
H,-0.9916096042,1.002322682,-5.3813659645
H,-1.2294827797,2.7142907381,-4.9975401422
H,1.2380475203,2.6392579422,-4.1727443059
H,1.3692029534.8887003933,-4.3224585028
H,1.648355992,1.6676485361,-2.7520833606
H,-4.612770469,4.0545053017.729223617
H,-5.1969191388,2.613917653,1.5763235829
H,-4.9560723084,2.5760122594,-0.1764903464
H,-1.5452450257,2.6932279081,2.5270606957
H,-3.1951892938,2.5524470662,3.1646483379
H,-2.6492193963,4.0736087026,2.4601099387

TS7-L2

Ni,-0.4325100626.3909258026.2944902477
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C,-0.1622233473,1.4198171,1.8804971002
H,-0.7072891739,2.3657879928,1.9004943602
H,-0.5463568108.7747830703,2.681479135
H,1.6932340463,2.1878063137,1.0665089209
Si,1.9051196449,2.6309369255,3.4828700019
C,1.1588412553,4.3681661017,3.4132002275
C,1.357291109,1.7749837462,5.0803727507
C,3.79674363,2.7660574027,3.4769178514
H,1.4132315224,4.8819163106,2.4784237728
H,1.5281296471,4.9886450254,4.2390730703
H.0657246269,4.3453429668,3.4873073481
H.2667541244,1.6898870356,5.144924711
H,1.6918376637,2.3403544906,5.9589997995
H,1.77337114.7644474069,5.1671625882
H,4.2765500822,1.78005629,3.4706279807
H,4.1521616294,3.2937972152,4.3708500406
H,4.1665341237,3.3196601418,2.6061422563
H,1.8856245657.6729489995,1.9519587956
C,-2.1719697008,1.1174636434.2462276089
C,-2.455045754,2.3038400622,-0.4243011222
C,-3.2780679368.4902032047.8108312015
C,-3.7372836638,2.82617609,-0.5697315154
F,-1.4450844296,3.0215176898,-0.9926760924
C,-4.5815010425.968274667.6983102416
F,-3.1215921025,-0.6670743287,1.5127149496
C,-4.8123563478,2.1504298985.0007662823
F,-3.9544227001,3.9700508005,-1.2470773723
F,-5.6180472693.310497034,1.2525753293
F,-6.0611703673,2.6322786559,-0.1247120334
C.7747391383,-0.9707435315,-0.689884754
N.8257372872,-2.3282274606,-0.5025926306
N,1.563396992,-0.7779805718,-1.7963583365
C,1.6202739719,-2.951801223,-1.4551517066
C.153117792,-3.0786292443.5377600533
C,2.0837388759,-1.9741434717,-2.2730494573
C,1.8786112452.4955943646,-2.411478302
H,1.7787020996,-4.0182745916,-1.4635263431
C.8218795798,-3.2907379364,1.761385933
C,-1.1095882595,-3.6419719402.2569457837
H,2.728134285,-2.0174472378,-3.1363361154
C,3.1386396215,1.0718047747,-2.1453687934
C.9532874315,1.0752887057,-3.3079455697
C.1790042985,-4.082489618,2.7216318659
C,2.2136582492,-2.7347106293,2.0492795044
C,-1.7028337185,-4.4267843196,1.2537125602
C,-1.8177362208,-3.4576328392,-1.0831577698
C,3.4512872758,2.2752586912,-2.7918583477

C,4.1725923072.4239632417,-1.225834814
C,1.3183544692,2.2819058744,-3.9170935957
C,-0.3713666975.4019735344,-3.6634855738
H.6650615446,-4.2635489803,3.6750843747
C,-1.0691751297,-4.6452883847,2.4732604036
H,2.4418836236,-1.9848630907,1.2868115381
C,3.2815538822,-3.841941339,1.9461673738
C,2.2902114627,-2.0304416984,3.4156083406
H,-2.675463986,-4.872410529,1.0716989675
H,-1.3425958305,-2.6207334424,-1.6026608301
C,-3.3074456653,-3.1059695338,-0.9175668539
C,-1.6532848455,-4.7099189478,-1.9681763599
H,4.4126568179,2.7447829635,-2.6079831304
C,2.5509251921,2.8781064531,-3.6630623533
H,3.6797084181,-0.3788544076,-0.6707768451
C,5.3161140605,-0.2106216571,-2.0428950801
C,4.737118423,1.410736035,-0.1888414912
H.6291599653,2.7622607531,-4.6025035194
H,-0.6952646044,-0.1724053582,-2.7906161829
C,-0.1824404105,-0.585052368,-4.8349322247
C,-1.4957917671,1.399232245,-3.9877517902
H,-1.5495876386,-5.2570762544,3.2317206647
H,3.1097104513,-4.6282787723,2.6898694929
H,4.2820315931,-3.4299158249,2.1205447993
H,3.2821360135,-4.3142950221.9582069472
H,1.5038007556,-1.2774260666,3.5187989448
H,3.2599708306,-1.5334078764,3.5297308165
H,2.1891507859,-2.7363943204,4.2471164005
H,-3.8895815577,-3.9582606591,-0.5501914808
H,-3.734631178,-2.8178698378,-1.8843401281
H,-3.4466317994,-2.2792099846,-0.2174298537
H,-0.6000718137,-4.9422176086,-2.1565523576
H,-2.1414010022,-4.5618024173,-2.9380910772
H,-2.1083663619,-5.5881461516,-1.4961990868
H,2.8098258429,3.8143973584,-4.1496617747
H,4.9463733368,-0.9658023009,-2.7440294488
H,6.0396024219,-0.6967444273,-1.3787452397
H,5.8531107977.5466677114,-2.6250061379
H,5.3347017119,2.200651272,-0.6558558028
H,5.3901083161.8849466108.5164130595
H,3.9367060517,1.8877325423.3820393804
H.1592610076,-0.0616801707,-5.7353942128
H,-1.1305417004,-1.07980878,-5.0743345992
H.5499895097,-1.3645468056,-4.6034764658
H,-1.5927396023,2.1602605075,-3.2103976125
H,-2.4493846886.866331101,-4.0662982133
H,-1.3342135695,1.9061198152,-4.9458647816

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Ni,-0.3988897056,-0.09693511,-0.0374662646
C,-2.468231569,-0.8496694164,-0.7477275651
C,-1.1978708512,-1.6757457205,-0.7074021196
H,-0.860332036,-2.0278666536,-1.6832507429
H,-1.1864741805,-2.4886941753.0242410681
H,-2.552484299,-0.310102865,-1.6981330907
Si,-4.0788145678,-1.853952389,-0.484128903
C,-4.2146255439,-3.0964016002,-1.9018315555
C,-4.0178081621,-2.7742054117,1.1653212826
C,-5.5721792729,-0.6895170586,-0.5245727617
H,-4.2039585443,-2.5968183173,-2.8779109012
H,-5.1465762469,-3.6712941876,-1.8397204638
H,-3.3839675761,-3.8109124124,-1.8890667948
H,-3.2015173882,-3.5042264044,1.1923861869
H,-4.9523952314,-3.3233830184,1.3332575212
H,-3.8798915551,-2.0964048038,2.015283371
H,-5.5130257616.0813243447.2524281727
H,-6.5064663528,-1.2417221109,-0.3651853047
H,-5.6575545895,-0.1802599776,-1.4916282794
H,-2.4632487093,-0.0623874323.0584790443
C,1.2728343145,-0.9793038278,-0.1617686897
C,2.0570087955,-0.9309953868,-1.3076368509
C,1.7756102362,-1.7855319383.852185379
C,3.2781095728,-1.5864145609,-1.4398128024
F,1.6359888956,-0.2142418946,-2.3876072373
C,2.9901937143,-2.4622062574.7738181815
F,1.0676756994,-1.9488307978,2.0053908808
C,3.7560297622,-2.3562761442,-0.3833559947
F,4.0054730699,-1.4793812524,-2.5703300537
F,3.4378477595,-3.2056450109,1.8060806899
F,4.9372640736,-2.9930044178,-0.4821263416
C,-0.0700755583,1.7520388424.6505630059
N,-0.0376089981,2.2096682485,1.9470291011
N.1217721966,2.8973346277,-0.0871986841
C.1468082116,3.588006681,2.0034902555
C,-0.2396259213,1.4329980176,3.1539618082
C.2469193925,4.0196439128.7258635873
C.178553423,3.0079252034,-1.5316313786
H.1807147345,4.12449993,2.9375612189

C,-1.544823488,1.3506669003,3.6834494295
C.879920819.8730697425,3.8100846197
H.3921587679,5.0076781936.3213487529
C,-1.0289208835,3.1700720649,-2.2470199354
C,1.4419997309,3.0556902998,-2.161695903
C,-1.7200422614.6376093546,4.8769980701
C,-2.7389140842,2.0582308487,3.0471952764
C.6433401027.1727299294,4.9994040623
C,2.3087793217,1.0626202779,3.3009015963
C,-0.943439465,3.3391263922,-3.6347695428
C,-2.3874092092,3.2363784074,-1.5508041638
C,1.4640219045,3.2320985415,-3.5511970092
C,2.7584105968,2.9796833892,-1.3882131955
H,-2.7130459812.5518628724,5.3069006721
C,-0.6401723268.0477048218,5.5245760869
H,-2.4410689687,2.3995517986,2.0522215074
C,-3.1353920219,3.3067949238,3.8612721623
C,-3.9534013491,1.1315913878,2.8677673123
H,1.4763064178,-0.2829499884,5.5232018333
H,2.2635672889,1.1429084869,2.2102790854
C,3.2439601688,-0.1107565748,3.6413425507
C,2.9180836629,2.3713945538,3.849439298
H,-1.8516638509,3.4591974045,-4.2158507957
C.2882625117,3.3663152536,-4.2821279297
H,-2.3071000884,2.6834938436,-0.610321301
C,-2.7529229118,4.6964639542,-1.2074327299
C,-3.5236435957,2.5922302155,-2.3635394527
H,2.4173740433,3.2623132628,-4.0677660333
H,2.5594040199,2.474536694,-0.4386059101
C,3.2911488237,4.3938302236,-1.0711501424
C,3.8509528163,2.1773292091,-2.1185260435
H,-0.7960231197,-0.5036563477,6.4477355428
H,-3.4588802953,3.0338691371,4.8719867463
H,-3.964281599,3.833949078,3.3753666226
H,-2.3024973178,4.0105259958,3.9585785323
H,-3.6865118467.2253280436,2.3173185781
H,-4.7426974341,1.65103534,2.3131617
H,-4.3818588729.8248287769,3.8279065691
H,3.4928284026,-0.1350722133,4.7084378555
H,4.1884673444.0031249844,3.0990857706
H,2.8106418852,-1.0747710763,3.3716172946
H,2.3425435868,3.2540277718,3.5585606248
H,3.9385407504,2.5027434947,3.4722565965
H,2.9664994747,2.3478189766,4.9442982509
H.3316528695,3.4983434435,-5.3597010728
H,-2.008059465,5.1631530753,-0.5562049525
H,-3.7196625406,4.7407636392,-0.6930280483
H,-2.8290176058,5.3025561445,-2.1173563186
H,-3.794593509,3.1924967624,-3.2388524849
H,-4.4227206537,2.5074712167,-1.7437013048
H,-3.258676141,1.5906529415,-2.7142989397
H,3.499411092,4.9458161379,-1.9947798658
H,4.2251618032,4.3309189255,-0.5015498021
H,2.5836607629,4.9843602531,-0.4827646849
H,3.4871705424,1.2091937752,-2.4640328817
H,4.6960104851,2.0059992629,-1.4430150042
H,4.2433174193,2.7205515414,-2.9856776262

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Ni,-0.3067008607,-0.2161572776,-0.6374054629
C,-3.1346055927,-0.6232485475,-1.6259416114
C,-1.6829858512,-0.2681185406,-1.9339947691
H,-1.6114767045.5901589367,-2.6128880652
H,-1.1452532732,-1.1246672045,-2.4134066741
H,-3.6300281466.2401043219,-1.1604525251
C,-4.1653735504.2437567413,-4.4387082753
C,-3.537888801,-2.7306933344,-3.8983614084
C,-5.980660077,-1.4075929518,-2.5557760371
H,-4.4709828119,1.2092814891,-4.017996189
H,-4.8472416025.017450237,-5.2675458924
H,-3.1647001019.374736305,-4.8661614994
H,-2.515343224,-2.6134267935,-4.2760692188
H,-4.1599703811,-3.0511914216,-4.7430582743
H,-3.5287404401,-3.551850753,-3.1711963025
H,-6.0406488744,-2.2010844666,-1.801172122
H,-6.6317758365,-1.6984487513,-3.3892797653
H,-6.4070246755,-0.5010776212,-2.1097361172
H,-3.1927893981,-1.4336101704,-0.8855150696
C,-1.155145248,1.2613373589.1416462058
C,-1.9722072985,1.1312143578,1.2592499668
C,-0.9987996089,2.5609574989,-0.326226702
C,-2.5720853524,2.210113399,1.9030274388
F,-2.2064597204,-0.0989507431,1.7917431936
C,-1.5759653093,3.6723395804.2828740258
F,-0.2323032166,2.8052506007,-1.4239206062
C,-2.370329131,3.4968627284,1.4121095502
F,-3.3285984629,2.0250711778,3.0031795657
F,-1.3622004698,4.9128251273,-0.1976894116

F,-2.9322634882,4.5556936993,2.0220873724
C,1.4154138017,-0.6561680332.3034100678
N,2.6775135495,-0.2521633478,-0.049745579
N,1.6400264101,-1.5264151818,1.3388931677
C,3.6504628258,-0.8638573193.7316417663
C,3.0112301325.6364740148,-1.1440126865
C,2.996673422,-1.6673774512,1.6060887063
C.6276854692,-2.2720769419,2.0576064961
H,4.7027944061,-0.6787662205.5878196768
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C,3.1848063108,2.0127293716,-0.8797206255
H,3.3651127507,-2.3239503054,2.3776459162
C.1668228579,-3.4873299674,1.5110776539
C.1839855358,-1.7884084854,3.3076934107
C,3.5956529111.9486549334,-3.4564864098
C,3.0809338585,-1.4122446266,-2.7145526723
C,3.5615731675,2.8320005515,-1.9507372612
C,3.0135216688,2.6081398383.5161977328
C,-0.778007058,-4.2140283532,2.248022604
C.6698628561,-4.0499409437.1840459494
C,-0.7564329397,-2.5594813501,4.0012298215
C.7162697897,-0.4976469256,3.9261230072
H,3.7611574913.549916099,-4.4527277843
C,3.7633204508,2.309823377,-3.2256596877
H,2.7389527386,-1.9067600148,-1.8012882236
C,4.4364873082,-2.0400324899,-3.0921694832
C,2.028332628,-1.6873456942,-3.8044930245
H,3.6958478938,3.8955812394,-1.78536203
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C,2.3425857901,3.9932980139.5030213922
C,4.3678989778,2.6839669502,1.251864478
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C,-1.2368235978,-3.757295039,3.4789480961
H,1.3609138659,-3.3247622348,-0.2538320306
C,1.4520495807,-5.361068126.3939058417
C,-0.4768300772,-4.2506382807,-0.8238462069
H,-1.122839898,-2.2132704728,4.9618267854
H,1.1356000772.1104023728,3.118819981
C,1.8505158096,-0.7955751517,4.928645572
C,-0.3799884064.3401371937,4.609037001
H,4.05294731,2.9675260564,-4.0404547278
H,4.8349430645,-1.6089143839,-4.0170745913
H,4.3281622132,-3.1191252516,-3.248668286
H,5.1843170863,-1.888225889,-2.3068461735
H,1.0601026089,-1.2472415679,-3.5456267152
H,1.8886158286,-2.766550246,-3.9343605573
H,2.3305538089,-1.2762512744,-4.7736666755
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H,1.8433166834,-5.7307528425,-0.5606482293
H.8144740224,-6.1454045086.8163862428
H,-1.1936648485,-5.0038898847,-0.4795675109
H,-0.0819241578,-4.5884581904,-1.7885714889
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H,1.4851725587,-1.4091364073,5.7601213829
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H,2.6832384752,-1.3307488791,4.4622400322
H,-1.2494965772.4769012899,3.9635156887
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H,-0.7234407393,-0.1194394073,5.5425879437
Si,-4.1954506861,-1.1261996283,-3.1302341053

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H,3.3219254009,-1.6428415378.3507272483
C,4.9146284452,-0.3783483731,-2.3341189274
C,4.4758918319,2.1158251659,-0.5642416844
C,6.1199116483,-0.2682193906.5145359393
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H,5.851214956.013956387,-2.7485739393
H,4.1066029172,-0.0611116604,-3.0036527574
H,3.6634578289,2.4560369181,-1.216543229
H,5.3980628019,2.5887701752,-0.9237495338
H,4.2797467055,2.5076184194.4408466981
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H,7.0483298188.1986591449.164232197
H,6.2760559887,-1.3536278064.5060559594
H,2.9033157494,-0.1465960191,1.1655030737

C.5146378273,-1.7101476534,-0.0505685451
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C.1876533342,-2.6698462776,-1.0244076624
C.5119144904,-3.5869369299,1.5477101093
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C.0094643986,-4.0194595953,-0.7550956568
F.012828241,-2.2731024443,-2.3119498527
C.1711411967,-4.4917210284.5451038009
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F,-0.3385359999,-4.8730631203,-1.7372713317
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C,-3.4573253738,1.9859107883,1.1231130141
C,-1.4842034889,1.5067802984,2.5584273116
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H,-3.9856615346,2.4771285251,1.9243112039
C,-0.6394065001,2.6106055178,2.7951935162
C,-1.7070015646.5058572111,3.5294472807
C,-2.2839458008,1.3955944209,-4.4485749361
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C,-2.6450823551,-0.6735109242,3.2847955652
H,-1.9198547185,2.1112531669,-5.1796830043
C,-2.7974971809.1767509122,-4.8785832008
H,-1.6670244507,3.1114372623,-1.5677104814
C,-2.5519390878,4.2307318739,-3.1616809502
C,-0.209847396,3.2512901065,-3.1206213922
H,-3.6558902345,-1.6999466768,-4.2993509655
H,-3.2828563339,-1.3228224817,-0.6223110514
C,-3.485109597,-2.956854837,-1.982727528
C,-5.2970997325,-1.3091670258,-1.3660793915
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C,-0.2005088539,1.7126388324,5.0123249433
H,-1.0277290959,3.4987881555.8926601682
C,-0.8078524154,5.09451529,2.2960575958
C,1.0630545641,3.7091429744,1.279344772
H,-1.1958740696,-0.1154535186,5.5246574848
H,-2.7300541163,-0.8055039731,2.2022486443
C,-4.056677593,-0.3853768386,3.8366368132
C,-2.1110375878,-1.9946789515,3.8666775887
H,-2.8324152415,-0.0542175893,-5.9397184192
H,-2.588978487,4.2647356294,-4.256278549
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H,-4.0906133335,-3.2774308224,-2.8380262346
H,-3.7267791943,-3.6291748179,-1.1524196283
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H,-5.8457344832,-1.4520809782,-2.30419735
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H,-1.8540465701,5.1089915373,2.6197176
H,-0.6864926086,5.8540862991,1.5156438561
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H,1.3366537821,2.7344922341.8629223293
H,-4.0289114048,-0.2348260285,4.9220312251
H,-4.7273790717,-1.2277624513,3.632219315
H,-4.4991295261.5090306315,3.3876138321
H,-1.0703835376,-2.1717961277,3.5884636683
H,-2.710811909,-2.8339771837,3.498265313
H,-2.1732368794,-2.0148579302,4.9606123959
Si,4.6431783008.2290769772,-0.5613952931

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C,-3.5723433211,-0.4443859455,-0.2776346863
C,-2.3184046221,-0.1144978517.5666222314
H,-1.8595993332,-1.0422618706.9221128915
H,-2.6088005652.4619864612,1.4499960781
H,-3.2646978044,-1.0056970176,-1.1694538643
Si,-4.9242289056,-1.4374638774.6244110399
C,-4.2592883038,-3.1389674561,1.1253217081
C,-5.4880911659,-0.5051406968,2.1738319263
C,-6.3878249156,-1.6565436029,-0.5556526428

H,-3.8957361866,-3.7006920718.2566141918
H,-5.0405249231,-3.7440266442,1.6016172703
H,-3.4296151011,-3.0637638462,1.8380393286
H,-4.6802941893,-0.4055529104,2.908460382
H,-6.3147633793,-1.0258644347,2.6722854166
H,-5.8377009885.5060061897,1.9326929891
H,-6.8168765352,-0.6913682868,-0.8498398089
H,-7.1905832838,-2.2450499605,-0.0953397894
H,-6.0884215847,-2.175035653,-1.4743065715
H,-4.0157188971.4910196637,-0.6458127277
C,-1.2810245242.6715171735,-0.2031407673
C,-1.2529298438,2.0504089248,-0.1944035187
C,-0.3250020171.0058452382,-1.0373458273
C,-0.379173375,2.8007988613,-1.0104604595
F,-2.0736734422,2.7485696573.6247378656
C.5713507669.7351105075,-1.8991633414
F,-0.6115926307,-1.3033711881,-1.3668855829
C.4870457954,2.1596755952,-1.8639628816
F,-0.3782499023,4.1440904677,-0.9201223265
F,1.0226480637.1786105397,-3.0740801508
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Ni,1.4870970011.1770427813,-0.317187247
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N,4.0385039494,-1.1834147087.3261507595
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C,5.1359063155,-1.1380924137,1.1771701756
C,3.8722011223,-2.18416324,-0.7047597392
C,4.9461670555,-0.0757388767,2.000378733
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H,5.9377456535,-1.8570805603,1.1207100936
C,3.177753835,-3.3712480872,-0.3931413333
C,4.4464520081,-1.95401996,-1.9721255482
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C,2.3035030331,1.4973383562,3.3615177813
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C,3.0700158739,-4.3420536334,-1.3969325641
C,2.5432981383,-3.6249693299.9710149639
C,4.3120090883,-2.9616921481,-2.9356773402
C,5.193539935,-0.6703753237,-2.3237627492
C,1.7688771533,2.6485461135,3.9541304653
C,1.9434792171.1249836647,3.9245803646
C,2.9782317147,4.0625170288,2.4197496097
C,4.5382043108,3.1499998973.6488343853
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C,3.6332380962,-4.1437569531,-2.6542296271
H,2.7323346457,-2.7508966736,1.599388159
C,3.1740567584,-4.8411993322,1.6749990588
C,1.0151527442,-3.7836036143.8562017107
H,4.7429494658,-2.8140183238,-3.9211491601
H,5.106247357.0145086081,-1.4761675192
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C,6.6939754346,-0.9376691602,-2.5509728125
H,1.0875548276,2.5469659121,4.7935711267
C,2.0962687777,3.918280406,3.4870804768
H,2.4441509282,-0.6335916637,3.3172839249
C,2.451530667,-0.0368951569,5.3704286861
C.4314305594,-0.1492314394,3.8371639491
H,3.2353149685,5.0575762536,2.0697522761
H,4.7769928206,2.1702237177.2267578315
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H,3.5398375882,-4.9106523425,-3.4181512837
H,3.0017112289,-5.7663820746,1.1140595798
H,2.7386026894,-4.9738018417,2.671820985
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H.5655661228,-3.866648632,1.8524976165
H.7459887818,-4.6865633781.2966647189
H,4.6753093709,-0.560112352,-4.4547906399
H,5.0663703295.996201526,-3.71751626
H,3.5029859007.2270351375,-3.3873367928
H,7.1628894706,-1.3924135246,-1.671633366
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H,6.8575041913,-1.6120616119,-3.3990813501
H,1.6679913093,4.7978587478,3.9595231189
H,3.5323483018.1269888821,5.4395588343
H,2.2403823789,-1.0472357669,5.738415027
H,1.9647845664.6710034542,6.050199757
H,-0.1463507489.5606496262,4.4390497494
H.2043377367,-1.1562402919,4.2053131735
H.0792749274,-0.077794057,2.8038719218
H,5.6918563128,4.7511669472,1.6070733661
H,6.5835954101,3.8569572394.3678425389
H,6.3027396905,3.1299046824,1.9576700448
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