

Supplementary information for

Mechanism and Regioselectivities of (NHC)Nickel(II)hydride-catalyzed Cycloisomerization of Dienes: A Computational Study

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I. β -Hydride transfer vs. β -hydride elimination

As compared with β -hydride transfer, a β -hydride elimination can occur from intermediate **7**, and eventually generate the intermediate **1** after extruded the product **10**. As shown in Figure S1, the β -hydride elimination transition state **TS-S1** is 7.2 kcal/mol higher than a β -hydride transfer transition state **TS8**. We hypothesis that this result is due to the instability of nickel-hydride bond in **int-S2**.

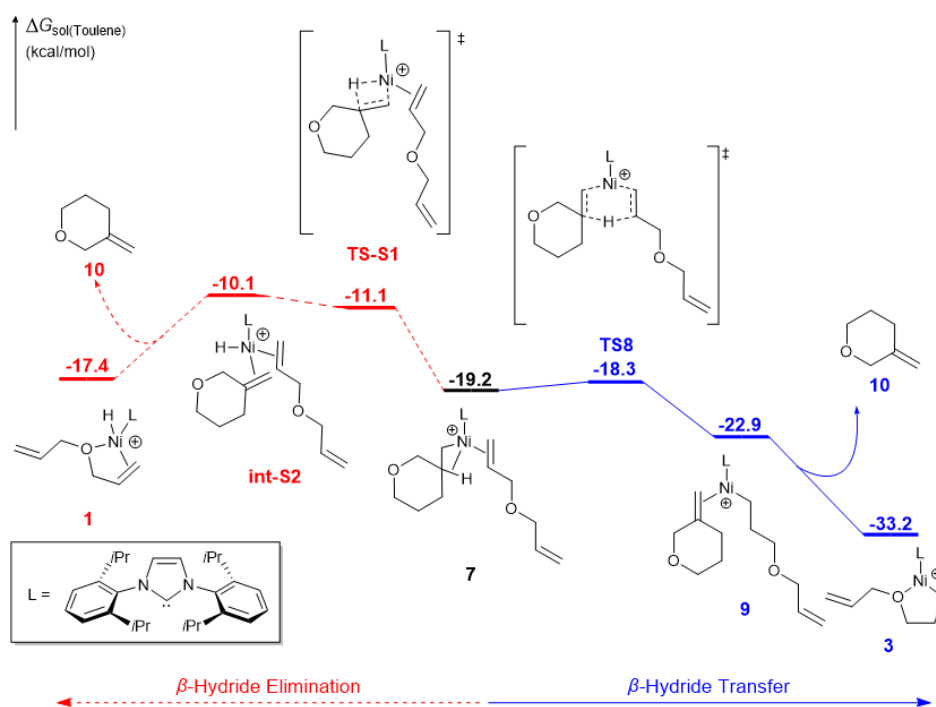


Figure S1. DFT-computed β -hydride transfer is favored than β -hydride elimination

II. Additional study on the selectivity of olefin insertion

As we discussed in the article, in **TS5** and **TS11**, we proved that the selectivity of the olefin insertion step is controlled by the ring strain rather than the steric effects of the bulky ligand *i*Pr. We also studied the degraded models of **TS16** and **TS19**. In figure S2, the free energy difference remain unchanged after the bulky 2,6-diisopropylphenyl groups was replaced by methyl groups (model 1).

Whereas the regioselectivity no longer exists after the carbocycle of the two transition states was removed (model 2).

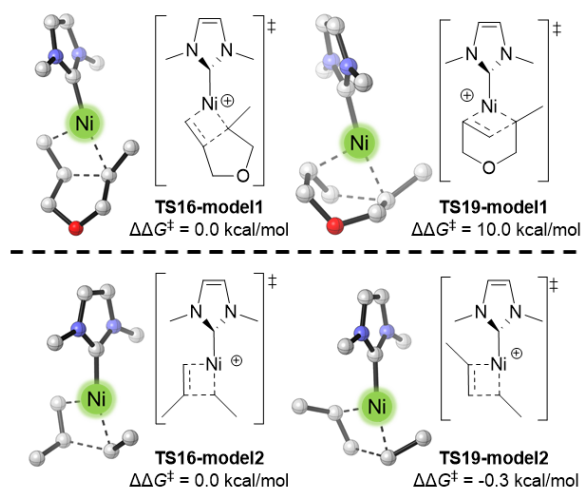


Figure S2. Relative Gibbs free energies of the degraded-truncated models of the competing olefin insertion transition states, **TS16** and **TS19**. All the hydrogens are hidden for clarity in the 3D diagrams of optimized species.

III. Selectivity of olefin insertion in the intermolecular hydroalkenylation

In the intermolecular hydroalkenylation¹, a rapid equilibrium occurs between the pre-insertion intermediates. Hence, the olefin insertion step determined the selectivity of both olefin substrates. As shown in Figure S3, the free energy of two β -hydride transfer transition states **TS-S4** and **TS-S6** and an olefin insertion with benzylic nickel species **TS23** are lower than the homobenzylic nickel species olefin insertion transition state **TS25**. From **int-S7**, an intermolecular β -hydride transfer process *via* **TS-S4** and **TS-S6**, generates **int-S5**. Subsequently, an olefin insertion with benzylic nickel species **TS23** occurs instead of an olefin insertion transition state with homobenzylic nickel species **TS25**.

¹ X. Hong, J. Wang, Y.-F. Yang, L. He, C.-Y. Ho and K. N. Houk, *ACS Catal.*, 2015, **5**, 5545.

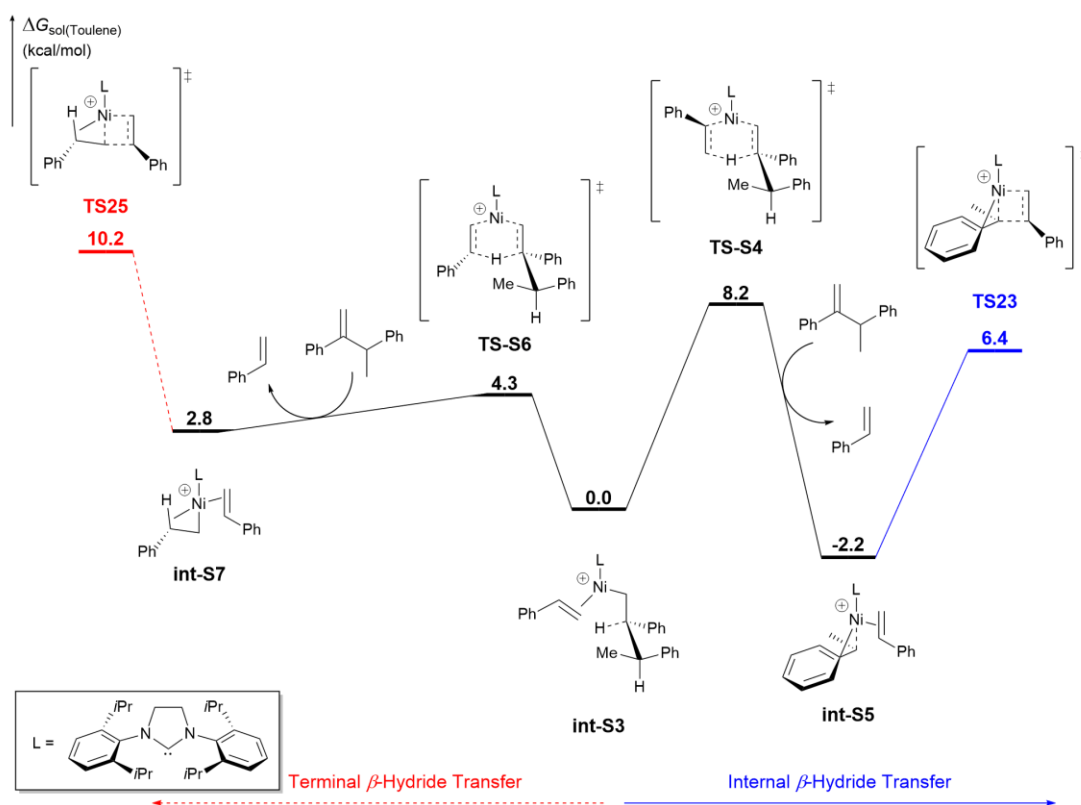


Figure S3. pre-insertion intermediates are in a rapid equilibrium through an intermolecular β -hydride transfer process.

IV. Additional study on the selectivity of β -hydride transfer

An alternative mechanism can occur with the initial hydride inserts on the terminal alkene position. As shown in Figure S4, β -hydride transfer also favors an internal position, which is similar to Figure 4. *Via* **TS-S9**, **int-S8** can produce the five-membered ring intermediate **3**. **3** is actually the active intermediate in the internal hydride insertion pathway, which produces the *n-exo* product in the next catalytic cycle. Only the unfavorable internal hydride transfer *via* **TS-S11** regenerates the four-membered ring intermediate **29**, leading to the catalytic turnover of the (*n-1*)-*exo* product. Similar to internal hydride insertion pathway (Figure 4), the regioselectivity of β -hydride transfer favors the internal position of alkene due to the steric repulsions between the IPr ligand and the

alkene substrate.

Therefore, the (*n*-1)-*exo* and *n*-*exo* products are both produced in the initial stage of catalysis. Once the nickel-hydride pre-catalyst is consumed, the catalytic cycle for the (*n*-1)-*exo* product formation cannot effectively produce turnover because it predominately generates the five-membered ring alkyl-nickel species **3** for the competing catalytic cycle of *n*-*exo* product formation.

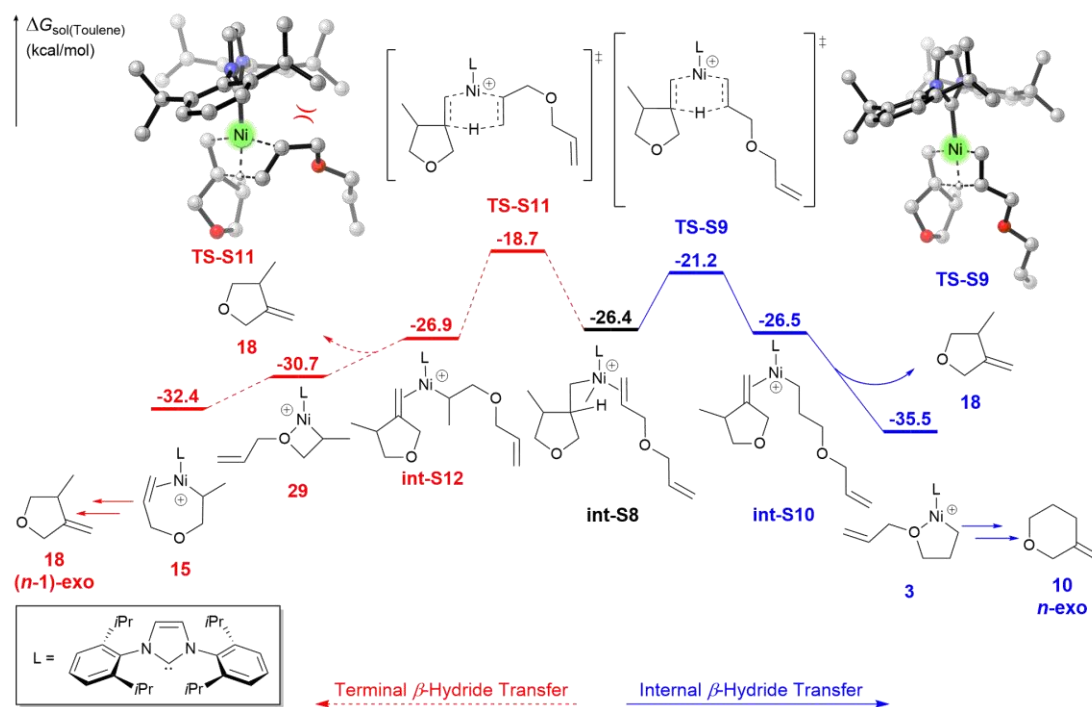


Figure S4. DFT-computed regioselectivity of β -hydride transfer steps that determine the competition between *n*-*exo* and (*n*-1)-*exo* products. All the hydrogens are hidden for clarity in the 3D diagrams of optimized species.

V. Energies, Enthalpies, and Free Energy of the Calculated Structures

Zero-point correction (ZPE), thermal correction to enthalpy (ΔH), thermal correction to Gibbs free energy (ΔG), energies (E), enthalpies (H), Gibbs free energies (G) (in Hartree), $\langle S^2 \rangle$ values (after annihilation) and imaginary frequencies of the transition states calculated at the B3LYP-D3/6-311+G(d,p)-SMD(Toluene)//B3LYP/6-31G(d) level of theory

Structures	ZPE	tcH	tcG	E	H	G	Imaginary Frequency
diallyl ether	0.146829	0.156234	0.113103	-309.673141	-309.516907	-309.560038	
1	0.732998	0.775382	0.657563	-1640.588329	-1639.812947	-1639.930766	
TS2	0.729513	0.772484	0.649419	-1640.565772	-1639.793288	-1639.916353	556.8i
3	0.737063	0.779148	0.660768	-1640.616699	-1639.837551	-1639.955931	
4	0.735970	0.777544	0.660609	-1640.593713	-1639.816169	-1639.933104	
TS5	0.736791	0.777438	0.663041	-1640.595019	-1639.817581	-1639.931978	121.5i
TS5-model1	0.291691	0.308944	0.246257	-785.797126	-785.488182	-785.550869	165.7i
TS5-model2	0.278748	0.295683	0.234488	-672.520071	-672.224388	-672.285583	222.8i
TS5-model3	0.182262	0.189931	0.151617	-349.001601	-348.811670	-348.849984	
6	0.740828	0.780858	0.668981	-1640.650416	-1639.869558	-1639.981435	
7	0.888351	0.938427	0.802746	-1950.321132	-1949.382705	-1949.518386	
TS8	0.885575	0.935129	0.801047	-1950.318050	-1949.382921	-1949.517003	894.4i
9	0.888364	0.938798	0.801453	-1950.325740	-1949.386942	-1949.524287	
10	0.151126	0.158759	0.120152	-309.707918	-309.549159	-309.587766	
TS11	0.736726	0.777295	0.663294	-1640.593055	-1639.815760	-1639.929761	256.4i
TS11-model1	0.291809	0.308868	0.246995	-785.795486	-785.486618	-785.548491	246.5i
TS11-model2	0.279095	0.296008	0.235448	-672.521572	-672.225564	-672.286124	226.9i
TS11-model3	0.182534	0.189958	0.152383	-348.999351	-348.809393	-348.846968	
12	0.740913	0.781372	0.667186	-1640.636875	-1639.855503	-1639.969689	
13	0.152127	0.159518	0.121793	-309.715134	-309.555616	-309.593341	
14	0.151729	0.159175	0.121136	-309.717709	-309.558534	-309.596573	
15	0.737155	0.778797	0.663709	-1640.614739	-1639.835942	-1639.951030	
TS16	0.737667	0.778046	0.665314	-1640.610301	-1639.832255	-1639.944987	165.7i
TS16-model1	0.292464	0.309600	0.247650	-785.811736	-785.502136	-785.564086	147.8i
TS16-model2	0.278748	0.295683	0.234488	-672.520071	-672.224388	-672.285583	222.8i
17	0.739673	0.780390	0.665465	-1640.639329	-1639.858939	-1639.973864	
18	0.149869	0.157883	0.118666	-309.710137	-309.552254	-309.591471	
TS19	0.736681	0.777238	0.664018	-1640.592775	-1639.815537	-1639.928757	303.9i
TS19-model1	0.291792	0.308939	0.247333	-785.795488	-785.486549	-785.548155	300.8i
TS19-model2	0.279095	0.296008	0.235448	-672.521572	-672.225564	-672.286124	226.9i
20	0.739745	0.780513	0.665396	-1640.630294	-1639.849781	-1639.964898	
21	0.151235	0.158861	0.120937	-309.723790	-309.564929	-309.602853	
22	0.150921	0.158541	0.120586	-309.716224	-309.557683	-309.595638	
TS23	0.883425	0.931432	0.803231	-1951.099933	-1950.168501	-1950.296702	218.6i
TS24	0.884295	0.932020	0.805774	-1951.097041	-1950.165021	-1950.291267	229.6i
TS25	0.882298	0.930607	0.798467	-1951.089144	-1950.158537	-1950.290677	175.9i
TS26	0.883095	0.931143	0.801194	-1951.086466	-1950.155323	-1950.285272	232.8i

TS27	0.885759	0.935209	0.801640	-1950.313588	-1949.378379	-1949.511948	984.0 <i>i</i>
28	0.888074	0.938648	0.800992	-1950.329291	-1949.390643	-1949.528299	
29	0.735718	0.778179	0.659301	-1640.607595	-1639.829416	-1639.948294	
31	0.879434	0.928104	0.795481	-1837.082905	-1836.154801	-1836.287424	
TS32	0.879982	0.926934	0.798391	-1837.068954	-1836.142020	-1836.270563	210.7 <i>i</i>
33	0.883822	0.930709	0.802129	-1837.108118	-1836.177409	-1836.305989	
TS35	0.875930	0.923150	0.795817	-1837.069654	-1836.146504	-1836.273837	923.5 <i>i</i>
36	0.879457	0.928130	0.794844	-1837.078601	-1836.150471	-1836.283757	
TS37	0.879871	0.926752	0.798524	-1837.066714	-1836.139962	-1836.268190	171.0 <i>i</i>
38	0.883462	0.930492	0.800180	-1837.113634	-1836.183142	-1836.313454	
TS40	0.904233	0.951393	0.823394	-1801.157806	-1800.206413	-1800.334412	196.0 <i>i</i>
TS41	0.903968	0.951200	0.822403	-1801.157104	-1800.205904	-1800.334701	187.8 <i>i</i>
styrene	0.13377	0.141482	0.102307	-309.4771924	-309.3357104	-309.3748854	
2,3-diphenyl- 1-butene	0.272252	0.286989	0.230124	-618.9875052	-618.7005162	-618.7573812	
TS-S1	0.884431	0.934468	0.79828	-1950.303733	-1949.369265	-1949.505453	147.7 <i>i</i>
int-S2	0.884849	0.935576	0.798238	-1950.30208	-1949.366504	-1949.503842	
int-S3	1.01945	1.07621	0.925529	-2260.614968	-2259.538758	-2259.689439	
TS-S4	1.016318	1.0722	0.92572	-2260.602112	-2259.529912	-2259.676392	941.6 <i>i</i>
int-S5	0.882371	0.931712	0.799932	-1951.110371	-1950.178659	-1950.310439	
TS-S6	1.015774	1.07177	0.924681	-2260.607235	-2259.535465	-2259.682554	773.0 <i>i</i>
int-S7	0.881099	0.930109	0.796562	-1951.099084	-1950.168975	-1950.302522	
int-S8	0.887797	0.938166	0.802692	-1950.332467	-1949.394301	-1949.529775	
TS-S9	0.883995	0.933942	0.798499	-1950.320078	-1949.386136	-1949.521579	922.4 <i>i</i>
int-S10	0.887121	0.937893	0.799845	-1950.329818	-1949.391925	-1949.529973	
TS-S11	0.884679	0.934488	0.800210	-1950.317835	-1949.383347	-1949.517625	973.9 <i>i</i>
int-S12	0.887028	0.937875	0.800520	-1950.331091	-1949.393216	-1949.530571	

VI. Cartesian Coordinates for the Optimized Structures

diallyl ether

C	-1.17019200	0.58180400	-0.16100700
H	-1.34679100	1.21184900	0.72757300
H	-1.04191300	1.26473800	-1.02188900
C	1.17017000	0.58175100	0.16110400
H	1.34689200	1.21216900	-0.72718900
H	1.04179800	1.26435000	1.02224400
C	-2.33645000	-0.33065800	-0.40251100
C	-3.49015800	-0.26971900	0.26136800
H	-2.19334400	-1.06509400	-1.19432300
H	-4.31977800	-0.93171900	0.02861200
H	-3.65242600	0.44840100	1.06282600
C	2.33639300	-0.33081300	0.40239600
C	3.49022700	-0.26962500	-0.26123700
H	2.19311900	-1.06556100	1.19389400
H	4.31979300	-0.93171500	-0.02856200
H	3.65264100	0.44877400	-1.06241800
O	0.00000900	-0.20408000	-0.00018100

1

Ni	-0.18208600	0.17062800	-1.46803400
H	-0.86742700	-1.09436900	-1.57235000
C	0.22438300	0.67839300	-3.52359000
C	-1.12728300	0.73224900	-3.34650300
H	0.67473200	-0.17307200	-4.02800800
H	-1.76882000	-0.06857000	-3.69870100
H	-1.62556500	1.63020500	-2.98610900
C	1.13127800	1.80989300	-3.08934600
H	2.18695700	1.53870500	-3.20134100
H	0.95068800	2.74874600	-3.62419400
O	0.81176600	1.96966600	-1.68549900
C	1.80502600	2.67145300	-0.89568700
H	2.75435500	2.12539800	-0.96090600
H	1.42229300	2.59590200	0.12527400
C	1.96032000	4.09811900	-1.32530900
C	3.11715600	4.61973500	-1.73852600
H	1.06692100	4.71778100	-1.26040500
H	3.20609400	5.66699100	-2.01199600
H	4.02495100	4.02295800	-1.80422300
C	-0.22558100	-0.40759200	0.34867300
N	-1.34721300	-0.42520200	1.12028300

N	0.73291900	-1.01956600	1.10161000
C	-1.09646700	-1.04073100	2.33973500
C	-2.64119000	0.09571800	0.72585400
C	0.20457300	-1.42275600	2.32469600
C	2.10996400	-1.24388600	0.70162200
H	-1.86170900	-1.14371500	3.09264300
C	-2.91012200	1.46395000	0.93388700
C	-3.59005000	-0.79838500	0.18594000
H	0.80022800	-1.94010000	3.05849200
C	2.38867300	-2.29199800	-0.20135700
C	3.12335000	-0.43573200	1.27054500
C	-4.17237400	1.93570900	0.55085200
C	-1.91514200	2.42026200	1.58551500
C	-4.83546600	-0.26873600	-0.17413900
C	-3.32746300	-2.29356600	0.02470700
C	3.72452200	-2.46898600	-0.58803300
C	1.33303400	-3.28043000	-0.69248000
C	4.43841000	-0.66864600	0.84965100
C	2.85268600	0.59703200	2.36559300
C	-5.12418200	1.08239800	-0.00022400
H	-4.41671100	2.98343800	0.69838800
C	-2.42848600	2.90242500	2.95777400
C	-1.58365000	3.61493900	0.67018800
H	-0.98067700	1.87688500	1.76130200
H	-5.59292200	-0.92563300	-0.59051700
C	-3.61215200	-2.78856000	-1.40586200
C	-4.13941200	-3.10550000	1.05584000
H	-2.26706500	-2.47869200	0.22388000
C	4.73693100	-1.66210900	-0.07995500
H	3.97540100	-3.26564200	-1.28153800
C	1.54772800	-4.66036800	-0.03455900
C	1.30378100	-3.40408100	-2.22698900
H	0.34866200	-2.92095000	-0.38110300
H	5.24378100	-0.07078500	1.26344900
C	3.66631600	1.89676300	2.21052900
C	3.13966700	-0.00653400	3.75971000
H	1.79038700	0.86635900	2.32837100
H	-6.09876900	1.46902200	-0.28437800
H	-2.63216900	2.06010600	3.62785300
H	-1.68432300	3.54730400	3.43874000
H	-3.35461000	3.47910400	2.85701900
H	-1.18347300	3.27644300	-0.29203200
H	-2.46792500	4.22959000	0.46983800
H	-0.83813200	4.26192800	1.14764800

H	-3.02773500	-2.22871100	-2.14423600
H	-3.34860900	-3.84833500	-1.49544600
H	-4.67097200	-2.69239200	-1.66913700
H	-3.90697700	-2.80261100	2.08301000
H	-5.21664100	-2.97094100	0.90671500
H	-3.91828700	-4.17435200	0.95966200
H	5.76568900	-1.82196600	-0.39010200
H	1.52461100	-4.59120100	1.05857000
H	0.76199500	-5.35711700	-0.34761300
H	2.51296800	-5.09257300	-0.32088500
H	1.12272100	-2.43175200	-2.69860300
H	2.24196100	-3.80573000	-2.62503800
H	0.50041500	-4.08319000	-2.53339500
H	3.56826200	2.33748900	1.21453100
H	3.32435300	2.63562000	2.94336100
H	4.73314200	1.73378900	2.39694700
H	2.55709500	-0.91249900	3.95191200
H	4.19875500	-0.27203700	3.85164200
H	2.90376800	0.71899500	4.54620500

TS2

Ni	-0.43918500	-0.83087300	-0.40037500
C	-2.45194900	-0.68615900	-1.23800400
C	-1.96767200	-1.97745000	-1.02056500
H	-2.29429600	-2.53820900	-0.14596400
H	-2.42519800	-0.28553600	-2.25060600
H	-1.22593400	0.35787100	-0.76415500
H	-1.56221400	-2.55862100	-1.84626200
C	-3.51016500	-0.06215100	-0.34416100
H	-3.41458200	1.03601800	-0.33886500
H	-3.39087400	-0.41431800	0.69501700
C	-5.86798500	0.16096500	-0.25559300
H	-5.83072700	-0.05305100	0.82688200
H	-5.81756400	1.25353700	-0.38296100
O	-4.74347500	-0.46155300	-0.88925300
C	-7.12445100	-0.38925800	-0.85749400
C	-8.08232200	0.36574100	-1.39426900
H	-7.23119900	-1.47217600	-0.81555900
H	-8.99514400	-0.06824500	-1.79186000
H	-7.99566900	1.44892600	-1.44982800
C	1.08503700	0.14282300	0.19580200
N	1.96984700	-0.82198300	0.54297700
N	1.71735900	1.31379000	0.43340800
C	3.16276500	-0.28140900	1.00121700

C	1.49376700	-2.17939500	0.36157200
C	2.99829900	1.06888900	0.92948000
C	1.16472100	2.63521300	0.20774000
H	3.99741900	-0.88267000	1.32706700
C	0.80685500	-2.80884100	1.43579200
C	1.73383000	-2.82507700	-0.88229400
H	3.66738500	1.87638900	1.18256100
C	1.34447300	3.23050900	-1.05675500
C	0.48780800	3.26894800	1.26854100
C	0.33078100	-4.10772300	1.21369300
C	0.64640300	-2.15907100	2.80682900
C	1.22994100	-4.12307500	-1.03347900
C	2.55289100	-2.18714800	-2.00028400
C	0.80329200	4.50873300	-1.24279500
C	2.09471200	2.55196400	-2.19931900
C	-0.03063700	4.54650600	1.02258500
C	0.30444200	2.62910800	2.64187500
C	0.53907600	-4.75560400	-0.00189800
H	-0.19338300	-4.62516600	2.01108100
C	1.51729200	-2.88794200	3.85229700
C	-0.82532100	-2.09897500	3.25707400
H	1.00837800	-1.12856500	2.74145200
H	1.39530500	-4.65162800	-1.96712700
C	1.75277400	-2.07432600	-3.31187500
C	3.87107500	-2.96038100	-2.21591900
H	2.81802000	-1.17096300	-1.69299900
C	0.12289300	5.16035500	-0.21765500
H	0.92035800	5.00201800	-2.20307300
C	3.34643700	3.35445300	-2.60699900
C	1.17475900	2.30771600	-3.41201600
H	2.43776300	1.57168200	-1.85166100
H	-0.55881800	5.06869200	1.81469600
C	-1.18595700	2.39041700	2.95545100
C	0.97761000	3.46339800	3.74993500
H	0.79333200	1.64913800	2.63365900
H	0.16876400	-5.76697500	-0.14320700
H	2.57301900	-2.89972500	3.55998800
H	1.43952300	-2.38540400	4.82233300
H	1.19579000	-3.92667700	3.98620900
H	-1.44016500	-1.54722100	2.53647100
H	-1.25825400	-3.09810600	3.37690300
H	-0.90050700	-1.59036000	4.22398300
H	0.83994500	-1.48353800	-3.17112100
H	2.35812200	-1.58110500	-4.07978100

H	1.46483800	-3.05755500	-3.70022600
H	4.46083100	-3.01631900	-1.29440700
H	3.68480300	-3.98486700	-2.55623500
H	4.47881000	-2.46069100	-2.97777200
H	-0.28554100	6.15291500	-0.38475200
H	4.02176200	3.50403500	-1.75742500
H	3.89829900	2.82481000	-3.39161000
H	3.08029600	4.34245800	-2.99843200
H	0.30244000	1.70486200	-3.13482000
H	0.80883500	3.24939400	-3.83566600
H	1.72027300	1.77951000	-4.20228800
H	-1.65615800	1.76160600	2.19060100
H	-1.29622900	1.89193700	3.92525900
H	-1.74252800	3.33288900	3.00206000
H	2.04483500	3.60909800	3.54992900
H	0.51899000	4.45382600	3.84327700
H	0.87851800	2.95976800	4.71801300

3

Ni	0.58537500	0.00035700	1.03122000
C	-0.25291900	-0.03466400	3.63278800
C	-0.72551300	-0.57469800	2.28536700
H	-0.81236600	-0.49999600	4.45812200
H	-0.66424000	-1.66900500	2.21734700
C	1.22781400	-0.32167100	3.80412300
H	1.69443700	0.25902100	4.60755400
H	1.42400200	-1.38651600	3.97107600
O	1.83539500	0.07223100	2.54284500
C	3.28046200	-0.08762300	2.46152500
H	3.72288300	0.50837600	3.26850000
H	3.54771000	0.36959300	1.50401600
C	3.71941900	-1.51897600	2.53408200
C	4.54621400	-1.99041100	3.46905600
H	3.34733000	-2.17485100	1.74780500
H	4.87463800	-3.02572100	3.47196600
H	4.94040500	-1.35513900	4.25982100
H	-1.72241600	-0.23724900	2.00910700
H	-0.42952300	1.04538700	3.69626900
C	-0.43344800	0.10134800	-0.55293700
N	-1.70516400	0.08214700	-1.03415900
N	0.34682300	0.33543000	-1.64628200
C	-1.70876000	0.30444500	-2.40964300
C	-2.92676400	-0.11725800	-0.27833700
C	-0.41777500	0.46632700	-2.79689900

C	1.78624200	0.43129900	-1.53379600
H	-2.62834900	0.32644000	-2.97277200
C	-3.44271400	-1.42456000	-0.16659000
C	-3.56931300	1.01217500	0.26845800
H	0.02137200	0.65685700	-3.76372700
C	2.35813000	1.68546800	-1.21421900
C	2.56064400	-0.72995600	-1.76623600
C	-4.64040400	-1.58072100	0.54213000
C	-2.77441000	-2.63862900	-0.80682400
C	-4.76091500	0.79182200	0.97123700
C	-3.03477200	2.43360500	0.11434200
C	3.75500800	1.74077000	-1.10338300
C	1.53405500	2.95913200	-1.04285700
C	3.94988200	-0.60785200	-1.64372500
C	1.94611300	-2.06843800	-2.16627100
C	-5.29101700	-0.48814600	1.10951100
H	-5.07174000	-2.57142200	0.64662500
C	-3.58727300	-3.13352100	-2.02143300
C	-2.54603800	-3.78212200	0.20002700
H	-1.78896900	-2.33312900	-1.17381700
H	-5.28442700	1.63661500	1.40868700
C	-2.71068400	3.07347300	1.47865400
C	-4.01163100	3.31383100	-0.69129000
H	-2.09773500	2.38951600	-0.45034000
C	4.54155500	0.61071800	-1.31480100
H	4.23243500	2.68702600	-0.86794900
C	1.82694600	3.95758300	-2.18197800
C	1.75717300	3.61088700	0.33567500
H	0.47424500	2.69394900	-1.10774600
H	4.57828000	-1.47560400	-1.81985300
C	2.24938600	-3.16996300	-1.13209700
C	2.40522100	-2.49021300	-3.57709400
H	0.85882100	-1.94975100	-2.19952000
H	-6.21908100	-0.63381100	1.65484500
H	-3.71155000	-2.34525900	-2.77239900
H	-3.08392900	-3.98125900	-2.49996100
H	-4.58732100	-3.46453000	-1.71943100
H	-1.97010700	-3.44322400	1.06814500
H	-3.49051000	-4.19822200	0.56682000
H	-1.99397800	-4.59888200	-0.27819700
H	-1.98131500	2.47467100	2.03563000
H	-2.29116700	4.07588600	1.33647000
H	-3.60658600	3.17614300	2.10083700
H	-4.21446100	2.88695900	-1.67970600

H	-4.97107800	3.42589000	-0.17442100
H	-3.59149200	4.31579800	-0.83352600
H	5.62268900	0.68218800	-1.23535100
H	1.63058200	3.51461900	-3.16447600
H	1.19442600	4.84577700	-2.07720200
H	2.87154200	4.28782100	-2.16710000
H	1.52054000	2.91589700	1.15025400
H	2.79299100	3.94367900	0.46585500
H	1.11347500	4.49060200	0.44350200
H	1.86456400	-2.89947100	-0.14162100
H	1.77510200	-4.11089500	-1.43181600
H	3.32543700	-3.35682000	-1.04161800
H	2.16323600	-1.72590000	-4.32369600
H	3.48660000	-2.66209800	-3.61428600
H	1.90987100	-3.42161200	-3.87194500

4

Ni	-0.59388800	1.17430900	-0.34696800
C	-2.00187500	3.88318300	-1.09994400
C	-1.86325800	2.55788800	-0.38167200
H	-2.98758800	4.31165000	-0.85305600
H	-1.84240500	2.68814800	0.71936500
C	-0.94982700	4.93305100	-0.74047400
H	-1.20398700	5.88308000	-1.21878400
H	-0.92893800	5.10024900	0.34873600
O	0.35934200	4.61827800	-1.20501900
C	1.13520500	3.77538900	-0.39455100
H	0.87963700	3.88998200	0.67095100
H	2.18136200	4.10232400	-0.49784200
C	1.11499700	2.31718200	-0.79332300
C	0.50383900	1.83960400	-1.94282500
H	1.85918400	1.70050600	-0.29190000
H	0.79354700	0.88305300	-2.36705100
H	-0.04428200	2.52233800	-2.58272700
H	-2.67083200	1.85614300	-0.66512400
H	-2.00874800	3.73562500	-2.18750100
C	0.09478800	-0.67280900	0.14303000
N	-0.89240300	-1.58989300	0.34831200
N	1.24550600	-1.37052500	0.35467300
C	-0.37843800	-2.83365600	0.68270500
C	-2.28907400	-1.22672200	0.24305300
C	0.97336300	-2.69323000	0.68816800
C	2.58586800	-0.82301500	0.28659900
H	-1.00763000	-3.68634500	0.88554100

C	-2.96325500	-0.79718200	1.40988600
C	-2.91851800	-1.31646400	-1.01999900
H	1.76018800	-3.39979900	0.90048400
C	3.31497000	-0.96135300	-0.91452000
C	3.11576600	-0.20254600	1.43745100
C	-4.30258100	-0.41361800	1.26908100
C	-2.31107600	-0.79386400	2.79066700
C	-4.25935400	-0.91831200	-1.09503000
C	-2.21579800	-1.86393300	-2.25925900
C	4.60849400	-0.42484800	-0.94315400
C	2.76844200	-1.70600300	-2.13108600
C	4.41240200	0.32127400	1.34452400
C	2.35995800	-0.11449200	2.76136200
C	-4.94191800	-0.46595400	0.03232600
H	-4.85651500	-0.07937700	2.14081900
C	-2.90614800	-1.91238900	3.67208800
C	-2.42027700	0.57301500	3.49209500
H	-1.24476500	-1.00940100	2.66819200
H	-4.77984500	-0.97447600	-2.04613800
C	-2.27944400	-0.88557800	-3.44772300
C	-2.79316600	-3.24108200	-2.64828800
H	-1.15855300	-2.01080100	-2.01629900
C	5.15013500	0.21562500	0.16891900
H	5.20226700	-0.51262200	-1.84715400
C	3.33860500	-3.13986800	-2.18997600
C	3.03728100	-0.97230000	-3.45887500
H	1.68119400	-1.78866600	-2.01911000
H	4.85342600	0.80684800	2.20981700
C	2.15483000	1.34400400	3.21448600
C	3.06784700	-0.93727100	3.85751900
H	1.36624800	-0.55110100	2.62014900
H	-5.98308400	-0.16739400	-0.05046700
H	-2.79195400	-2.89641200	3.20420800
H	-2.40274800	-1.93832400	4.64477800
H	-3.97499100	-1.75127400	3.85139400
H	-1.97061400	1.37158900	2.89034200
H	-3.46114700	0.84961600	3.69125700
H	-1.89957800	0.54312100	4.45539900
H	-1.85836900	0.09195400	-3.18492400
H	-1.71039900	-1.28454900	-4.29458500
H	-3.30741000	-0.72581000	-3.79076600
H	-2.70997100	-3.95899800	-1.82500500
H	-3.85207500	-3.16663200	-2.91981200
H	-2.25408200	-3.64931700	-3.51026600

H	6.15553300	0.62404200	0.12154000
H	3.10484500	-3.70874100	-1.28365900
H	2.92294800	-3.68239100	-3.04641500
H	4.42879400	-3.12122200	-2.29864800
H	2.69134400	0.06697500	-3.43151600
H	4.10295500	-0.95925500	-3.71096600
H	2.51941000	-1.48274400	-4.27809800
H	1.60493600	1.92284200	2.46281600
H	1.58255200	1.37411000	4.14836500
H	3.10867900	1.85130400	3.39610000
H	3.18713600	-1.98418600	3.55792500
H	4.06406800	-0.53863700	4.07878700
H	2.48596000	-0.91332700	4.78564700

TS5

Ni	-0.40720400	0.92703800	-0.76227200
C	-1.27874800	3.71146500	-0.54050200
C	-1.53729900	2.42524600	-1.30467300
H	-0.53128500	3.54379700	0.24643000
H	-2.16305600	1.69334200	-0.71877600
C	-0.85788800	4.86908200	-1.46780800
H	-1.73937700	5.38196900	-1.86231400
H	-0.26285100	5.60323300	-0.90453500
O	-0.14209000	4.43882000	-2.62029600
C	0.85192500	3.47551800	-2.36518400
H	1.36419700	3.64747300	-1.40629100
H	1.60297100	3.58337000	-3.15832000
C	0.33204200	2.04851500	-2.45581700
C	1.11483800	0.97389500	-1.95629400
H	-0.26439700	1.85799100	-3.34481700
H	1.11541600	0.02449200	-2.48630500
H	2.01704300	1.18644900	-1.38543500
H	-2.05295000	2.58971600	-2.25049600
H	-2.19565600	4.00322100	-0.00776800
C	0.06417500	-0.61844000	0.29572200
N	-0.93950200	-1.42515500	0.74969000
N	1.20024100	-1.16794100	0.81125900
C	-0.44409700	-2.45270900	1.53834700
C	-2.33971300	-1.19245300	0.46117800
C	0.90299900	-2.28773000	1.57933400
C	2.55327200	-0.67866900	0.63249000
H	-1.08711700	-3.19095700	1.99150800
C	-3.10722000	-0.46650600	1.39871500
C	-2.87828200	-1.70515200	-0.73885400

H	1.67412900	-2.85159400	2.07943500
C	3.37846900	-1.31560500	-0.31956300
C	3.00140300	0.37996400	1.44859500
C	-4.45049600	-0.22952700	1.07965100
C	-2.54696200	0.02880900	2.73028200
C	-4.22655000	-1.43197000	-1.00326800
C	-2.06876600	-2.54572800	-1.72237400
C	4.68783000	-0.83716300	-0.45339300
C	2.91376400	-2.50559900	-1.15738500
C	4.31803400	0.82146300	1.26066100
C	2.13920000	1.02620400	2.52967100
C	-5.00354700	-0.69892300	-0.10969700
H	-5.07422000	0.32203900	1.77667400
C	-3.22256400	-0.69244300	3.91489000
C	-2.66966400	1.55793600	2.87725700
H	-1.48032500	-0.21488500	2.76886100
H	-4.67637500	-1.80777300	-1.91722200
C	-1.96353300	-1.86471100	-3.10111700
C	-2.65091500	-3.96790500	-1.85173900
H	-1.05130000	-2.64628200	-1.33126800
C	5.15242200	0.22344100	0.32065100
H	5.35455300	-1.30320300	-1.17189800
C	3.50310600	-3.82335800	-0.60977300
C	3.25322500	-2.35315100	-2.65282700
H	1.82299200	-2.57359100	-1.07866800
H	4.69854800	1.63568600	1.87005200
C	1.95618700	2.53697100	2.28897600
C	2.71602700	0.75768700	3.93462800
H	1.14443800	0.57095400	2.49561900
H	-6.04841800	-0.50456600	-0.33421000
H	-3.10597900	-1.77930800	3.84245300
H	-2.77900800	-0.36535100	4.86170700
H	-4.29568400	-0.47557000	3.95589700
H	-2.15355600	2.08157800	2.06372100
H	-3.71544200	1.88402400	2.87516100
H	-2.22459800	1.88387900	3.82375500
H	-1.51361200	-0.86800300	-3.01684700
H	-1.34184400	-2.46441000	-3.77533800
H	-2.94630900	-1.74923400	-3.57133400
H	-2.70255000	-4.46974700	-0.87948700
H	-3.66181000	-3.95234000	-2.27375800
H	-2.02385500	-4.57452900	-2.51437200
H	6.17190000	0.57755000	0.19763500
H	3.22747700	-3.99012600	0.43720500

H	3.14101600	-4.67641100	-1.19436000
H	4.59735500	-3.81600400	-0.66685200
H	4.33320300	-2.38206800	-2.83179600
H	2.80884000	-3.17711000	-3.22170100
H	2.87391200	-1.41153700	-3.06462300
H	1.52051500	2.72998600	1.30107400
H	1.29031700	2.96537800	3.04663200
H	2.90858800	3.07557400	2.34391100
H	2.81066300	-0.31612500	4.12908800
H	3.70841300	1.20636500	4.05391000
H	2.06228900	1.18599700	4.70273400

TS5-modell1

Ni	0.10698000	-0.36345800	-0.23540700
C	2.55100600	0.57767700	-1.44010400
C	1.82849500	-0.71197800	-1.09166900
H	1.92684400	1.44651200	-1.18763000
H	0.99151600	-0.95885400	-1.81097900
C	3.93097100	0.66690000	-0.75365400
H	4.69803500	0.20083200	-1.37760000
H	4.20869100	1.72037800	-0.60419700
O	3.99067500	-0.03693200	0.48215500
C	2.89271400	0.18464900	1.33261100
H	2.53676700	1.22591600	1.28981200
H	3.24585300	0.00308600	2.35549800
C	1.74735800	-0.79049400	1.08871600
C	0.46048200	-0.52321000	1.64857500
H	2.05937200	-1.83169500	1.06209500
H	-0.13370600	-1.34955500	2.03439500
H	0.28422800	0.43133600	2.14500600
H	2.48798200	-1.57861300	-1.08303900
H	2.68882400	0.62950400	-2.52931800
C	-1.75860300	0.06513300	-0.09021400
N	-2.80561700	-0.80320600	-0.14836600
N	-2.33663700	1.28851500	0.06106300
C	-4.01265200	-0.13393500	-0.04423400
C	-3.71691600	1.18579900	0.08747100
H	-4.96271100	-0.64533100	-0.07333800
H	-4.35956800	2.04638600	0.19410100
C	-2.69291400	-2.25128100	-0.31879800
H	-3.10745200	-2.55180400	-1.28509100
H	-1.63846500	-2.52647000	-0.27734300
H	-3.23089300	-2.76381800	0.48291600
C	-1.61740500	2.55721300	0.15775500

H	-1.93905000	3.10077800	1.04994000
H	-0.54974200	2.34807600	0.22964400
H	-1.80679900	3.16961700	-0.72832100

TS5-model2

Ni	-0.67975400	-0.27596400	0.17657400
C	-2.52947400	-0.92300900	0.70821800
C	-3.22324900	1.31902200	-0.88129100
H	-2.61413600	2.08605300	-0.39197900
H	-3.50885300	1.70208200	-1.86825900
C	-2.45531600	0.02224100	-1.06697000
C	-1.11838100	0.09736800	-1.62809800
H	-3.05758300	-0.79808300	-1.45482400
H	-0.79019800	-0.71089800	-2.28164200
H	-0.73633600	1.07792400	-1.91045200
H	-2.45369500	-1.97974600	0.43617100
C	1.20189500	0.01558700	0.05524200
N	2.15894600	-0.90540900	-0.23695000
N	1.88438500	1.17823300	0.23482300
C	3.41939000	-0.32829100	-0.23392600
C	3.24658500	0.98487000	0.06302500
H	4.31454600	-0.89465400	-0.44063600
H	3.96150900	1.78685700	0.16531300
C	1.91529500	-2.32155200	-0.50434600
H	2.34534700	-2.93735900	0.29066600
H	0.83830300	-2.48687700	-0.54737300
H	2.36080000	-2.60203800	-1.46233800
C	1.28424500	2.46548500	0.57853600
H	1.59672400	3.22681800	-0.14102700
H	0.19917800	2.36306800	0.54418600
H	1.58783400	2.77060800	1.58404600
H	-3.57657000	-0.63896700	0.75696600
H	-4.14135100	1.18577500	-0.30155400
C	-1.84867900	-0.60872800	2.04686900
H	-0.71980300	-0.56571400	2.03749900
H	-2.19816300	0.32732300	2.48690400
H	-2.03163800	-1.43290200	2.74560700

TS5-model3

C	1.77749200	0.40885600	0.46037200
C	0.91047400	1.39188600	-0.33335100
C	-0.69874000	-0.67207400	-0.65786700
C	0.37701600	-1.44013000	0.12631200
H	0.91059000	2.37628000	0.15551100

H	1.48952200	0.40291200	1.52663300
H	2.83478800	0.68607700	0.40271100
H	-0.75694900	-1.05087700	-1.68415100
H	0.14216800	-1.43562200	1.20557300
H	0.42230200	-2.48589600	-0.19436800
H	1.36895200	1.52461800	-1.32202100
O	1.68085900	-0.90764800	-0.06719400
C	-2.03613000	-0.53414800	0.12404800
H	-2.89223500	-0.42481100	-0.54972500
H	-2.27085400	-1.31240900	0.85943900
C	-0.51836700	0.87249500	-0.51522800
H	-0.98405300	1.37270600	-1.37295000
C	-1.54237300	0.83977800	0.65692100
H	-2.26883000	1.65736000	0.70790800
H	-1.05850900	0.75086300	1.63574900

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Ni	0.22213200	-0.97637000	0.84210500
C	-1.94931500	-2.58973100	2.56726200
C	-1.81584400	-1.53457600	3.68113200
H	-2.26351800	-2.10696900	1.63387800
H	-2.70054700	-0.88804800	3.68619800
C	-0.63143500	-3.32533200	2.32863500
O	0.48125000	-2.38579300	2.20164500
C	0.65869200	-1.62953300	3.44426100
H	1.61509000	-1.11216200	3.34043200
H	0.72035500	-2.34273200	4.27417800
C	-0.53565600	-0.68580100	3.51498800
C	-0.51037500	0.14540900	2.21707600
H	-0.43360000	-0.01965900	4.38441600
H	-1.49547800	0.49355900	1.89840900
H	0.17955100	0.99285200	2.28387500
H	-1.78287100	-2.03044700	4.66033700
H	-2.72433500	-3.32350700	2.81917100
C	0.14421700	0.33057000	-0.52229600
N	-0.88653800	0.90204700	-1.20681500
N	1.27061000	0.81025200	-1.12250500
C	-0.40477300	1.71204200	-2.22889000
C	-2.29931800	0.69392100	-0.95330700
C	0.95068900	1.65618900	-2.17575800
C	2.61829700	0.46321400	-0.71791300
H	-1.06837900	2.24070700	-2.89432300
C	-2.91398100	-0.46419200	-1.47168600
C	-3.00872300	1.68414300	-0.23852600

H	1.70874700	2.12778900	-2.78111800
C	3.33321800	1.36192800	0.09960900
C	3.15883400	-0.75805300	-1.17292600
C	-4.28035900	-0.63618700	-1.21241000
C	-2.18034000	-1.48210600	-2.34132600
C	-4.37374900	1.45977500	-0.01977000
C	-2.36502700	2.98546000	0.23860800
C	4.63052200	0.98903600	0.47521900
C	2.76488600	2.70370800	0.55377300
C	4.45276100	-1.08477500	-0.74992900
C	2.37704000	-1.70691500	-2.07925600
C	-5.00240800	0.30990300	-0.49103900
H	-4.78889300	-1.51504600	-1.59725700
C	-2.70259500	-1.43880100	-3.79263700
C	-2.26723200	-2.90948600	-1.76964200
H	-1.12064200	-1.20973900	-2.37117100
H	-4.95451900	2.19886500	0.52271800
C	-2.72858500	3.34416800	1.69204000
C	-2.73857200	4.15086400	-0.70338200
H	-1.27699800	2.86229900	0.19885700
C	5.18187900	-0.22141600	0.06468100
H	5.21713400	1.65731400	1.09799100
C	3.45807600	3.87148800	-0.17882900
C	2.85458000	2.88936700	2.08083200
H	1.70277700	2.73304800	0.28789100
H	4.90284300	-2.01828500	-1.07167700
C	1.71286900	-2.83253600	-1.26345000
C	3.23842000	-2.30344900	-3.20842100
H	1.57645400	-1.13422300	-2.56024400
H	-6.06247400	0.15887700	-0.30824600
H	-2.60473400	-0.43635100	-4.22325000
H	-2.13804800	-2.13588900	-4.42216400
H	-3.75972400	-1.72179500	-3.84546700
H	-1.86206100	-2.95431300	-0.75191100
H	-3.29988800	-3.27306900	-1.73426700
H	-1.69635000	-3.60466500	-2.39560200
H	-2.49010600	2.53051100	2.38465300
H	-2.16753000	4.23113100	2.00600300
H	-3.79245800	3.57964400	1.80227300
H	-2.44314300	3.95172400	-1.73921300
H	-3.82014900	4.32694500	-0.69653700
H	-2.24474500	5.07493100	-0.38272500
H	6.18844200	-0.48974700	0.37233100
H	3.35645400	3.78419300	-1.26633700

H	3.02016300	4.82810900	0.12700400
H	4.52880100	3.90341500	0.05205000
H	2.36709400	2.06615700	2.61536600
H	3.89279200	2.94244100	2.42552500
H	2.36465500	3.82418400	2.37458600
H	0.96839000	-2.43510900	-0.54840700
H	1.17379000	-3.52760100	-1.91674500
H	2.44814700	-3.39848800	-0.68186000
H	3.75047900	-1.51868300	-3.77430800
H	3.99722100	-2.99554300	-2.82821700
H	2.60534000	-2.86552900	-3.90341300
H	-0.37851300	-3.99785000	3.15685600
H	-0.63337200	-3.90440500	1.40224800

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Ni	0.14795000	-0.03617200	-1.25331600
C	4.70755600	-0.32498400	-2.28003000
C	3.27518900	-0.68980200	-2.69599300
H	5.42195800	-1.03034900	-2.71861200
H	3.19539200	-0.64585900	-3.78736800
C	5.04583700	1.10707000	-2.73554800
H	5.81727700	1.54869000	-2.08732300
H	5.42343600	1.11135100	-3.76231600
O	3.89144600	1.95704500	-2.75908400
C	2.96747200	1.65548000	-1.73881300
H	2.24926400	2.48051200	-1.70466200
H	3.45690400	1.59437100	-0.75646200
C	2.25275000	0.32368400	-2.09393900
C	1.00498700	0.49363800	-2.88721800
H	1.94928400	-0.12887500	-1.05478400
H	0.76829600	1.50855100	-3.20989800
H	0.83655900	-0.23833900	-3.68085700
H	3.02727300	-1.71438200	-2.40041000
H	4.81171600	-0.41359700	-1.19249800
C	-1.66924600	-0.00707100	-2.35875400
C	-1.71749300	1.01848500	-1.44513900
H	-2.02764500	-0.99977700	-2.10652300
H	-1.50350900	0.19575500	-3.41206500
H	-2.12307400	0.84296800	-0.45463200
C	-1.54247200	2.48100300	-1.78763800
H	-0.53816000	2.84449100	-1.51144100
H	-1.65396000	2.63333700	-2.87417400
O	-2.53096900	3.17981400	-1.06344300
C	-2.62823800	4.55912900	-1.43873300

H	-1.65641100	5.05978900	-1.30870900
H	-2.89491500	4.61812100	-2.50796300
C	-3.67861300	5.21246200	-0.59361000
C	-3.47555500	6.32071600	0.11873600
H	-4.65758300	4.73553200	-0.60838900
H	-4.27326600	6.78549600	0.69089600
H	-2.50751100	6.81707000	0.14405700
C	-0.21242700	-0.73091200	0.61686400
N	-1.19380200	-1.59847600	1.02204200
N	0.45098600	-0.43131100	1.77572300
C	-1.13127600	-1.83327100	2.38968200
C	-2.15867300	-2.26004300	0.16784400
C	-0.10275500	-1.09168900	2.86537900
C	1.64371800	0.38177300	1.89782600
H	-1.81487400	-2.50359700	2.88512000
C	-3.50726900	-1.83675200	0.20642300
C	-1.71918500	-3.33223800	-0.63859600
H	0.29268700	-0.97824300	3.86202900
C	2.88556300	-0.28090500	2.00851400
C	1.51307300	1.78510300	1.98132700
C	-4.40820200	-2.49317300	-0.64205900
C	-4.02143400	-0.75632200	1.15882100
C	-2.66572000	-3.93962200	-1.47445700
C	-0.29138100	-3.87323700	-0.61056500
C	4.02806500	0.51791100	2.15552300
C	3.01723300	-1.80351900	2.05558300
C	2.69078900	2.52896600	2.12961200
C	0.15256500	2.47854200	2.00463400
C	-3.99354000	-3.52199200	-1.48401000
H	-5.45189700	-2.19586100	-0.64169300
C	-4.77255100	-1.40092300	2.34508600
C	-4.92786700	0.28543300	0.47308100
H	-3.15935000	-0.21766600	1.56848600
H	-2.36087400	-4.76239300	-2.11421600
C	0.40712500	-3.71632600	-1.97473200
C	-0.26194100	-5.34226500	-0.14192600
H	0.28377300	-3.29157900	0.11602900
C	3.93487800	1.90601600	2.20816100
H	5.00053500	0.04426600	2.24954900
C	3.38928300	-2.26760100	3.48059800
C	4.02593000	-2.35645000	1.03277900
H	2.04460800	-2.24288300	1.81255300
H	2.63394000	3.61013300	2.19755900
C	0.15041100	3.85109500	1.30861900

C	-0.35290300	2.62084900	3.45737000
H	-0.56187200	1.84396200	1.47037200
H	-4.71136500	-4.01091700	-2.13633300
H	-4.14973300	-2.12132400	2.88625300
H	-5.09533700	-0.63156000	3.05502700
H	-5.66441400	-1.93382800	1.99695100
H	-4.43496300	0.77696000	-0.37127500
H	-5.85837100	-0.16192800	0.10765900
H	-5.20401600	1.06181800	1.19467600
H	0.43049600	-2.66575200	-2.29111800
H	1.43972600	-4.07953500	-1.91880700
H	-0.10261000	-4.28667600	-2.75930800
H	-0.73105600	-5.45710000	0.84105900
H	-0.78764200	-6.00096300	-0.84176300
H	0.77294600	-5.69515400	-0.06840900
H	4.83285300	2.50533100	2.32881700
H	2.66428300	-1.91934600	4.22431800
H	3.42447200	-3.36168700	3.52804200
H	4.37339300	-1.88708500	3.77622800
H	3.74691600	-2.08889600	0.00856800
H	5.04104100	-1.98651800	1.21455100
H	4.06187300	-3.44963800	1.09695300
H	0.61540900	3.80526900	0.31703300
H	-0.88024400	4.19898600	1.18736800
H	0.68681400	4.60763900	1.89200200
H	-0.44301100	1.64913800	3.95426200
H	0.33356400	3.23775800	4.04838600
H	-1.33781600	3.10092000	3.47167500

TS8

Ni	0.47892000	-0.44905800	-0.02277800
C	3.82622600	-2.04160000	-2.16491000
C	2.37602700	-1.59268400	-2.38889200
H	4.04635300	-2.93235300	-2.76273900
H	2.21589200	-1.36733900	-3.45068200
C	4.79378900	-0.90355000	-2.54782200
H	5.71857500	-0.97124000	-1.95717000
H	5.06076300	-0.95187100	-3.60750400
O	4.20351000	0.39382000	-2.37782900
C	3.35866200	0.47194100	-1.24533500
H	3.13141000	1.52929900	-1.08441300
H	3.84959900	0.07199400	-0.35088700
C	2.07854900	-0.30717600	-1.59995400
C	0.87778300	0.39235500	-1.81111500

H	1.90836400	-1.03678500	-0.13130100
H	0.85986100	1.46262300	-1.63744100
H	0.14067500	0.00634100	-2.51062900
H	1.67174400	-2.39035800	-2.13047900
H	3.96680300	-2.31794100	-1.11430400
C	0.20778500	-1.53944600	1.66413400
C	1.50883200	-1.88499700	1.27478600
H	-0.61551300	-2.19950200	1.41735100
H	0.05602400	-0.86787400	2.50556600
H	1.64496100	-2.81782200	0.72671200
C	2.70355500	-1.48474200	2.11139600
H	2.56546100	-0.48054100	2.54104400
H	2.75042100	-2.19674200	2.95347600
O	3.88823900	-1.55949500	1.34953800
C	5.07326300	-1.50995900	2.16129900
H	5.01066500	-0.63626900	2.83096600
H	5.12632500	-2.41162000	2.78925200
C	6.27930600	-1.40266000	1.27903800
C	7.24767600	-2.31806900	1.23527400
H	6.35072900	-0.49893500	0.67494900
H	8.12600100	-2.19111100	0.60892400
H	7.20569600	-3.22520400	1.83448900
C	-1.28414100	0.36226200	0.06227400
N	-2.51069500	-0.23797100	-0.03990000
N	-1.57335500	1.69171700	0.22060400
C	-3.53455400	0.70104900	0.04668000
C	-2.78347100	-1.65451400	-0.20020400
C	-2.94807700	1.90716400	0.22199000
C	-0.61966100	2.77309100	0.38776300
H	-4.57180200	0.41758800	-0.02619700
C	-2.73592100	-2.21470000	-1.49439500
C	-3.16695700	-2.40031200	0.93882800
H	-3.36880200	2.89109000	0.34951000
C	-0.05744500	2.98639300	1.66522000
C	-0.34631400	3.61551000	-0.71480300
C	-3.01169100	-3.58347000	-1.61478800
C	-2.50772400	-1.37452600	-2.74831700
C	-3.43555700	-3.76249700	0.75316900
C	-3.36565700	-1.77237100	2.31947900
C	0.86410300	4.03347300	1.79733600
C	-0.50055800	2.20319100	2.89904800
C	0.57990800	4.64835800	-0.51786300
C	-1.06585100	3.49467600	-2.05952000
C	-3.34588600	-4.35284200	-0.50459100

H	-2.98246900	-4.04940300	-2.59448000
C	-3.85923900	-1.04272400	-3.41810200
C	-1.55593100	-2.03687800	-3.76096600
H	-2.05488100	-0.42571100	-2.44456400
H	-3.72828200	-4.36857600	1.60423100
C	-2.79158300	-2.62092800	3.47110600
C	-4.86555500	-1.50379000	2.57698000
H	-2.84861500	-0.80620800	2.33400000
C	1.19061500	4.84783200	0.71679100
H	1.31821400	4.22766700	2.76347400
C	-1.59713700	2.98404900	3.65640000
C	0.65778500	1.85178900	3.84904400
H	-0.94428000	1.26062900	2.56411300
H	0.82062000	5.31215400	-1.34174900
C	-0.13483700	3.65549600	-3.27753500
C	-2.20928000	4.53057700	-2.15000200
H	-1.51594500	2.49725600	-2.11927400
H	-3.55868200	-5.41148400	-0.62261900
H	-4.52850500	-0.50953900	-2.73415000
H	-3.70403400	-0.41185200	-4.30071700
H	-4.37063400	-1.95629900	-3.74149100
H	-0.60647000	-2.32664800	-3.29768600
H	-1.99452800	-2.93422200	-4.21022500
H	-1.33974400	-1.34232500	-4.58056700
H	-1.73874200	-2.87663300	3.31491100
H	-2.86920000	-2.06580200	4.41235500
H	-3.34580800	-3.55604700	3.60431400
H	-5.30542600	-0.85427800	1.81359100
H	-5.43218800	-2.44166600	2.58007300
H	-5.00535500	-1.02176200	3.55102600
H	1.90629600	5.65517700	0.84294200
H	-2.46269400	3.18665100	3.01657400
H	-1.94422500	2.41285700	4.52507700
H	-1.21389300	3.94594400	4.01523700
H	1.48118300	1.36066800	3.31826700
H	1.06575100	2.73771600	4.34690000
H	0.30456400	1.17772300	4.63760800
H	0.71895600	2.97133800	-3.24574300
H	-0.69474700	3.45277300	-4.19695000
H	0.25685000	4.67486000	-3.35965500
H	-2.92980700	4.42619200	-1.33252800
H	-1.81142900	5.55077700	-2.11036900
H	-2.75244800	4.41680900	-3.09476900

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Ni	0.33747200	-0.43830100	-0.06214200
C	4.08549400	-1.63193300	-2.40912400
C	2.79047100	-0.93941500	-2.86082500
H	4.36637100	-2.41498700	-3.12060500
H	2.94533200	-0.48461500	-3.85039900
C	5.22530100	-0.59896100	-2.29063000
H	5.93069300	-0.89999200	-1.50412400
H	5.77652300	-0.51074100	-3.23126300
O	4.73824200	0.72539300	-2.02946500
C	3.61115300	0.75458200	-1.17405000
H	3.44165600	1.80087300	-0.90340700
H	3.79760100	0.18454700	-0.24893800
C	2.41584000	0.18111300	-1.91597100
C	1.16218800	0.69772100	-1.81423900
H	-0.62342300	-2.44049100	1.10924800
H	1.00310600	1.63619000	-1.28870200
H	0.37128900	0.35961900	-2.48162500
H	1.96397900	-1.64906000	-2.97579700
H	3.92398500	-2.12223100	-1.44254100
C	1.54097000	-2.06931800	0.90225100
C	0.15276200	-1.71092400	1.32590600
H	1.87375900	-1.36588000	0.04397800
C	-1.38503900	0.35011300	0.09067500
N	-2.60832900	-0.24436400	-0.05446600
N	-1.67238600	1.65932600	0.36800000
C	-3.63181800	0.68062100	0.11880700
C	-2.87518600	-1.63967700	-0.34905300
C	-3.04663900	1.86978400	0.39512400
C	-0.71382700	2.72159000	0.60816100
H	-4.66889900	0.40134600	0.02716200
C	-2.77654700	-2.08341600	-1.68383800
C	-3.29624300	-2.48083100	0.70583200
H	-3.46906400	2.83835900	0.60741900
C	-0.11743000	2.81899700	1.88402700
C	-0.46653200	3.65481300	-0.42512000
C	-3.06567900	-3.43101700	-1.93745500
C	-2.45675800	-1.15068100	-2.84890600
C	-3.57609300	-3.81592200	0.38838600
C	-3.50755300	-1.98336300	2.13616800
C	0.80070100	3.85800700	2.08596400
C	-0.51131400	1.91306700	3.04830100
C	0.45900500	4.67282700	-0.15962600
C	-1.20587900	3.63688800	-1.76413800

C	-3.45424600	-4.29087600	-0.91486700
H	-3.00311800	-3.80670600	-2.95381700
C	-3.73887800	-0.82204400	-3.64341000
C	-1.36992300	-1.71605700	-3.78184700
H	-2.07743200	-0.20851000	-2.44085200
H	-3.90087300	-4.49246700	1.17238900
C	-2.89114900	-2.91192100	3.20060600
C	-5.01206900	-1.78492600	2.42446200
H	-3.01942200	-1.00752000	2.23443100
C	1.09469000	4.76875900	1.07508400
H	1.27906400	3.96731600	3.05375600
C	-1.56885600	2.61299600	3.92966100
C	0.68764200	1.46321600	3.90184600
H	-0.97240100	1.00991500	2.63769700
H	0.67919200	5.40626300	-0.92845700
C	-0.28777200	3.87268400	-2.97952600
C	-2.34025200	4.68607100	-1.76532400
H	-1.66529400	2.64991300	-1.88951700
H	-3.67848700	-5.33046700	-1.13593400
H	-4.50148100	-0.36481700	-3.00346500
H	-3.51645300	-0.12388200	-4.45849600
H	-4.17223000	-1.72681100	-4.08425200
H	-0.46111000	-1.97563100	-3.22676500
H	-1.70682100	-2.61688000	-4.30547800
H	-1.10806400	-0.97664300	-4.54727300
H	-1.82695600	-3.09388600	3.02040900
H	-2.99460200	-2.45738500	4.19210400
H	-3.39592800	-3.88314000	3.23799900
H	-5.47791800	-1.08681000	1.72098000
H	-5.55165900	-2.73585500	2.35148500
H	-5.15837000	-1.39161900	3.43666200
H	1.80771500	5.56797900	1.25621100
H	-2.46204300	2.87808800	3.35350100
H	-1.87857100	1.95701700	4.75129600
H	-1.16734300	3.53455200	4.36622900
H	1.47499700	1.01315400	3.28652000
H	1.13318000	2.29435200	4.45869000
H	0.36288500	0.72139400	4.64010600
H	0.54887600	3.16797700	-3.01139400
H	-0.86454400	3.75459000	-3.90341900
H	0.12648000	4.88645700	-2.98819500
H	-3.05027000	4.53027900	-0.94663900
H	-1.93223700	5.69750000	-1.65958200
H	-2.89713300	4.64393900	-2.70794200

C	2.63844500	-1.90230200	1.95239700
H	2.60376000	-2.76094700	2.64095700
H	2.46403200	-0.99213300	2.54845200
C	5.00064800	-1.91677200	2.19342300
H	4.84673900	-1.20162700	3.01888900
H	5.05055000	-2.92566700	2.62925200
C	6.26391400	-1.58890700	1.45709400
C	7.28579300	-2.43469300	1.32211700
H	6.32734000	-0.58168400	1.04658300
H	8.20125300	-2.14825700	0.81228900
H	7.25131700	-3.44354300	1.72792300
O	3.88677600	-1.83389900	1.29254300
H	0.04856800	-1.25687100	2.31240900
H	1.60151900	-3.04748800	0.41440600

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C	-1.04173700	1.19891100	0.37151100
C	0.27805700	1.20676700	-0.42039500
H	-1.66665600	2.05472600	0.09192300
H	0.04811000	1.15648000	-1.49420700
C	-1.80848700	-0.12404400	0.11582300
H	-2.25568800	-0.49637500	1.05249500
H	-2.61845800	0.02451400	-0.60488300
O	-0.98678000	-1.13441200	-0.46263000
C	0.27174600	-1.24648900	0.18481200
H	0.75702800	-2.13356800	-0.23384200
H	0.12739300	-1.42906200	1.26559100
C	1.11088500	0.00432000	-0.03381200
C	2.43539500	0.02481700	0.12445600
H	2.99716900	-0.87056800	0.38357400
H	3.01166600	0.93854000	0.00012600
H	0.83421700	2.13546700	-0.25334100
H	-0.81569900	1.30945000	1.43923000

TS11

Ni	-0.50052300	-0.41249200	1.29499700
C	-1.08662900	-2.84734300	2.95777000
C	-1.55109100	-1.44079700	2.59169900
H	-1.84357200	-3.56223400	2.60335300
H	-2.11101300	-1.43271600	1.61604700
C	0.27950700	-3.27096900	2.39293800
H	0.41479700	-4.34355200	2.56676600
H	0.33450500	-3.09933500	1.30710000
O	1.35678800	-2.61790200	3.05960600

C	1.96728800	-1.52794000	2.39809400
H	2.27156400	-1.79787300	1.37710800
H	2.88909100	-1.32247400	2.95816200
C	1.12328500	-0.26625100	2.38058200
C	0.03058500	-0.15762800	3.28696900
H	1.62320400	0.62985500	2.02528800
H	-0.39056500	0.82337600	3.49751000
H	-0.01596700	-0.85686500	4.11495400
H	-2.21443900	-1.00010400	3.33771100
H	-1.04389500	-2.96272800	4.04663900
C	-0.03500400	0.34547900	-0.43856000
N	-1.09464100	0.71271000	-1.21840600
N	1.05802800	0.69198900	-1.17631600
C	-0.67758300	1.27592600	-2.41473500
C	-2.46993200	0.49980400	-0.81937000
C	0.67965100	1.26160400	-2.38760200
C	2.44664100	0.48539100	-0.81378500
H	-1.37372800	1.62488800	-3.16135000
C	-3.10857900	-0.69555300	-1.22024300
C	-3.11733300	1.49848600	-0.05762900
H	1.40839200	1.59426100	-3.10947300
C	3.12934100	1.51819000	-0.13542700
C	3.07146200	-0.71432300	-1.21464100
C	-4.42985300	-0.88780200	-0.79700900
C	-2.43582000	-1.74090900	-2.10675900
C	-4.43898400	1.24795700	0.33363800
C	-2.45802000	2.82921000	0.29463500
C	4.47715600	1.29692800	0.17539500
C	2.47404200	2.85923800	0.19326200
C	4.42240100	-0.87558100	-0.87792000
C	2.36001800	-1.78219200	-2.04401800
C	-5.08646900	0.06798100	-0.02454400
H	-4.95576300	-1.79254100	-1.08648200
C	-3.13277500	-1.82896500	-3.48004500
C	-2.37862000	-3.12468600	-1.43085100
H	-1.40290700	-1.42571300	-2.28609600
H	-4.97264000	1.99300500	0.91558800
C	-2.50268600	3.12511500	1.80542100
C	-3.09570800	3.98067900	-0.51077900
H	-1.40294300	2.77449200	0.00821900
C	5.11601100	0.11292900	-0.18538000
H	5.03814300	2.06596700	0.69640400
C	2.84833900	3.91495000	-0.87015300
C	2.81906800	3.38134500	1.60082700

H	1.38706300	2.72444000	0.15546600
H	4.94075500	-1.78289400	-1.17156800
C	2.55945700	-3.20695500	-1.49368600
C	2.81149600	-1.70754700	-3.51846400
H	1.28471900	-1.57546000	-2.01853400
H	-6.11334100	-0.10107500	0.28682600
H	-3.14793900	-0.85742300	-3.98586700
H	-2.60804200	-2.54064800	-4.12687300
H	-4.16958900	-2.16920700	-3.38170900
H	-1.84600300	-3.08059600	-0.47343700
H	-3.37955800	-3.52673700	-1.23948100
H	-1.85450700	-3.83884500	-2.07541500
H	-2.03671400	2.31794900	2.38281900
H	-1.96441400	4.05407600	2.02325500
H	-3.52816700	3.24776200	2.17043000
H	-3.02590600	3.80276200	-1.58947300
H	-4.15578500	4.10134400	-0.26108600
H	-2.58910200	4.92651700	-0.28920900
H	6.16332700	-0.03364100	0.06267100
H	2.55369600	3.60042100	-1.87693400
H	2.35185500	4.86780000	-0.65489600
H	3.92968000	4.09205000	-0.87982400
H	2.59364600	2.64652500	2.38218800
H	3.87702100	3.64907200	1.69210300
H	2.23924700	4.28621000	1.81281400
H	2.24596700	-3.28730800	-0.44693900
H	1.96711700	-3.91872000	-2.07918200
H	3.60430600	-3.52942000	-1.55403000
H	2.62628700	-0.71753300	-3.94926600
H	3.88328500	-1.91559500	-3.61223600
H	2.27149200	-2.44607600	-4.12154900

TS11-modell

Ni	0.28556800	-0.46598800	-0.52370900
C	3.11520700	0.29613900	-1.17354800
C	1.98326800	-0.68701300	-1.45409400
H	3.31247100	0.86655000	-2.09264400
H	1.21853600	-0.25062300	-2.16673700
C	2.87616900	1.29457300	-0.02765600
H	3.68706900	2.02956700	-0.02934300
H	1.93201100	1.84466700	-0.16245600
O	2.90973600	0.66618400	1.25120900
C	1.67945700	0.38297700	1.88147000
H	1.02683900	1.27016000	1.90228400

H	1.92809800	0.15103000	2.92551500
C	0.94597000	-0.80911900	1.28501100
C	1.66745800	-1.68521700	0.42126200
H	0.10379000	-1.18580000	1.86227100
H	1.27534000	-2.68016700	0.21947000
H	2.75038000	-1.62269000	0.43163100
H	2.32744900	-1.62233400	-1.89851600
H	4.03911200	-0.24901400	-0.95096200
C	-1.54182300	0.07312300	-0.16300500
N	-2.59736700	-0.75723100	0.07253300
N	-2.08480200	1.32236800	-0.13210900
C	-3.76946600	-0.04145200	0.24386100
C	-3.44596200	1.27146700	0.11487500
H	-4.71785900	-0.51977700	0.43565600
H	-4.05765300	2.15887700	0.17250300
C	-2.53323300	-2.21712800	0.11452000
H	-3.13804400	-2.64393300	-0.69025300
H	-1.49589200	-2.52481400	-0.01861800
H	-2.90061600	-2.58256000	1.07736800
C	-1.35729300	2.56899600	-0.35872000
H	-1.73201100	3.06578400	-1.25798400
H	-1.47558400	3.23537200	0.49995800
H	-0.30057200	2.33787700	-0.49179200

TS11-model2

Ni	0.87726000	-0.19206000	-0.20948000
C	2.78673500	-0.32821400	-0.87411700
C	2.54206700	0.10105900	1.07859300
C	1.25031100	0.58305700	1.51373600
H	2.88947300	-0.83638600	1.50671900
H	0.73207300	-0.04127200	2.24249400
H	3.73790500	-0.77813400	-0.60306600
C	-1.03421800	-0.11685800	-0.12550500
N	-1.88178200	-1.00638800	0.45822000
N	-1.84766100	0.83802000	-0.65233200
C	-3.20205700	-0.61484300	0.29578000
C	-3.18059900	0.54751300	-0.40468600
H	-4.02754500	-1.18931100	0.68742600
H	-3.98367900	1.18346600	-0.74447900
C	-1.47886000	-2.22768300	1.15277600
H	-1.85721200	-3.10596400	0.62229300
H	-0.38965200	-2.26778700	1.18329200
H	-1.86940900	-2.22501300	2.17401300
C	-1.39700700	2.00324800	-1.41063800

H	-1.82666600	2.91430000	-0.98629700
H	-0.30954200	2.05824800	-1.34976500
H	-1.69792800	1.91467000	-2.45850000
H	2.96083600	0.65825100	-1.31039600
H	3.32986400	0.84423900	0.97206600
C	0.98948300	2.06732100	1.65822600
H	1.47539500	2.65181000	0.86926700
H	-0.08165100	2.29084400	1.64424100
H	1.38180600	2.42490000	2.62037600
C	2.00943200	-1.25930700	-1.81083300
H	2.16529800	-2.31459200	-1.57879400
H	0.89301900	-1.09788500	-1.86069500
H	2.30871300	-1.05986700	-2.84597100

TS11-model3

C	-0.94270800	-1.05300300	0.10090400
C	0.49903800	-1.58099500	0.12010300
C	1.59325800	0.54301200	0.29205800
C	-0.90977900	1.10794800	-0.09472600
C	0.54867900	1.59083300	-0.12356500
H	0.77230200	-1.87704300	1.14859300
H	1.55186500	0.36468000	1.37893600
H	-1.62234400	-1.90973800	0.18904000
H	0.57082300	-2.47146100	-0.51417400
H	2.59642200	0.92109100	0.06513200
H	-1.57704600	1.97237100	-0.19033400
H	0.66485300	2.45462600	0.54742100
H	0.78205800	1.94527300	-1.13671500
O	1.47537300	-0.69087200	-0.40356200
C	-1.19844800	-0.06942500	-1.07541300
H	-2.24586600	-0.08064000	-1.39469900
H	-0.55078400	-0.16258300	-1.95265600
C	-1.22786700	0.12900000	1.07221300
H	-0.63128300	0.20045100	1.98992200
H	-2.28702400	0.16573700	1.34858900

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Ni	0.59447600	-0.35106700	1.14108400
C	0.46315700	-3.18467400	3.28740100
C	-0.56404900	-3.06591600	2.14582700
H	0.90301100	-4.19023100	3.28150600
C	1.65071500	-2.21570200	3.22655100
H	2.17671200	-2.18612600	4.18726600
H	2.36388200	-2.51160700	2.45319600

O	1.32100900	-0.83222100	2.88950700
C	0.07202000	-0.30611800	3.49255600
H	0.27668900	0.73972800	3.72828000
H	-0.14723500	-0.84670900	4.42018000
C	-0.90117500	-0.49572400	2.35029200
C	-1.53772800	-1.87412800	2.26242300
H	-1.60676200	0.32107000	2.20206200
H	-2.23080400	-1.89547600	1.41609000
H	-2.15836000	-2.02001900	3.16436200
H	-0.05150100	-3.09601800	4.25195700
H	-1.15825400	-3.98705800	2.12533600
H	-0.04079400	-3.01728000	1.17961700
C	-0.03480900	0.34468900	-0.49752300
N	-1.17843000	0.66800100	-1.15832100
N	0.97079200	0.71797600	-1.33783300
C	-0.88101200	1.23861100	-2.39353800
C	-2.53639900	0.44230200	-0.70258100
C	0.47190400	1.27017500	-2.50822300
C	2.36238900	0.52490200	-0.98294300
H	-1.65841100	1.56073000	-3.06786300
C	-3.18251400	-0.74980500	-1.09236800
C	-3.17063900	1.44975400	0.05434200
H	1.11454200	1.62585100	-3.29838400
C	3.03192900	1.55509700	-0.28283800
C	2.99413000	-0.68238500	-1.36260700
C	-4.50436900	-0.92937100	-0.66330600
C	-2.52775000	-1.78805500	-2.00210800
C	-4.49103800	1.21067300	0.45599200
C	-2.50136800	2.78576000	0.37201800
C	4.37077500	1.32892300	0.05999700
C	2.37130700	2.88317900	0.07538900
C	4.33410400	-0.84727100	-0.98974500
C	2.29683300	-1.76284100	-2.18488700
C	-5.14935600	0.03389100	0.10767300
H	-5.03906000	-1.83090800	-0.94539500
C	-3.09104400	-1.67967000	-3.43550300
C	-2.67208500	-3.22881300	-1.47744500
H	-1.45529900	-1.57155800	-2.05254900
H	-5.01571100	1.96074100	1.03900700
C	-2.70572500	3.23753900	1.83002100
C	-2.99703700	3.87705700	-0.60166400
H	-1.42274900	2.67217800	0.21846200
C	5.01429300	0.14302000	-0.28503100
H	4.91916600	2.09698600	0.59655200

C	3.03653000	4.05303200	-0.67826100
C	2.37428700	3.13064100	1.59638600
H	1.32512200	2.84364300	-0.24416800
H	4.85550500	-1.75816000	-1.26760600
C	2.30483000	-3.12811700	-1.47090000
C	2.92196300	-1.87216500	-3.59101500
H	1.24960800	-1.47226200	-2.31670500
H	-6.17511900	-0.12666200	0.42702500
H	-2.94981400	-0.67650400	-3.85243900
H	-2.59127000	-2.39529500	-4.09795900
H	-4.16469700	-1.89818100	-3.45288300
H	-2.26564500	-3.33498000	-0.46617600
H	-3.71722900	-3.55561300	-1.45625600
H	-2.13060600	-3.91929500	-2.13351800
H	-2.37546300	2.47532700	2.54478000
H	-2.13077700	4.15045500	2.02021800
H	-3.75462400	3.46606300	2.04695500
H	-2.80895600	3.60415200	-1.64577300
H	-4.07481000	4.04076000	-0.48992700
H	-2.48891100	4.82748400	-0.40330900
H	6.05532600	-0.00565400	-0.01275900
H	3.00387300	3.90250800	-1.76290400
H	2.52089700	4.99234300	-0.45011600
H	4.08685100	4.17063700	-0.38955000
H	1.88072800	2.31083100	2.13164100
H	3.39202100	3.22224000	1.99150400
H	1.84427700	4.06093400	1.82901700
H	1.83508600	-3.06354900	-0.48217200
H	1.75117500	-3.86673300	-2.06084900
H	3.32202500	-3.51131400	-1.33433200
H	2.88601000	-0.91446800	-4.12169100
H	3.97069400	-2.18502100	-3.53920900
H	2.38131100	-2.61309900	-4.19015300

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C	-0.47360900	-1.48096800	-0.29109200
C	0.92767700	-1.24520900	0.27135400
C	-1.53548200	-0.53269800	0.27463900
C	1.16958000	1.14695400	0.03100900
C	-1.39349000	0.92310700	-0.19099600
C	-0.08357600	1.61524600	0.10076900
H	-0.43744000	-1.41572600	-1.38732800
H	0.87586000	-1.16351400	1.36805600
H	-1.49568200	-0.57017400	1.37268800

H	-2.20594600	1.51147200	0.25384200
H	-0.74826700	-2.51650900	-0.04578200
H	1.57864000	-2.08879000	0.02239700
H	-2.53181900	-0.89157400	-0.01472300
H	2.01039700	1.82626000	0.16029200
H	-0.14881800	2.68016800	0.31564100
O	1.62588200	-0.11069300	-0.24251400
H	-1.57057900	0.95532800	-1.27906100

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C	-1.31440600	-0.89580800	-0.28029100
C	-0.03468400	-1.52800300	0.26818800
C	-1.59374400	0.53635000	0.19645200
C	1.63014200	0.19478600	0.16517700
C	-0.53011900	1.57740900	-0.06739200
C	0.80054500	1.43748300	-0.07525500
H	-1.25260700	-0.91890100	-1.37530600
H	0.02536100	-1.40402500	1.36420700
H	-1.79136900	0.51628000	1.28175100
H	-0.91470700	2.58566900	-0.22381300
H	-2.16579100	-1.52879100	0.00728400
H	-0.03760000	-2.60356300	0.05763800
H	-2.53362700	0.87566200	-0.25804900
H	2.60985500	0.32561000	-0.30736800
H	1.39615300	2.33846900	-0.22726300
O	1.13781400	-1.02638500	-0.35156800
H	1.81541900	0.09135800	1.25219000

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Ni	-0.49696000	-0.50658200	1.23917900
C	0.97623300	0.23129400	2.26988500
C	0.43468500	1.43928200	3.02234700
H	1.71475400	0.53529200	1.52781900
H	1.28126700	1.99062500	3.46084600
H	-0.22544700	1.16450300	3.84838500
C	1.60014100	-0.84733800	3.14677300
H	2.12304800	-1.59158500	2.52864700
H	2.35530000	-0.35975100	3.78077200
O	0.71556800	-1.49788800	4.04891200
C	0.01413900	-2.56522900	3.45179500
H	-0.40005600	-3.16719400	4.27063600
H	0.70045100	-3.21401900	2.88538800
C	-1.12267400	-2.11181300	2.56062500
C	-1.86674800	-0.98719100	2.78974000

H	-1.47018300	-2.83999900	1.82500700
H	-2.79833600	-0.81290200	2.25298400
H	-1.66177000	-0.34843000	3.64164600
H	-0.09261200	2.13702500	2.36490200
C	0.00957500	0.21462100	-0.48888400
N	1.10796500	0.41889300	-1.26843000
N	-1.04486600	0.55545400	-1.28603600
C	0.73708900	0.87154500	-2.52947200
C	2.48859100	0.15210300	-0.90900500
C	-0.61835200	0.95946700	-2.54131500
C	-2.42328400	0.42917700	-0.85183500
H	1.46903500	1.07881100	-3.29389400
C	3.30796000	1.23691600	-0.52788300
C	2.96460400	-1.17141800	-1.00650600
H	-1.30675500	1.26295900	-3.31421200
C	-3.09768800	-0.78644900	-1.10974200
C	-3.03430300	1.52711800	-0.20382400
C	4.63908500	0.94866100	-0.20219300
C	2.81346100	2.68215800	-0.50337800
C	4.30234700	-1.39789700	-0.65600800
C	2.11567500	-2.33182500	-1.52013400
C	-4.41718300	-0.89445000	-0.64903400
C	-2.48081200	-1.91923000	-1.92840300
C	-4.35490500	1.35689800	0.22915900
C	-2.33242400	2.87251600	-0.03695500
C	5.13005400	-0.35366000	-0.25395800
H	5.30127000	1.75599900	0.09366700
C	3.34462900	3.45978900	-1.72676200
C	3.18200400	3.41845100	0.79877400
H	1.71966700	2.67072300	-0.56920400
H	4.70421800	-2.40482000	-0.71604700
C	1.97850800	-3.45619200	-0.47628900
C	2.67689000	-2.87898700	-2.84899500
H	1.10802400	-1.95685800	-1.72556300
C	-5.03605600	0.15912600	0.01847000
H	-4.97237900	-1.80944900	-0.82926200
C	-3.05280900	-1.91033400	-3.36296800
C	-2.66751500	-3.30498100	-1.28428900
H	-1.40305400	-1.74164400	-2.00511000
H	-4.86221800	2.17391300	0.73108500
C	-2.62010900	3.54736700	1.31646900
C	-2.70986700	3.81847400	-1.19845200
H	-1.25167200	2.69987700	-0.09037200
H	6.16558400	-0.55248500	0.00668100

H	3.05243300	2.98591200	-2.67026700
H	2.95495600	4.48382900	-1.72741400
H	4.43878700	3.51597200	-1.71036600
H	2.82979900	2.87911500	1.68433900
H	4.26381700	3.55649800	0.89914300
H	2.72643500	4.41463900	0.80487400
H	1.53240500	-3.08183700	0.45242600
H	1.33962700	-4.25798400	-0.86369100
H	2.94863200	-3.89955600	-0.22672800
H	2.74217300	-2.09350100	-3.60968000
H	3.67964200	-3.30013600	-2.71814600
H	2.02978100	-3.67421800	-3.23571400
H	-6.06115900	0.05346100	0.36197200
H	-2.88235200	-0.94961100	-3.86094200
H	-2.58086800	-2.69341400	-3.96655000
H	-4.13297200	-2.09389200	-3.35624600
H	-2.25885000	-3.33776500	-0.26781300
H	-3.72155700	-3.59689400	-1.23051000
H	-2.15019800	-4.06532700	-1.87909300
H	-2.41336000	2.87815900	2.15860300
H	-1.99127900	4.43735300	1.42651000
H	-3.66066200	3.87921000	1.39787600
H	-2.45021200	3.39071000	-2.17281900
H	-3.78629700	4.02356400	-1.20008000
H	-2.18384600	4.77427600	-1.09806300

TS16

Ni	-0.19022500	0.94675700	-0.89016900
C	-0.85704300	2.30893100	-2.44772600
C	-1.62966100	0.97756400	-2.51311600
H	-0.17516600	2.36313000	-3.29652800
H	-1.86968000	0.77046700	-3.56275200
H	-2.55765900	0.98474700	-1.93483800
C	-1.84519500	3.48843000	-2.46173400
H	-2.25410500	3.64149200	-3.46461500
H	-2.67913200	3.27447200	-1.77116200
O	-1.17827600	4.66701200	-2.08550200
C	-0.46444600	4.34671200	-0.91323500
H	-1.14741000	4.20095700	-0.05936400
H	0.20460700	5.18185900	-0.68971400
C	0.34302300	3.07407000	-1.16226500
C	0.75822000	2.29216200	0.00510800
H	1.15241800	3.23952200	-1.87227400
H	1.81088400	2.02981100	0.07980200

H	0.29068700	2.53447500	0.96099100
H	-1.06123500	0.03912200	-2.24561200
C	0.14994800	-0.50632400	0.27815800
N	1.32444400	-1.10032400	0.63540900
N	-0.81480800	-1.23372100	0.91272800
C	1.09095400	-2.18806000	1.46925600
C	2.65103800	-0.69784500	0.21099700
C	-0.25085100	-2.26712000	1.65044400
C	-2.24063500	-0.98939100	0.81984200
H	1.89690300	-2.79661500	1.84693600
C	3.08617200	-1.05491700	-1.08166300
C	3.46826800	-0.00102700	1.12878000
H	-0.85333900	-2.95251600	2.22497100
C	-2.82022900	-0.03069100	1.67808200
C	-2.99419200	-1.75327900	-0.09816700
C	4.37498200	-0.65449500	-1.45883700
C	2.24687400	-1.88200400	-2.05194400
C	4.74960400	0.36353300	0.69611000
C	3.03167300	0.32182600	2.55758800
C	-4.20223000	0.17276800	1.56978400
C	-2.01969200	0.71510200	2.74253300
C	-4.37184300	-1.50648700	-0.15752400
C	-2.37910300	-2.85250900	-0.96280700
C	5.19733200	0.04951500	-0.58461600
H	4.74435200	-0.91163100	-2.44710300
C	2.89733800	-3.25562300	-2.31578900
C	1.98989800	-1.13133400	-3.37287500
H	1.27231900	-2.07145200	-1.59108500
H	5.40852400	0.89793900	1.37303100
C	3.28091800	1.79272100	2.94368500
C	3.72864800	-0.61805200	3.56496100
H	1.95308100	0.14650100	2.63502200
C	-4.96954900	-0.55132400	0.66089300
H	-4.68681000	0.89781900	2.21588100
C	-2.25585600	0.08625100	4.13257900
C	-2.32331000	2.22442200	2.77236500
H	-0.95594300	0.60431300	2.50922400
H	-4.98704700	-2.07674700	-0.84626300
C	-2.82610000	-2.78426400	-2.43545300
C	-2.69573000	-4.24504000	-0.37532000
H	-1.29012900	-2.73065100	-0.94871000
H	6.19506300	0.34396100	-0.89710000
H	3.04564200	-3.81183700	-1.38391000
H	2.26134900	-3.85821900	-2.97400500

H	3.87418800	-3.15129600	-2.80047000
H	1.50965900	-0.16162300	-3.19133400
H	2.91993000	-0.94150400	-3.91952300
H	1.33822300	-1.72210300	-4.02693600
H	2.80377200	2.48529400	2.24235000
H	2.87503900	1.98842500	3.94224500
H	4.34900700	2.03205000	2.97621400
H	3.52939100	-1.67273200	3.34591500
H	4.81512300	-0.47720700	3.54559400
H	3.38086400	-0.41234800	4.58338000
H	-6.04054900	-0.38034200	0.59989800
H	-1.98487500	-0.97514700	4.14575500
H	-1.65436800	0.59906800	4.89152400
H	-3.30842300	0.16535100	4.42668300
H	-2.18929500	2.68288600	1.78566000
H	-3.34779600	2.43214400	3.09912400
H	-1.65228700	2.72752900	3.47741000
H	-2.63406300	-1.79993900	-2.87703000
H	-2.28325600	-3.53123100	-3.02470700
H	-3.89427200	-2.99648200	-2.55040600
H	-2.33535600	-4.34401500	0.65417100
H	-3.77574700	-4.42965300	-0.36722400
H	-2.22338200	-5.03033900	-0.97589100

TS16-modell

Ni	-0.17142900	-0.24401400	0.20059300
C	-2.25265700	-0.65424000	0.72876900
C	-1.37684400	-0.44988700	1.98586400
H	-2.51261700	-1.71057300	0.65835900
H	-1.79744700	-1.05736200	2.79584900
H	-1.34110500	0.59034200	2.32360000
C	-3.52178900	0.21646200	0.83967300
H	-4.24009700	-0.22659400	1.53494600
H	-3.24522300	1.21865400	1.21032500
O	-4.13610100	0.30443400	-0.41996700
C	-3.10700700	0.62505100	-1.32614800
H	-2.75478300	1.66043400	-1.18070700
H	-3.50577300	0.52709000	-2.33891100
C	-1.95477200	-0.35834200	-1.10628300
C	-0.62242800	0.04702800	-1.58812700
H	-2.22307000	-1.36447200	-1.42680100
H	-0.10661700	-0.63762000	-2.26051800
H	-0.49217500	1.09573500	-1.86457400
H	-0.32141900	-0.85049000	1.95623700

C	1.69418400	0.03301400	0.05341700
N	2.64979900	-0.91210800	-0.15234200
N	2.37458200	1.20755700	0.12781700
C	3.91042900	-0.33681200	-0.19667500
C	3.73717200	0.99792400	-0.02075900
H	4.80598900	-0.91991900	-0.34750100
H	4.45223300	1.80565100	0.01105800
C	2.40615600	-2.34745800	-0.28526700
H	1.33054000	-2.51378000	-0.35431600
H	2.88610400	-2.72308100	-1.19251100
H	2.80169400	-2.88226500	0.58301700
C	1.77493100	2.52206700	0.34883700
H	2.07151200	3.20647600	-0.45030300
H	0.69001600	2.41431700	0.34533300
H	2.09614800	2.92738500	1.31242300

TS16-model2

Ni	-0.67975400	-0.27596400	0.17657400
C	-2.52947400	-0.92300900	0.70821800
C	-3.22324900	1.31902200	-0.88129100
H	-2.61413600	2.08605300	-0.39197900
H	-3.50885300	1.70208200	-1.86825900
C	-2.45531600	0.02224100	-1.06697000
C	-1.11838100	0.09736800	-1.62809800
H	-3.05758300	-0.79808300	-1.45482400
H	-0.79019800	-0.71089800	-2.28164200
H	-0.73633600	1.07792400	-1.91045200
H	-2.45369500	-1.97974600	0.43617100
C	1.20189500	0.01558700	0.05524200
N	2.15894600	-0.90540900	-0.23695000
N	1.88438500	1.17823300	0.23482300
C	3.41939000	-0.32829100	-0.23392600
C	3.24658500	0.98487000	0.06302500
H	4.31454600	-0.89465400	-0.44063600
H	3.96150900	1.78685700	0.16531300
C	1.91529500	-2.32155200	-0.50434600
H	2.34534700	-2.93735900	0.29066600
H	0.83830300	-2.48687700	-0.54737300
H	2.36080000	-2.60203800	-1.46233800
C	1.28424500	2.46548500	0.57853600
H	1.59672400	3.22681800	-0.14102700
H	0.19917800	2.36306800	0.54418600
H	1.58783400	2.77060800	1.58404600
H	-3.57657000	-0.63896700	0.75696600

H	-4.14135100	1.18577500	-0.30155400
C	-1.84867900	-0.60872800	2.04686900
H	-0.71980300	-0.56571400	2.03749900
H	-2.19816300	0.32732300	2.48690400
H	-2.03163800	-1.43290200	2.74560700

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Ni	0.59382400	-0.19968900	1.12811800
C	0.55170800	-2.75560100	3.13557300
C	0.13837000	-3.85189100	2.15177000
H	0.66111300	-3.21190400	4.12659100
H	0.86012800	-4.67618400	2.16743100
H	0.08168900	-3.47830500	1.12354100
C	1.88924900	-2.04995900	2.77359800
H	2.67946900	-2.22335700	3.51032900
H	2.27223000	-2.28098600	1.77767700
O	1.58568600	-0.60948200	2.79095000
C	0.54585400	-0.49581500	3.82504100
H	0.18428500	0.53333300	3.81273700
H	0.99345200	-0.72755700	4.79825600
C	-0.42172900	-1.54712200	3.29430000
C	-0.94608600	-0.98406200	1.96643300
H	-1.24104400	-1.78723700	3.98488400
H	-1.40705200	-1.71873100	1.30494000
H	-1.63804600	-0.14986300	2.11902700
H	-0.83959300	-4.26802300	2.41774100
C	-0.12453600	0.32785000	-0.53293800
N	-1.29794000	0.56614600	-1.17468700
N	0.84168000	0.70265800	-1.41669100
C	-1.05818400	1.08936000	-2.44314500
C	-2.63370200	0.34896600	-0.65320200
C	0.28870400	1.17757700	-2.59678600
C	2.24411600	0.59503900	-1.06972900
H	-1.86765400	1.34840800	-3.10695100
C	-3.27712100	-0.87245800	-0.94224100
C	-3.24721400	1.38892700	0.07394700
H	0.89319300	1.52687800	-3.41925000
C	2.84318200	1.64896000	-0.34046500
C	2.95274200	-0.56103200	-1.47383300
C	-4.57874500	-1.03924600	-0.45350600
C	-2.63304900	-1.96425800	-1.79418400
C	-4.54904900	1.16170900	0.53908200
C	-2.57769200	2.73818100	0.32410200
C	4.18980800	1.49218400	0.01787900

C	2.11312500	2.94304400	0.01133200
C	4.29618800	-0.65147600	-1.09295400
C	2.32625900	-1.65759300	-2.33079800
C	-5.20713400	-0.03780300	0.28247400
H	-5.11131300	-1.96280000	-0.65728300
C	-3.21534100	-1.95157700	-3.22386900
C	-2.76572500	-3.36686800	-1.17211500
H	-1.56186700	-1.74823700	-1.87254700
H	-5.05807400	1.93945000	1.10012200
C	-2.55716100	3.11553200	1.81760900
C	-3.25132600	3.84574900	-0.51263000
H	-1.53501400	2.67136200	-0.00330200
C	4.90666000	0.35763100	-0.34961100
H	4.68558700	2.27884200	0.57798000
C	2.73692600	4.14324600	-0.73073000
C	2.07762500	3.19157400	1.53163800
H	1.07623500	2.85682100	-0.32896200
H	4.87632000	-1.52012600	-1.38883200
C	2.48200500	-3.05513100	-1.70267400
C	2.90919600	-1.62941900	-3.75966400
H	1.25288900	-1.45874400	-2.41211300
H	-6.21841800	-0.18955100	0.64885000
H	-3.07384600	-0.98052500	-3.71112200
H	-2.72932700	-2.71448800	-3.84245500
H	-4.29048000	-2.16276600	-3.21114700
H	-2.36909400	-3.39711300	-0.15130700
H	-3.80744000	-3.70321600	-1.13654800
H	-2.21095500	-4.09531600	-1.77377000
H	-2.06126600	2.34496600	2.41883000
H	-2.01650500	4.05788900	1.96015700
H	-3.56684700	3.25444400	2.21881300
H	-3.22315900	3.61356600	-1.58304300
H	-4.30149300	3.97510500	-0.22805400
H	-2.74199200	4.80390600	-0.35969700
H	5.95145000	0.26381500	-0.06754500
H	2.73258600	3.99050000	-1.81542900
H	2.17170800	5.05633800	-0.51403000
H	3.77429400	4.31177100	-0.42133800
H	1.60403800	2.35618400	2.06200300
H	3.08346200	3.32018600	1.94638400
H	1.50890800	4.10147200	1.75269800
H	2.03655800	-3.09560400	-0.70190700
H	1.98073700	-3.80436900	-2.32508000
H	3.53326300	-3.35094300	-1.61717700

H	2.76356500	-0.65309600	-4.23518000
H	3.98463400	-1.83909800	-3.75467500
H	2.42238600	-2.38687600	-4.38374000

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C	1.40002800	0.78381200	0.10991900
O	1.75220200	-0.58228100	-0.10057200
C	0.59139000	-1.36341400	0.15991100
C	-0.58351800	-0.53954700	-0.39736400
H	1.96979800	1.39148700	-0.60274500
H	1.67854100	1.10581800	1.12721100
H	0.46161300	-1.52953700	1.24425800
H	0.72515400	-2.33387600	-0.32661700
C	-0.10626600	0.87208800	-0.09044200
C	-0.84678000	1.97310700	0.02715200
H	-0.40425700	2.93861200	0.26232500
H	-1.92464100	1.95864700	-0.11032100
C	-1.95589000	-0.91825400	0.15789700
H	-2.19574500	-1.96354600	-0.07006900
H	-2.74738900	-0.29825800	-0.27707100
H	-1.98810200	-0.78825100	1.24571800
H	-0.58637300	-0.66960100	-1.49055700

TS19

Ni	-0.15667100	-0.21728700	1.44608700
C	-0.00375800	-0.90075800	3.37585400
C	-0.59184000	-2.11536500	2.64640700
H	-0.46714200	-0.84484200	4.35680200
H	0.01072500	-3.00741900	2.85903400
H	-0.58172900	-2.08043500	1.52179700
C	1.54037600	-0.85541800	3.47090400
H	1.87801900	-1.47358900	4.31056000
H	1.99766700	-1.26343600	2.55437300
O	2.02948000	0.45143600	3.72257100
C	1.93043800	1.33540900	2.60646100
H	2.60082500	1.01134600	1.79774600
H	2.29730300	2.30081100	2.97726000
C	0.48943300	1.46446900	2.11830400
C	-0.47367700	1.03275600	3.10859100
H	0.25583500	2.26474900	1.42141600
H	-1.53386100	1.21041500	2.92832500
H	-0.19013500	1.16320000	4.14679200
H	-1.62582500	-2.29933100	2.94390500
C	-0.12847200	-0.00989700	-0.45664600

N	-1.26258000	0.11690800	-1.20758900
N	0.88519000	-0.01943400	-1.36917000
C	-0.96068900	0.17911700	-2.56174000
C	-2.60695700	0.17414700	-0.66762500
C	0.38908700	0.08865200	-2.66370900
C	2.29745900	-0.12466800	-1.06299000
H	-1.72636300	0.27889600	-3.31446100
C	-3.34969900	-1.02294300	-0.57874300
C	-3.12843000	1.43037000	-0.28768300
H	1.03929700	0.09040000	-3.52394300
C	3.07137000	1.05618500	-1.04846100
C	2.84928000	-1.40485700	-0.84431900
C	-4.64546500	-0.93567500	-0.05306300
C	-2.82189900	-2.36087400	-1.09313500
C	-4.42869500	1.45276600	0.23201200
C	-2.36172800	2.73431400	-0.49780800
C	4.43528300	0.92435300	-0.75559900
C	2.49729900	2.42715100	-1.40418000
C	4.21771300	-1.47137100	-0.55117200
C	2.04071300	-2.69062600	-1.00421800
C	-5.17712500	0.28449800	0.35490700
H	-5.25043900	-1.83308300	0.02816500
C	-3.41014300	-2.67244600	-2.48666900
C	-3.09300700	-3.53118600	-0.12932100
H	-1.73497500	-2.27846400	-1.20768400
H	-4.86776500	2.39822600	0.53328700
C	-2.49274700	3.71651000	0.68059800
C	-2.80819600	3.41174300	-1.81192400
H	-1.29862500	2.48966300	-0.59955000
C	5.00118100	-0.32159100	-0.49837100
H	5.06492800	1.80821800	-0.73612500
C	2.90425800	2.82462400	-2.83999400
C	2.90593400	3.53491400	-0.41522000
H	1.40434000	2.35670900	-1.37922100
H	4.68031300	-2.43760500	-0.37741100
C	2.28746100	-3.70784200	0.12489500
C	2.32548700	-3.33319000	-2.37927000
H	0.97693400	-2.43169800	-0.97998000
H	-6.18548000	0.32807700	0.75654600
H	-3.18065300	-1.88343000	-3.21070100
H	-3.00401400	-3.61417100	-2.87266100
H	-4.50040700	-2.77029000	-2.43650500
H	-2.72627900	-3.32154400	0.88140600
H	-4.16099300	-3.76084700	-0.05311200

H	-2.59436600	-4.43663700	-0.49200700
H	-2.21549800	3.25220200	1.63364200
H	-1.83746900	4.57968700	0.52014700
H	-3.51209600	4.10350100	0.78255100
H	-2.65878000	2.75572100	-2.67617200
H	-3.87105300	3.67561700	-1.77340900
H	-2.23762200	4.33160800	-1.98273100
H	6.06082800	-0.39847300	-0.27247900
H	2.58251400	2.08062700	-3.57648700
H	2.45534200	3.78638200	-3.11193500
H	3.99218300	2.92441300	-2.92455000
H	2.63183200	3.28632700	0.61527200
H	3.98406100	3.72628500	-0.43586500
H	2.40641800	4.47301200	-0.68082400
H	2.11638100	-3.26617700	1.11330200
H	1.61264200	-4.56353800	0.01110500
H	3.30975400	-4.09997100	0.10998700
H	2.09733700	-2.64538600	-3.20064700
H	3.37942100	-3.61989200	-2.46730600
H	1.71787200	-4.23523500	-2.51378400

TS19-modell

Ni	-0.39722100	-0.41693200	0.32615500
C	-2.35860000	-0.49663600	0.90144000
C	-1.61239100	-0.55408100	2.24321700
H	-3.22014900	-1.15470000	0.96918500
H	-1.99965000	0.21840900	2.91937400
H	-0.50864900	-0.32114000	2.22011200
C	-2.75408800	0.92106500	0.41437800
H	-3.70220800	1.21913800	0.87526100
H	-1.99581800	1.65987600	0.72637400
O	-2.96408100	0.98922100	-0.98594500
C	-1.78411600	0.87228700	-1.77814000
H	-1.13523500	1.75147500	-1.64012400
H	-2.13615200	0.88574400	-2.81680200
C	-1.03596600	-0.42568300	-1.48334900
C	-1.86807900	-1.40699000	-0.82063700
H	-0.24951700	-0.72536100	-2.17178800
H	-1.49577200	-2.42361600	-0.69511700
H	-2.92781100	-1.37417700	-1.04719900
H	-1.71266900	-1.53125100	2.71923200
C	1.44989700	0.03362400	0.10086300
N	2.46159900	-0.83644900	-0.17325300
N	2.06014900	1.24784700	0.18423100

C	3.67801300	-0.17782500	-0.25538500
C	3.42487900	1.13657600	-0.03166800
H	4.60287100	-0.69488300	-0.46069000
H	4.08543600	1.98974700	-0.00681400
C	2.31554100	-2.28179500	-0.33270700
H	1.25359600	-2.52829200	-0.31654900
H	2.74588800	-2.59791900	-1.28661900
H	2.81892100	-2.80658200	0.48427200
C	1.39410800	2.51570000	0.47119100
H	1.54886400	3.21808900	-0.35249000
H	0.32675000	2.33053500	0.58859500
H	1.78871600	2.94798800	1.39493000

TS19-model2

Ni	0.87726000	-0.19206000	-0.20948000
C	2.78673500	-0.32821400	-0.87411700
C	2.54206700	0.10105900	1.07859300
C	1.25031100	0.58305700	1.51373600
H	2.88947300	-0.83638600	1.50671900
H	0.73207300	-0.04127200	2.24249400
H	3.73790500	-0.77813400	-0.60306600
C	-1.03421800	-0.11685800	-0.12550500
N	-1.88178200	-1.00638800	0.45822000
N	-1.84766100	0.83802000	-0.65233200
C	-3.20205700	-0.61484300	0.29578000
C	-3.18059900	0.54751300	-0.40468600
H	-4.02754500	-1.18931100	0.68742600
H	-3.98367900	1.18346600	-0.74447900
C	-1.47886000	-2.22768300	1.15277600
H	-1.85721200	-3.10596400	0.62229300
H	-0.38965200	-2.26778700	1.18329200
H	-1.86940900	-2.22501300	2.17401300
C	-1.39700700	2.00324800	-1.41063800
H	-1.82666600	2.91430000	-0.98629700
H	-0.30954200	2.05824800	-1.34976500
H	-1.69792800	1.91467000	-2.45850000
H	2.96083600	0.65825100	-1.31039600
H	3.32986400	0.84423900	0.97206600
C	0.98948300	2.06732100	1.65822600
H	1.47539500	2.65181000	0.86926700
H	-0.08165100	2.29084400	1.64424100
H	1.38180600	2.42490000	2.62037600
C	2.00943200	-1.25930700	-1.81083300
H	2.16529800	-2.31459200	-1.57879400

H	0.89301900	-1.09788500	-1.86069500
H	2.30871300	-1.05986700	-2.84597100
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Ni	0.50823600	0.13145800	1.26919700
C	0.03188800	-1.79295300	3.57627000
C	0.63891900	-2.76662900	2.55462400
H	-0.21087100	-2.37663300	4.47313400
H	1.55869600	-3.22073900	2.94033100
H	0.88161700	-2.26650400	1.60679700
C	1.04954700	-0.71988100	4.02376300
H	0.84294800	-0.36061800	5.03876300
H	2.07575500	-1.09251800	3.98843500
O	1.03805700	0.46207000	3.16500300
C	-0.29121100	1.11975300	3.27083700
H	-0.16386600	2.14138200	2.90936000
H	-0.59049600	1.13962000	4.32918600
C	-1.07355700	0.20523900	2.36551100
C	-1.28658600	-1.14196700	3.05204300
H	-1.94343100	0.61399600	1.85605200
H	-1.79961300	-1.84166400	2.38547900
H	-1.96781900	-0.97145000	3.90272300
H	-0.06475000	-3.57385900	2.32583000
C	-0.03115000	0.12406100	-0.53995900
N	-1.15550500	0.16705400	-1.30373700
N	0.99869600	0.22032800	-1.42784700
C	-0.82395300	0.29723000	-2.65001800
C	-2.52530100	0.08907100	-0.83454800
C	0.53108600	0.33308700	-2.72916100
C	2.38159200	0.20958100	-0.99303900
H	-1.58212700	0.35179400	-3.41493700
C	-3.14343700	-1.17730500	-0.77488700
C	-3.19524300	1.28825800	-0.51393600
H	1.19430100	0.42662700	-3.57446200
C	2.96137700	1.42236400	-0.55273900
C	3.09712100	-1.01059700	-1.04521500
C	-4.47433100	-1.21818900	-0.33885300
C	-2.44852800	-2.45802300	-1.23297600
C	-4.52479300	1.18280500	-0.08534600
C	-2.55149300	2.66388800	-0.67260800
C	4.29278700	1.37260900	-0.11705900
C	2.23360900	2.76349500	-0.60953400
C	4.42533600	-0.99042800	-0.60489900
C	2.49568900	-2.29185900	-1.61752600

C	-5.15620500	-0.05485000	0.00812300
H	-4.98764500	-2.17263600	-0.28102600
C	-2.93840100	-2.86047700	-2.64110300
C	-2.62627900	-3.62910800	-0.24962000
H	-1.37409100	-2.25730600	-1.30309700
H	-5.07663600	2.08264800	0.16784600
C	-2.71844600	3.55154700	0.57531300
C	-3.10504800	3.37767400	-1.92425600
H	-1.47600500	2.52354700	-0.82405600
C	5.01477700	0.18343300	-0.13878000
H	4.77352900	2.28247400	0.22801200
C	2.79554300	3.63272500	-1.75456800
C	2.28762000	3.52112100	0.73076400
H	1.17890000	2.57434200	-0.83307400
H	5.00992200	-1.90412600	-0.63200600
C	2.81868000	-3.54149700	-0.77770100
C	2.95723200	-2.49609700	-3.07733400
H	1.40563800	-2.18141300	-1.62801500
H	-6.18892600	-0.11156200	0.34009000
H	-2.76907800	-2.06316400	-3.37300500
H	-2.41100800	-3.75616700	-2.98797700
H	-4.01148500	-3.08246000	-2.63429600
H	-2.28619700	-3.36653700	0.75787400
H	-3.67022100	-3.95212900	-0.17792500
H	-2.04339100	-4.49228700	-0.58930400
H	-2.33193400	3.06072400	1.47577300
H	-2.17277800	4.49201100	0.44071800
H	-3.76685500	3.80865300	0.76027800
H	-2.94381700	2.78411900	-2.83089800
H	-4.18216200	3.55659800	-1.83161800
H	-2.61327000	4.34723800	-2.06165500
H	6.04785400	0.17235400	0.19676700
H	2.71464600	3.12502100	-2.72198700
H	2.24461100	4.57753300	-1.81997300
H	3.85234500	3.87051000	-1.58988800
H	1.91020700	2.90592000	1.55586000
H	3.30746300	3.82761700	0.98718700
H	1.67912600	4.43033500	0.67249000
H	2.53705000	-3.41052200	0.27217500
H	2.27027300	-4.40386100	-1.17184800
H	3.88362300	-3.79501900	-0.81181600
H	2.68805300	-1.64637300	-3.71405200
H	4.04505100	-2.61766800	-3.12940200
H	2.49642300	-3.39538600	-3.50077800

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C	1.86015200	-0.01311200	-0.06314800
C	-0.15835600	-1.17704200	0.26915300
C	-0.91066700	0.00607000	-0.34869500
C	-0.23784200	1.31603700	0.10386100
C	1.26336800	1.17716700	0.06722700
H	-0.57835100	-2.13434000	-0.05328900
H	2.93501900	-0.14169000	-0.15182900
H	-0.56040100	2.13960100	-0.54850000
H	-0.58354900	1.58433400	1.11543100
H	1.88558100	2.06606200	0.11199400
H	-0.21775700	-1.12415500	1.36757000
O	1.22199000	-1.21855800	-0.11137800
C	-2.40013900	-0.04367900	0.00454500
H	-2.54952100	-0.01639700	1.09166000
H	-2.93180000	0.81374800	-0.42389900
H	-2.87489100	-0.95570500	-0.37682300
H	-0.79933300	-0.07564300	-1.43893900

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C	1.06295200	1.27739900	0.10396100
C	-0.16067600	-1.18642800	0.15930600
C	-0.99903100	-0.02813900	-0.40020900
C	-0.23906600	1.26293300	-0.19132200
H	1.58936500	2.21162800	0.29307400
H	-1.12814800	-0.19260800	-1.48151400
H	-0.79638100	2.19597300	-0.27159700
H	-0.19429100	-1.16420800	1.26294000
O	1.18385200	-1.12837500	-0.29463700
C	1.87327200	0.01075200	0.19279300
H	2.19947800	-0.15451200	1.23767100
H	2.78423100	0.09323800	-0.41319700
C	-2.39174800	0.01496200	0.24647400
H	-2.99561500	0.82679500	-0.17524700
H	-2.93402200	-0.92403200	0.08226300
H	-2.31887400	0.18011100	1.32836100
H	-0.55076900	-2.15425400	-0.17166600

TS23

C	0.76519900	0.73879600	0.35149600
N	0.19550400	1.80388800	0.95582400
N	2.11463400	0.88609000	0.40434500
C	1.19967800	2.67993500	1.60480000

C	-1.20820800	2.13208700	1.06978400
Ni	-0.09817700	-0.76640900	-0.42943900
C	2.50463300	2.20038600	0.97274500
C	3.11376000	0.10350900	-0.29292700
H	0.98338300	3.73023700	1.40606600
H	1.17589900	2.52020800	2.68846500
C	-1.97043000	1.60488000	2.13724200
C	-1.75472700	3.07294400	0.16003600
C	-0.94603700	0.17409400	-1.83164100
H	3.31144400	2.08630300	1.69646800
H	2.85123600	2.85943000	0.16896000
C	3.33622800	0.32570500	-1.67607300
C	3.93504200	-0.78349600	0.44920100
C	-1.36790000	0.73144200	3.23437900
C	-3.31920000	1.97826400	2.22459000
C	-0.92329200	3.79324800	-0.90246500
C	-3.10740600	3.40725100	0.29801200
C	-1.50731600	-1.11879000	-2.22743800
H	-1.63120200	0.89741300	-1.39976400
H	-0.22169800	0.61336800	-2.51276300
C	2.61992300	1.40527600	-2.48596200
C	4.33160300	-0.42886500	-2.31186500
C	3.85154100	-0.92775300	1.96801000
C	4.91670400	-1.50561100	-0.24214200
C	-2.26579500	-0.45887700	3.61443100
C	-1.06727000	1.57973600	4.49080900
H	-0.42083500	0.32187200	2.86624000
C	-3.88848900	2.85833400	1.31015300
H	-3.92818100	1.58783300	3.03337100
C	-1.56843400	3.78321700	-2.30261600
C	-0.65152300	5.25388500	-0.47482200
H	0.04220100	3.28175400	-0.98415200
H	-3.55284200	4.11933000	-0.38960700
C	-2.95813300	-1.38830200	-1.96849100
H	-1.20351100	-1.42146500	-3.22887200
C	2.10884700	0.89727400	-3.84910100
C	3.54840500	2.62137000	-2.70529900
H	1.75155900	1.74850300	-1.91501900
C	5.10675500	-1.34548500	-1.61058000
H	4.51644800	-0.27915400	-3.37077400
C	4.00062600	-2.38584700	2.44891300
C	4.93753400	-0.07067300	2.65963700
H	2.86945500	-0.56118300	2.28922100
H	5.55285200	-2.19576500	0.30218500

H	-1.74231800	-1.10732500	4.32477600
H	-3.19160100	-0.13210700	4.10020700
H	-2.53199600	-1.05951300	2.73987200
H	-1.99299900	1.98509900	4.91486200
H	-0.58521200	0.96682300	5.26117800
H	-0.41069400	2.42860700	4.27140900
H	-4.93516900	3.13494200	1.39994900
H	-2.49980800	4.35901800	-2.32410300
H	-0.88848900	4.24491500	-3.02747100
H	-1.79458300	2.77013700	-2.64769200
H	-1.58550200	5.82476800	-0.42726000
H	0.00673400	5.74895700	-1.19778400
H	-0.18215200	5.31880400	0.51288900
C	-3.63183400	-0.87372200	-0.84927700
C	-3.67380700	-2.18670000	-2.87531500
H	2.93373200	0.68029500	-4.53588100
H	1.48667000	1.66222300	-4.32720800
H	1.51509100	-0.01710600	-3.74930900
H	4.42237800	2.34126700	-3.30397300
H	3.01700500	3.41724800	-3.23968900
H	3.91910700	3.03422100	-1.76100900
H	5.87502000	-1.91619000	-2.12443500
H	5.03201600	-2.73955000	2.34771200
H	3.74661100	-2.45732300	3.51263600
H	3.36160900	-3.07901900	1.89363000
H	5.93689900	-0.43137200	2.39127200
H	4.83885900	-0.13409800	3.74932300
H	4.88863900	0.98509000	2.37591000
C	-4.98476700	-1.14955900	-0.64861500
H	-3.10470900	-0.25390500	-0.12993100
C	-5.02657300	-2.46182100	-2.67495600
H	-3.17039300	-2.58487800	-3.75438200
C	-5.68611700	-1.94464300	-1.55784100
H	-5.49154200	-0.73863100	0.21999600
H	-5.56508200	-3.07275100	-3.39362500
H	-6.73995300	-2.15506800	-1.40051000
C	-0.55183100	-2.67516700	-1.50781700
C	0.77638200	-2.84050000	-2.24340900
C	-0.57484400	-2.94312800	-0.03998500
H	-1.32205900	-3.28745900	-1.96990000
H	0.63525200	-2.71656800	-3.32185800
H	1.16915900	-3.85065300	-2.07244900
H	1.54760600	-2.12938200	-1.93065300
C	0.54837000	-2.70656300	0.79161400

C	-1.76099100	-3.44229400	0.55776200
C	0.47102700	-2.97129700	2.17368800
H	1.51452400	-2.46083800	0.35779200
C	-1.80691800	-3.73022700	1.91111600
H	-2.62555600	-3.63631100	-0.06843800
C	-0.68852400	-3.49078300	2.72742700
H	1.34318200	-2.81081400	2.79673600
H	-2.71103200	-4.15168700	2.34101200
H	-0.72883600	-3.72814700	3.78624900

TS24

C	-0.12740100	-0.37820400	-0.62880800
N	0.83594200	-0.23398000	-1.56700900
N	-1.22253200	-0.91893400	-1.23398400
C	0.32972300	-0.51538400	-2.93322300
C	2.25203900	0.01456200	-1.40004000
Ni	-0.14429100	0.20694700	1.23724600
C	-0.95809100	-1.27993600	-2.64985600
C	-2.41038900	-1.45121200	-0.60047300
H	1.05729000	-1.08710000	-3.50920600
H	0.14691400	0.43342800	-3.45133600
C	2.74925400	1.33610500	-1.36669800
C	3.12169700	-1.10454400	-1.43034200
C	-1.69961700	1.44630500	1.02329500
H	-1.78365000	-0.97448000	-3.29199200
H	-0.83779200	-2.36584700	-2.73795400
C	-3.66937700	-0.87822500	-0.91681400
C	-2.31738900	-2.59721100	0.23214600
C	1.84753500	2.55802400	-1.49631800
C	4.13798900	1.51213600	-1.29336700
C	2.64104200	-2.54104100	-1.64386200
C	4.49957200	-0.86707400	-1.34973300
C	-1.82085000	0.96594600	2.36958700
C	-1.40950100	2.86417100	0.71579400
H	-2.30245800	0.93685200	0.28377100
C	-3.85264900	0.27313600	-1.90678700
C	-4.81477700	-1.42771900	-0.32655600
C	-1.02235600	-3.37923900	0.45285800
C	-3.49863800	-3.09371200	0.79964800
C	2.23652400	3.70157400	-0.54262200
C	1.84268700	3.07149600	-2.95321700
H	0.82666300	2.25754800	-1.24465300
C	5.00724900	0.42611900	-1.27466400
H	4.54509600	2.51780000	-1.27150800

C	3.09472900	-3.50450100	-0.53214500
C	3.10135100	-3.07304900	-3.01938900
H	1.54688200	-2.54356700	-1.63234200
H	5.18603000	-1.70843900	-1.37030400
H	-2.40050700	0.05439400	2.49907600
H	-1.99753100	1.69537300	3.15331400
C	-0.96002000	3.78396400	1.68407700
C	-1.67070400	3.35345300	-0.57941500
C	-4.71474900	1.42240300	-1.34445700
C	-4.47685500	-0.23360100	-3.22699000
H	-2.86324700	0.68569100	-2.13649300
C	-4.73518400	-2.51415200	0.53596900
H	-5.78583900	-0.99866900	-0.55214700
C	-0.87594700	-3.91746400	1.88888300
C	-0.92719500	-4.55482400	-0.54564100
H	-0.17371000	-2.71350000	0.27019300
H	-3.45309700	-3.96642700	1.44234400
H	2.29290100	3.36028500	0.49607000
H	3.20407900	4.14336300	-0.80535600
H	1.48898300	4.49781200	-0.59385200
H	1.14872000	3.91338600	-3.05765600
H	2.83994200	3.41744400	-3.24863800
H	1.54274600	2.29269000	-3.66304800
H	6.08063900	0.58821700	-1.22687700
H	4.18685100	-3.56632500	-0.46766200
H	2.72238400	-4.51490200	-0.73699100
H	2.71601000	-3.18950400	0.44353700
H	2.80033700	-2.41459800	-3.84189700
H	2.67790200	-4.06656300	-3.20569200
H	4.19236500	-3.16377300	-3.06092200
C	-0.80478100	5.13437600	1.37678300
H	-0.75409800	3.45513300	2.69831100
C	-1.51578500	4.70297400	-0.88898500
H	-2.02161800	2.66632900	-1.34372400
H	-5.75225900	1.10832800	-1.19009100
H	-4.73321000	2.25724200	-2.05387100
H	-4.33545100	1.79969700	-0.39007800
H	-5.49317500	-0.60541500	-3.05629300
H	-4.53763900	0.57968300	-3.95893600
H	-3.90380200	-1.05341400	-3.67332700
H	-5.63591500	-2.92284400	0.98492500
H	-1.06950100	-3.13994900	2.63557900
H	0.13845300	-4.30149700	2.04260600
H	-1.56356200	-4.74594800	2.08884400

H	-1.74878000	-5.26312800	-0.38956400
H	0.01575300	-5.09714600	-0.41063200
H	-0.97878000	-4.21833600	-1.58616000
C	-1.08629400	5.60233300	0.09064400
H	-0.47222000	5.82535100	2.14620800
H	-1.74300100	5.05626000	-1.89094800
H	-0.97702900	6.65711200	-0.14372000
C	-0.07516600	0.55942200	3.38924900
C	-0.74170100	-0.19569000	4.53515200
C	1.21099600	-0.01371400	2.89750700
H	0.08632600	1.60638400	3.64053000
H	-1.09164300	-1.18891600	4.23640300
H	-0.02797900	-0.32495400	5.35710300
H	-1.60305400	0.35337800	4.92524600
C	1.52408700	-1.39088100	3.00548100
C	2.22040700	0.86070400	2.41729500
C	2.81086100	-1.84910900	2.73021400
H	0.78217300	-2.08550200	3.37964900
C	3.49815600	0.39158400	2.12778000
H	2.00616600	1.92365700	2.34601200
C	3.80029500	-0.96114400	2.30077300
H	3.04693900	-2.89945700	2.87229500
H	4.25931000	1.08048700	1.77862600
H	4.80432400	-1.32218000	2.10087500

TS25

C	0.25666000	-1.27884700	0.11364100
N	-0.71772900	-2.21088700	0.11020400
N	1.38260900	-1.83757000	0.60552900
C	-0.22660300	-3.54815900	0.51612900
C	-2.08101000	-2.04051300	-0.32866800
Ni	-0.02838700	0.49702800	-0.55702800
C	1.15022300	-3.21786600	1.10081700
C	2.62069000	-1.17293000	0.93340900
H	-0.90424300	-4.00633700	1.23918700
H	-0.16777700	-4.19950200	-0.36406200
C	-2.39049500	-2.13055600	-1.70612400
C	-3.08681200	-1.88727900	0.65570300
C	1.32459600	0.46649800	-1.88615300
H	1.93585800	-3.89045900	0.75362300
H	1.15591000	-3.21660700	2.19723900
C	2.68748100	-0.35249000	2.08396600
C	3.76386800	-1.44231400	0.14190400
C	-1.34077700	-2.42079700	-2.77549800

C	-3.73547000	-2.01273100	-2.08072000
C	-2.78764000	-1.87337100	2.15384200
C	-4.41479100	-1.78714400	0.22246400
C	0.95221200	1.86016700	-2.02680900
H	2.28379000	0.23772000	-1.43284200
H	1.03092500	-0.20799700	-2.68909900
C	1.50856700	-0.13861300	3.03106500
C	3.92011400	0.24024000	2.39231500
C	3.74607400	-2.41251300	-1.03890200
C	4.96783400	-0.82401600	0.50070400
C	-1.38364300	-1.40866400	-3.93681500
C	-1.49266400	-3.86042800	-3.31213100
H	-0.35159900	-2.34433200	-2.31273100
C	-4.73867700	-1.84231100	-1.13058100
H	-4.00419600	-2.07850600	-3.13074100
C	-3.33037500	-0.61355000	2.85640900
C	-3.33695100	-3.14338700	2.83870200
H	-1.69972800	-1.87012400	2.28210800
H	-5.20687200	-1.66994200	0.95592800
C	1.84581000	2.95024600	-1.53220600
H	0.46989000	2.10040800	-2.97266800
C	1.21753900	1.35297200	3.28510000
C	1.73989500	-0.87574900	4.36785900
H	0.61274900	-0.56719700	2.57074100
C	5.04778800	0.01499700	1.60864300
H	4.00057200	0.87287400	3.27126200
C	4.35198200	-1.81574900	-2.32474200
C	4.48034400	-3.72284100	-0.67652600
H	2.70061700	-2.65849400	-1.25681600
H	5.85889600	-1.00931400	-0.09113100
H	-1.29636000	-0.37770700	-3.57549400
H	-0.56102700	-1.59892600	-4.63569800
H	-2.31606400	-1.48200200	-4.50664000
H	-2.45746200	-3.99480300	-3.81379800
H	-0.70315300	-4.08425600	-4.03856200
H	-1.43476000	-4.60112300	-2.50676300
H	-5.77602100	-1.76772600	-1.44470500
H	-4.42423100	-0.56959600	2.82128000
H	-3.03707200	-0.61751700	3.91221200
H	-2.95176600	0.30679200	2.40009000
H	-3.05909400	-3.15645400	3.89858300
H	-2.95378100	-4.05907800	2.37429800
H	-4.43048100	-3.18118800	2.78089900
C	1.86880200	4.17059600	-2.22553200

C	2.67214600	2.79583500	-0.40810400
H	1.07856000	1.90113400	2.34692900
H	0.30865200	1.46352200	3.88738700
H	2.03235900	1.83811000	3.83336000
H	1.91170400	-1.94738200	4.21652300
H	0.87057300	-0.75929500	5.02500900
H	2.61298400	-0.47380600	4.89387200
H	5.99392000	0.48010400	1.87051500
H	5.42089500	-1.60642300	-2.21076500
H	4.24722100	-2.52795000	-3.15079900
H	3.85891800	-0.88352300	-2.61780900
H	4.40075200	-4.44631200	-1.49573200
H	5.54528500	-3.53621100	-0.49795900
H	4.07650400	-4.18741500	0.22993800
C	2.69998800	5.21144400	-1.81103100
H	1.24079700	4.30265500	-3.10437600
C	3.49967800	3.83812800	0.00750600
H	2.67544700	1.86197900	0.14614600
C	3.51647300	5.04845600	-0.69061300
H	2.71195200	6.14526400	-2.36540500
H	4.13587500	3.70159400	0.87728400
H	4.16446600	5.85709200	-0.36552100
C	-0.85742900	2.26715200	-1.17624300
C	-1.34727500	2.14192900	0.27483800
H	-1.58671800	1.88969000	-1.89925400
H	-0.63493400	3.30923500	-1.38512300
C	-2.76834400	2.68007300	0.39912000
H	-0.67767700	2.68589500	0.94599100
C	-2.97396000	3.95274900	0.94502500
C	-3.86749200	1.94583900	-0.06417000
C	-4.26254700	4.48353300	1.03012800
H	-2.12634900	4.53006000	1.30707600
C	-5.15399600	2.47872800	0.02059000
H	-3.72289800	0.95348900	-0.48372700
C	-5.35489100	3.74857000	0.56686700
H	-4.41038500	5.47015700	1.45965200
H	-6.00024100	1.89946300	-0.33789600
H	-6.35715600	4.16164500	0.63267600
H	-1.38486900	1.07904700	0.65188600

TS26

C	0.61495400	-0.27036000	0.75924100
N	0.09976000	0.22811100	1.90090200
N	1.66764000	-1.06631100	1.07088100

C	0.90334000	-0.13767000	3.09063900
C	-1.12503300	0.98487000	2.03399800
Ni	-0.12016500	0.11467100	-0.99141700
C	1.79690700	-1.25135100	2.54025300
C	2.32482900	-2.01301100	0.19575900
H	0.25901500	-0.46301200	3.90936600
H	1.47691300	0.73404200	3.42533000
C	-1.10653500	2.39140700	1.89456600
C	-2.30896400	0.28413700	2.37268400
C	1.49976900	0.64198400	-1.98251700
H	2.83631900	-1.15840200	2.85565000
H	1.44157900	-2.25354100	2.81021100
C	1.60320000	-3.12687700	-0.29980800
C	3.70982800	-1.86078000	-0.06504800
C	0.18129100	3.18303600	1.68854200
C	-2.32252100	3.07536900	2.03185400
C	-2.34114000	-1.21525800	2.66495800
C	-3.49239500	1.02161900	2.50103400
C	0.57878300	0.14040500	-2.97598000
C	1.88724400	2.07070500	-1.92680300
H	2.24796500	-0.05657100	-1.61847200
C	0.15766500	-3.44012700	0.07991500
C	2.27880200	-4.03382800	-1.12755700
C	4.56164700	-0.75216000	0.55020700
C	4.33291400	-2.80676400	-0.88866700
C	0.03298700	4.32200300	0.66517900
C	0.68214900	3.74678000	3.03730400
H	0.94612100	2.49986300	1.30479000
C	-3.50528900	2.40144400	2.32147000
H	-2.34023200	4.15511600	1.92769200
C	-3.40036300	-1.96918400	1.83778100
C	-2.56660100	-1.47149300	4.17153800
H	-1.36588000	-1.63716900	2.40102500
H	-4.41466000	0.50788200	2.75452500
H	0.64021400	-0.92589600	-3.18551100
H	0.42189600	0.72738800	-3.87522300
C	1.33351800	3.04741800	-2.77836800
C	2.90421300	2.47666400	-1.04147600
C	-0.75181200	-3.59507900	-1.15313400
C	0.08421500	-4.69974200	0.96888200
H	-0.23890400	-2.60698300	0.66645300
C	3.62646700	-3.87566000	-1.42993700
H	1.74339500	-4.89239200	-1.52169500
C	5.45816000	-0.04049800	-0.48343800

C	5.44102200	-1.30437200	1.69520300
H	3.88264700	-0.00396100	0.97677800
H	5.39160500	-2.70699300	-1.10503900
H	-0.34217200	3.95666600	-0.29621400
H	-0.64378000	5.10651200	1.02066900
H	1.00574500	4.78832600	0.48588900
H	1.63362700	4.27346900	2.90126100
H	-0.03944800	4.45874700	3.45403000
H	0.83263400	2.95863900	3.78348800
H	-4.43382400	2.95524900	2.42870200
H	-4.41685200	-1.65477700	2.09720000
H	-3.33304700	-3.04514200	2.03533500
H	-3.27470100	-1.81203400	0.76159100
H	-2.52405300	-2.54494600	4.38793200
H	-1.81555500	-0.96868900	4.79131100
H	-3.54908800	-1.10515400	4.48944200
C	1.79906300	4.36099000	-2.76515700
H	0.55125900	2.78456300	-3.48397500
C	3.37118400	3.78900400	-1.02712800
H	3.34029900	1.74667400	-0.36794400
H	-1.79053500	-3.75423800	-0.84245800
H	-0.71556200	-2.69972100	-1.78528600
H	-0.45948800	-4.45017500	-1.77215800
H	0.70072100	-4.59347200	1.86841200
H	-0.94919600	-4.88586300	1.28328200
H	0.43490700	-5.58818800	0.43233500
H	4.13070700	-4.59507600	-2.06868000
H	6.24931100	-0.70126800	-0.85301700
H	5.95111200	0.82221500	-0.02133600
H	4.89220000	0.31640000	-1.34931600
H	6.16997200	-2.02628700	1.31037400
H	5.99754200	-0.49198200	2.17624600
H	4.85331400	-1.81714800	2.46412000
C	2.82454200	4.73777600	-1.89491800
H	1.36671300	5.08956300	-3.44497500
H	4.16960900	4.06943100	-0.34576000
H	3.19523800	5.75853500	-1.89567000
C	-1.36919900	0.47102800	-2.59600400
C	-2.30099300	0.29150600	-1.37873000
H	-1.41058000	1.49566300	-2.96073300
H	-1.63845800	-0.22485400	-3.38811800
C	-3.68658400	-0.21044500	-1.76914300
H	-2.39776000	1.22821500	-0.82345400
C	-4.79508900	0.62233100	-1.57907300

C	-3.87579800	-1.48063100	-2.33086800
C	-6.07269000	0.19459700	-1.94757500
H	-4.65999600	1.60708000	-1.13866900
C	-5.15221400	-1.90788900	-2.69667000
H	-3.02645600	-2.14237800	-2.48223200
C	-6.25430400	-1.07036900	-2.50731800
H	-6.92394000	0.85227800	-1.79673200
H	-5.28604400	-2.89562400	-3.12857500
H	-7.24744000	-1.40325100	-2.79408300
H	-1.89911600	-0.45990000	-0.63508400

TS27

Ni	-0.30996500	-0.67883000	0.59817800
C	-2.64789700	-2.48940100	3.69973500
C	-1.67180600	-1.31127400	3.57794200
H	-2.53008400	-2.98469400	4.66897500
H	-1.87692300	-0.58207100	4.37101800
C	-4.10177900	-1.99243100	3.53414100
H	-4.72400100	-2.76389600	3.05660800
H	-4.54515900	-1.75005300	4.50368400
O	-4.17644400	-0.77651300	2.78227900
C	-3.29024200	-0.75567300	1.68211700
H	-3.56397600	0.10230500	1.06284400
H	-3.39687500	-1.66149400	1.06682500
C	-1.86152000	-0.58530100	2.23599100
C	-1.13926200	0.58682100	1.93967700
H	-1.16447600	-1.72061900	1.38200900
H	-1.60925900	1.35742400	1.33864700
H	-0.35411800	0.91933700	2.61595700
H	-0.63561600	-1.63609200	3.71247400
H	-2.41197000	-3.24365400	2.93806900
C	0.10473900	-2.32277100	-0.62882600
C	-0.40405700	-2.84362100	0.56746000
H	1.17889700	-2.26604100	-0.75512000
H	0.28544100	-3.15547600	1.34975100
C	0.87512500	0.62775100	-0.22452100
N	2.23970200	0.50684900	-0.32647000
N	0.62128600	1.87643500	-0.73589100
C	2.80942800	1.64794200	-0.87896700
C	3.06201500	-0.61315900	0.08978000
C	1.79430200	2.49927700	-1.14798400
C	-0.65605000	2.55830900	-0.85950800
H	3.87391800	1.74022600	-1.01943200
C	3.39183400	-0.74331200	1.45555000

C	3.57897100	-1.47850000	-0.90312700
H	1.78787100	3.48148400	-1.59130800
C	-1.44870800	2.31115400	-1.99929600
C	-1.00262200	3.52512200	0.11365200
C	4.21447300	-1.81775200	1.82081800
C	2.97512500	0.27821100	2.51107500
C	4.40074000	-2.52952900	-0.47599900
C	3.32482500	-1.27939400	-2.39857900
C	-2.65908500	3.00962400	-2.10692800
C	-0.98761800	1.41296900	-3.14347400
C	-2.22223100	4.19366600	-0.05190100
C	-0.08680500	3.90394200	1.27848600
C	4.70765200	-2.70653000	0.87050300
H	4.49045800	-1.94670800	2.86263000
C	4.16440400	1.19676300	2.86550300
C	2.39881400	-0.37589800	3.77957300
H	2.18970200	0.90988200	2.08574900
H	4.81310200	-3.21533300	-1.20910400
C	2.97189700	-2.58629900	-3.13636700
C	4.54717000	-0.62149700	-3.07655800
H	2.47406600	-0.59795900	-2.51287500
C	-3.04924800	3.93119800	-1.14058600
H	-3.29568500	2.84345900	-2.96952300
C	-0.37292400	2.26652000	-4.27434000
C	-2.10746400	0.51316200	-3.69300400
H	-0.19901800	0.75522800	-2.76283100
H	-2.52528900	4.93653700	0.67848200
C	-0.83537000	4.08747700	2.61359000
C	0.70155800	5.19220300	0.95214400
H	0.64007700	3.09542300	1.41680200
H	5.34840400	-3.52838100	1.17695000
H	4.54798600	1.71730600	1.98128900
H	3.85864800	1.95244100	3.59794700
H	4.99062000	0.62229700	3.29930100
H	1.56841400	-1.04904000	3.53918500
H	3.15227400	-0.95636700	4.32250500
H	2.02857000	0.39442200	4.46549900
H	2.14278000	-3.12179000	-2.66222300
H	2.68479100	-2.36237000	-4.16954700
H	3.82474400	-3.27177400	-3.18141900
H	4.80180700	0.34190200	-2.62386600
H	5.42888600	-1.26718600	-2.99761500
H	4.34754100	-0.45156900	-4.14042100
H	-3.99075200	4.46254600	-1.24615400

H	0.46558300	2.87296300	-3.91490100
H	-0.00320000	1.62399400	-5.08175000
H	-1.11838200	2.94756100	-4.70036500
H	-2.54804500	-0.09752800	-2.89923500
H	-2.90682300	1.09262600	-4.16670100
H	-1.70303700	-0.15589700	-4.46147600
H	-1.46116800	3.22480100	2.86184300
H	-0.11293900	4.22927000	3.42500300
H	-1.47868400	4.97377500	2.60069500
H	1.30409600	5.08960500	0.04435100
H	0.01938100	6.03684000	0.80419700
H	1.37690100	5.44483400	1.77731500
C	-0.72448100	-2.39000800	-1.88960900
H	-0.50058000	-3.34789800	-2.39265500
H	-0.44947200	-1.59038000	-2.59159400
C	-2.96080800	-2.96564500	-2.50822200
H	-2.79489600	-2.52330200	-3.50319700
H	-2.71521500	-4.03645600	-2.57089100
C	-4.38328000	-2.77022000	-2.07944700
C	-5.22526700	-3.77139600	-1.82115600
H	-4.72139200	-1.73690400	-2.00966400
H	-6.26021500	-3.59048600	-1.54538000
H	-4.91668700	-4.81245700	-1.89174700
O	-2.09883700	-2.32606000	-1.55506600
H	-1.36397000	-3.35478300	0.53818700

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Ni	0.08685600	-0.55362700	-0.83082500
C	3.85850700	-1.77712200	-2.86446800
C	2.90035900	-0.69568900	-3.39090700
H	4.23052600	-2.39217300	-3.69001000
H	3.44515900	-0.03571900	-4.08186400
C	5.04159900	-1.11657800	-2.12287700
H	5.37087200	-1.75246900	-1.28906200
H	5.89119500	-0.96457400	-2.79447400
O	4.71968600	0.19286500	-1.64013300
C	3.40615100	0.29331000	-1.12629000
H	3.32880400	1.26235300	-0.62691300
H	3.20925700	-0.48969400	-0.37318200
C	2.40177800	0.17073300	-2.25755400
C	1.20546200	0.81148800	-2.26672300
H	0.61403800	-1.87602800	-2.12151300
H	0.99839900	1.58761000	-1.53573300
H	0.54976700	0.75941700	-3.13413100

H	2.06891200	-1.12197100	-3.96346300
H	3.31628900	-2.44749000	-2.18715200
C	-0.47882700	-2.27210100	-0.26720000
C	-0.03673200	-2.67559700	-1.65359100
H	-1.54838800	-2.35249300	-0.09115000
H	-0.86814800	-2.82051200	-2.34668400
C	-0.97334700	0.56292100	0.29145300
N	-2.34186800	0.55367400	0.38033000
N	-0.59710900	1.63541900	1.05979500
C	-2.79764400	1.59418600	1.17964400
C	-3.26755700	-0.35780600	-0.26533900
C	-1.70518800	2.26387000	1.61471000
C	0.74983000	2.11848800	1.30568700
H	-3.84880700	1.75472400	1.35630200
C	-3.57472500	-0.16689500	-1.62880100
C	-3.88813400	-1.35239700	0.52408900
H	-1.60645200	3.11835300	2.26373400
C	1.50527500	1.50874200	2.32982200
C	1.20950400	3.24513300	0.58338200
C	-4.50358800	-1.04297000	-2.20686200
C	-3.00800300	0.98008600	-2.46234400
C	-4.81359700	-2.19153200	-0.10899800
C	-3.62159500	-1.51760500	2.02065100
C	2.79295700	2.00862800	2.56347600
C	0.92870700	0.42756500	3.24033000
C	2.50471700	3.69994900	0.86583800
C	0.33533300	4.02283400	-0.40320100
C	-5.11374500	-2.04672300	-1.46082500
H	-4.76699300	-0.92374100	-3.25316600
C	-4.08073400	2.06779700	-2.68265200
C	-2.43102000	0.50335000	-3.80852100
H	-2.18632800	1.44008100	-1.90468900
H	-5.31056000	-2.96592300	0.46659500
C	-3.32411600	-2.97625300	2.41987000
C	-4.80585600	-0.97692200	2.85099200
H	-2.73726600	-0.92480100	2.27874300
C	3.29376500	3.08244700	1.83294800
H	3.40525800	1.56438200	3.34116900
C	0.41854400	1.05988000	4.55390500
C	1.92243500	-0.70772600	3.53702700
H	0.06798400	-0.02174500	2.73409900
H	2.89685500	4.55769000	0.32957700
C	1.08373300	4.47524400	-1.67314100
C	-0.28282800	5.26062200	0.28627100

H	-0.48911100	3.37210200	-0.71859500
H	-5.83623400	-2.70840800	-1.92995300
H	-4.46132700	2.45426400	-1.73084000
H	-3.66307100	2.90856300	-3.24805000
H	-4.93304200	1.67344100	-3.24719300
H	-1.68101700	-0.28318400	-3.66616600
H	-3.20762400	0.10624300	-4.47087900
H	-1.95691500	1.34107500	-4.33285500
H	-2.50060200	-3.40110000	1.83638500
H	-3.04884500	-3.02307200	3.47923500
H	-4.19667100	-3.62384000	2.28332000
H	-5.01514700	0.07550900	2.63176300
H	-5.72001200	-1.54480400	2.64450300
H	-4.59181100	-1.06237300	3.92219900
H	4.29464200	3.45418300	2.03268300
H	-0.33542900	1.83227700	4.36698100
H	-0.03267300	0.29464200	5.19575100
H	1.24101300	1.52410000	5.10991000
H	2.28804700	-1.15891700	2.61035100
H	2.78368300	-0.36200400	4.11853400
H	1.42942300	-1.48622600	4.13065200
H	1.59536200	3.64912300	-2.17605000
H	0.37280400	4.91451900	-2.38127700
H	1.83022600	5.24508200	-1.45096600
H	-0.87280800	4.99531400	1.16875500
H	0.50245300	5.95354600	0.60852700
H	-0.93935100	5.79482300	-0.40951100
C	0.33128600	-2.86793300	0.86208000
H	0.08181800	-3.94292800	0.93845400
H	0.07151600	-2.41012600	1.82813300
C	2.52070300	-3.68492700	1.30274500
H	2.27782200	-3.63396300	2.37644400
H	2.27674400	-4.69966800	0.95392800
C	3.97428400	-3.38858500	1.09276800
C	4.84484000	-4.26379500	0.58708000
H	4.31421300	-2.40707300	1.42170500
H	5.90241200	-4.03152800	0.49810100
H	4.53714800	-5.25520200	0.26108400
O	1.72174700	-2.72550700	0.59481800
H	0.63620900	-3.53931200	-1.65419600

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Ni	-0.16327600	1.10750600	-0.49371400
C	0.81130000	0.82771200	-2.12742400

C	0.06536800	-0.03240800	-3.12972500
H	1.79794200	0.43832600	-1.87146300
H	0.59592400	-0.03615500	-4.09512400
H	-0.94678000	0.34201300	-3.31813900
C	0.80907900	2.32037400	-2.40893900
H	1.75561800	2.80694400	-2.15051600
H	0.51504900	2.60547800	-3.42475500
O	-0.22688700	2.78547100	-1.47014600
C	-0.14319000	4.17729900	-1.05416800
H	0.84974800	4.36542200	-0.62584900
H	-0.89475000	4.26768300	-0.26424500
C	-0.43190200	5.09981400	-2.19785200
C	0.42720500	6.02435800	-2.63061600
H	-1.41299700	4.99477400	-2.65922200
H	0.17557000	6.70228900	-3.44084100
H	1.40894600	6.15235600	-2.17869400
H	-0.01146000	-1.07104300	-2.79661700
C	-0.04920200	-0.57700000	0.35909500
N	-1.13417100	-1.27542700	0.80522200
N	1.02727400	-1.27786200	0.81876700
C	-0.74153100	-2.38269900	1.54467100
C	-2.51437100	-0.89383300	0.57644200
C	0.61578000	-2.38373500	1.55249500
C	2.42263300	-0.93243800	0.62405000
H	-1.45757400	-3.05258400	1.99359400
C	-3.07543300	0.10889900	1.39537400
C	-3.24651700	-1.55955200	-0.42895900
H	1.32334600	-3.05547500	2.01158100
C	3.16041100	-1.63620600	-0.35319600
C	2.99755600	0.05320900	1.45203600
C	-4.40397200	0.47487700	1.14681700
C	-2.29047000	0.78797000	2.51513800
C	-4.57643300	-1.16276500	-0.61845300
C	-2.66561200	-2.69833500	-1.26304200
C	4.51136400	-1.29802600	-0.50221300
C	2.56232800	-2.75947800	-1.19858700
C	4.35106200	0.35361100	1.24890600
C	2.23330000	0.76173100	2.56693700
C	-5.14695900	-0.15185300	0.14995300
H	-4.86841500	1.24833100	1.75034200
C	-3.08296200	0.86512400	3.83431100
C	-1.81812000	2.18984500	2.08681800
H	-1.39655100	0.18876400	2.71792900
H	-5.17478000	-1.65327300	-1.37949700

C	-2.94280000	-2.53276400	-2.76929600
C	-3.19260600	-4.06203700	-0.76678700
H	-1.57783900	-2.69680400	-1.13154100
C	5.10058800	-0.30997600	0.28236400
H	5.11242000	-1.81894100	-1.24059000
C	3.01438900	-4.13889500	-0.67229100
C	2.90104000	-2.62709000	-2.69586700
H	1.47142300	-2.71194000	-1.10757200
H	4.82732000	1.10754200	1.86851100
C	2.18740600	2.28649800	2.34984400
C	2.82138600	0.41739000	3.95047200
H	1.19946800	0.40256300	2.55790300
H	-6.17905100	0.14054900	-0.02058300
H	-3.44308300	-0.12289900	4.13841000
H	-2.44286800	1.25443500	4.63352600
H	-3.94958500	1.52999300	3.75713700
H	-1.15922000	2.14249100	1.20070300
H	-2.66392400	2.83445400	1.82335400
H	-1.24565400	2.67563800	2.88455400
H	-2.60517300	-1.55882500	-3.13760200
H	-2.41793700	-3.31221500	-3.33261800
H	-4.00875700	-2.62895400	-3.00182900
H	-2.95870200	-4.23052200	0.29022700
H	-4.28081300	-4.12600400	-0.87889800
H	-2.74633000	-4.87795600	-1.34610700
H	6.15042800	-0.06582100	0.14772000
H	2.74162500	-4.28624300	0.37827500
H	2.55191200	-4.94176700	-1.25721000
H	4.10186300	-4.24949500	-0.74996700
H	2.61545800	-1.64772100	-3.09324900
H	3.97024800	-2.76717800	-2.88666900
H	2.36756100	-3.39441600	-3.26750400
H	1.72013700	2.53379400	1.38845900
H	1.60834400	2.76797500	3.14619900
H	3.18992400	2.72806800	2.35780700
H	2.82702500	-0.66412200	4.12378200
H	3.85171600	0.77611000	4.05069700
H	2.22765400	0.88572200	4.74358500

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Ni	-0.26395400	-0.52413100	-0.44057000
C	-0.35033100	-2.18562200	-2.62707400
C	0.69793500	-1.60384700	-1.68283100
H	0.05693700	-3.04494500	-3.18039900

H	1.16901600	-2.36224100	-1.04737600
C	-1.55994100	-2.63092400	-1.82686700
H	-2.41890700	-2.88268900	-2.45470500
H	-1.32717700	-3.48598200	-1.17752200
O	-1.89229100	-1.49543000	-0.98608800
C	-3.06560700	-1.65978900	-0.12315600
H	-2.98499400	-2.66140000	0.31977400
H	1.46144300	-1.01798500	-2.19464000
H	-0.66061000	-1.44271000	-3.37022800
C	1.20611600	0.54983100	0.07618700
N	1.10814900	1.90997300	0.15441100
N	2.48834200	0.27422600	0.45589500
C	2.30568500	2.47263600	0.57181700
C	-0.10121800	2.66572300	-0.10806900
C	3.16925700	1.44505200	0.76752100
C	3.09397000	-1.03719700	0.59026300
H	2.42521200	3.53727800	0.69348300
C	-0.43215500	2.97549900	-1.44443900
C	-0.87269300	3.09759200	0.99493800
H	4.19365200	1.43186800	1.10301400
C	2.76923500	-1.81797500	1.71868900
C	4.02743000	-1.45314700	-0.38445200
C	-1.60830700	3.70589000	-1.65960600
C	0.45998000	2.61169600	-2.62797300
C	-2.03503900	3.82699300	0.71423700
C	-0.44916100	2.86898200	2.44544900
C	3.38316600	-3.07265400	1.82989200
C	1.82583800	-1.34975500	2.82345800
C	4.61794900	-2.71078400	-0.21016500
C	4.43531100	-0.58612600	-1.57476400
C	-2.40489200	4.12105800	-0.59620700
H	-1.89530300	3.96583100	-2.67376300
C	1.16191100	3.86985000	-3.18101600
C	-0.31090000	1.87720500	-3.74060800
H	1.24043900	1.93157000	-2.27397000
H	-2.65192000	4.18246300	1.53363200
C	-1.59212100	2.35828000	3.34180200
C	0.15251400	4.16201900	3.03857200
H	0.33530800	2.10445200	2.45906100
C	4.29493300	-3.51758200	0.87770600
H	3.15524200	-3.70246000	2.68464500
C	2.56034600	-1.23091600	4.17410900
C	0.59339600	-2.26697200	2.94373100
H	1.46115000	-0.35033400	2.56699500

H	5.34218100	-3.06376300	-0.93732900
C	4.41594400	-1.35628400	-2.90988300
C	5.82904300	0.03856000	-1.34759800
H	3.71434000	0.23426800	-1.66390700
H	-3.30878100	4.69241500	-0.78789100
H	1.75711100	4.36944200	-2.40865600
H	1.83198900	3.60120700	-4.00544500
H	0.43440500	4.59517500	-3.56227600
H	-0.81289700	0.98469100	-3.35100800
H	-1.07103900	2.51616300	-4.20282800
H	0.37879700	1.56557600	-4.53306900
H	-2.05325800	1.44821500	2.94618500
H	-1.20501900	2.13457000	4.34205200
H	-2.38326100	3.10623200	3.46379200
H	1.00168800	4.52665000	2.45062800
H	-0.59564500	4.96205300	3.06844800
H	0.50008700	3.98678500	4.06276500
H	4.76459200	-4.49069300	0.98911100
H	3.41864700	-0.55408000	4.10333500
H	1.88209900	-0.84164700	4.94184500
H	2.92954000	-2.20276500	4.51936400
H	0.05065100	-2.32239600	1.99216800
H	0.87470600	-3.28754800	3.22606100
H	-0.09097800	-1.88768600	3.71157400
H	3.45085200	-1.84247100	-3.08570800
H	4.60777500	-0.66726700	-3.73974400
H	5.19095700	-2.12933200	-2.94587000
H	5.86924200	0.63420700	-0.42920900
H	6.59686300	-0.73937500	-1.26934700
H	6.09632500	0.69189800	-2.18566000
C	-2.91746300	-0.59971500	0.97728500
H	-1.90796800	-0.70605100	1.41627500
H	-2.98280500	0.39779600	0.52348300
C	-3.93325300	-0.72884500	2.08287100
C	-4.83352400	0.20477000	2.39651600
H	-3.90067600	-1.65607300	2.65563600
H	-5.53837600	0.06386800	3.21074900
H	-4.89803400	1.14501800	1.85324500
C	-4.36527200	-1.52228400	-0.93663800
C	-5.51535000	-2.45639200	-0.49258600
H	-4.15247400	-1.71334200	-1.99601600
H	-4.69995300	-0.47866900	-0.88023900
C	-6.84144800	-1.98100100	-1.10423100
H	-5.60847500	-2.38719200	0.59968900

H	-7.66932000	-2.62955500	-0.79800100
H	-7.08182400	-0.95864700	-0.79058000
H	-6.79711600	-1.99480500	-2.20090400
C	-5.24383200	-3.92316400	-0.86247200
H	-5.18658000	-4.04711900	-1.95189700
H	-4.30868500	-4.30278800	-0.43230000
H	-6.05027400	-4.56992400	-0.50044600

TS32

Ni	-0.00775100	-0.61712000	-0.80563200
C	-0.82565700	-2.69796200	-0.23795100
C	-0.74258000	-2.26366400	-1.69758200
H	-0.23842400	-2.03805900	0.46348800
H	0.21286100	-2.48429700	-2.18848500
C	-2.82184400	-0.18297600	-1.99286100
H	-2.80498700	0.70408200	-1.34935600
H	-3.40693200	0.08354900	-2.88372400
C	-1.39681700	-0.46532000	-2.46728500
C	-0.40540300	0.56329100	-2.25168000
H	-1.32286600	-0.97402700	-3.42623500
H	0.42744500	0.63638600	-2.94990800
H	-0.73368400	1.50816100	-1.82803900
H	-1.54173600	-2.72350300	-2.27099700
H	-0.32352200	-3.66781200	-0.11500800
C	1.16623300	0.49485100	0.21956000
N	2.44056400	0.12268500	0.54154600
N	1.02099400	1.73251900	0.77530300
C	3.07664100	1.10843400	1.28527400
C	3.04609000	-1.14725500	0.19498800
C	2.18214100	2.11619000	1.43759400
C	-0.17416800	2.55429200	0.74454900
H	4.09157500	0.99731600	1.63216200
C	3.03795000	-2.17933700	1.15974800
C	3.65647800	-1.28697300	-1.06960400
H	2.25552500	3.06013700	1.95309500
C	-0.24173300	3.61319300	-0.18805300
C	-1.19045500	2.29887600	1.68962200
C	3.64598700	-3.39098600	0.80776000
C	2.45909400	-1.99623700	2.56204900
C	4.24643700	-2.52333300	-1.36384100
C	3.75289000	-0.14109200	-2.07350200
C	-1.39817300	4.40358500	-0.17607500
C	0.90310300	3.95323200	-1.14255800
C	-2.32342000	3.12230800	1.64858900

C	-1.05734100	1.24120300	2.78360800
C	4.23908800	-3.56506500	-0.44022300
H	3.66580700	-4.20588300	1.52443200
C	3.59067700	-1.77914000	3.59015700
C	1.55975400	-3.16688100	3.00204900
H	1.83792400	-1.09381600	2.56156000
H	4.73225300	-2.66680300	-2.32392000
C	3.32562600	-0.55761700	-3.49334100
C	5.17974900	0.44756200	-2.08474800
H	3.07273300	0.65349400	-1.75118100
C	-2.43101000	4.15804500	0.72474500
H	-1.48831500	5.22791000	-0.87610700
C	1.73238200	5.13529400	-0.59387600
C	0.43061600	4.26864800	-2.57499500
H	1.56595900	3.08272900	-1.20380500
H	-3.12627100	2.95922200	2.36009600
C	-2.34374500	0.42385300	3.00048300
C	-0.60147100	1.89912400	4.10436900
H	-0.27639700	0.53531900	2.48190700
H	4.70956900	-4.51221300	-0.68851700
H	4.21352000	-0.91591100	3.33245800
H	3.17315400	-1.60898900	4.58880300
H	4.24524800	-2.65645300	3.64252400
H	0.75550100	-3.35649300	2.28254000
H	2.12558200	-4.09698200	3.12124900
H	1.10083700	-2.94075400	3.97065000
H	2.31861400	-0.99071100	-3.49981700
H	3.32629200	0.31436500	-4.15698100
H	4.00820500	-1.29550700	-3.92837700
H	5.47606000	0.80299900	-1.09175600
H	5.91343600	-0.30169700	-2.40291700
H	5.23948800	1.29339700	-2.77895000
H	-3.31735900	4.78610700	0.71598000
H	2.14237900	4.92342600	0.39908500
H	2.56994400	5.35840000	-1.26422700
H	1.11616400	6.03770700	-0.51167600
H	-0.14873600	5.19695600	-2.62000600
H	1.29912900	4.39995100	-3.22971100
H	-0.18842200	3.46709200	-2.99107100
H	-2.69193200	-0.03857300	2.07173400
H	-2.15453100	-0.37077200	3.73182200
H	-3.15628900	1.03811400	3.40421200
H	0.34841100	2.43224100	3.98652100
H	-1.34636900	2.62038800	4.45929400

H	-0.46955800	1.14048300	4.88428600
C	-2.27672300	-2.73659300	0.25391300
H	-2.81257700	-3.55349700	-0.25026900
H	-2.31089400	-2.92935200	1.33066400
C	-3.58544200	-1.27366200	-1.22143600
H	-3.59653600	-2.21174200	-1.79177700
C	-5.02786600	-0.83038900	-0.94361900
C	-5.91233200	-1.85889300	-0.21106500
H	-5.49966100	-0.56502900	-1.90064300
H	-4.98093900	0.09312300	-0.35044800
C	-7.23188000	-1.20155200	0.22231400
H	-5.37603000	-2.16698000	0.69703200
H	-7.86080100	-1.90926200	0.77369800
H	-7.05393900	-0.33559500	0.87065100
H	-7.80576600	-0.85627500	-0.64729100
O	-2.92794000	-1.49700800	0.04202200
C	-6.19058700	-3.10899700	-1.06096100
H	-6.71795600	-2.84487300	-1.98690400
H	-5.27445200	-3.64309300	-1.34162000
H	-6.82182900	-3.81743800	-0.51332300

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Ni	-0.34215300	-0.54209700	-0.06039800
C	-1.66931300	-3.36102300	-2.00475000
C	-1.06145800	-2.24993700	-2.87484200
H	-1.18939500	-4.31916500	-2.24224400
H	0.02914000	-2.24184700	-2.75330500
C	-3.04091700	-0.82086700	-2.01427000
H	-3.47408700	0.17834900	-2.13523000
H	-3.67715900	-1.49875900	-2.59381200
C	-1.61635200	-0.81504200	-2.61149700
C	-0.64641100	0.07912500	-1.83691600
H	-1.71617600	-0.33277100	-3.59781100
H	0.32797800	0.14030400	-2.33064300
H	-1.03946600	1.09110100	-1.68386600
H	-1.24826600	-2.52014000	-3.92052800
H	-2.72786700	-3.49001400	-2.25590900
C	1.13297600	0.58030600	0.31315600
N	2.38201500	0.10437000	0.58647400
N	1.22130400	1.92481000	0.52483100
C	3.23185300	1.13043200	0.97573400
C	2.76055100	-1.29094500	0.49749200
C	2.50162400	2.27463800	0.93626300
C	0.13630500	2.87664500	0.38736200

H	4.26110100	0.95013100	1.24308600
C	2.47232900	-2.13856900	1.58755200
C	3.41751800	-1.73760100	-0.66890800
H	2.76567400	3.29451800	1.16658600
C	0.06835300	3.65739200	-0.78682500
C	-0.78119800	3.00999000	1.44916900
C	2.83368000	-3.48712800	1.46446500
C	1.82698600	-1.64497700	2.88083100
C	3.76565300	-3.09262400	-0.72792700
C	3.78829200	-0.80292900	-1.81764200
C	-0.98641100	4.57336900	-0.88559200
C	1.11254000	3.57689200	-1.89929800
C	-1.82139400	3.93460400	1.28666200
C	-0.66407400	2.23422600	2.75874100
C	3.47114600	-3.96084300	0.32098700
H	2.62782200	-4.17072400	2.28282300
C	2.76835700	-1.84360900	4.08617600
C	0.46198700	-2.31429300	3.13525500
H	1.64897600	-0.56861900	2.78832500
H	4.27844500	-3.47300900	-1.60583300
C	3.35521000	-1.34869500	-3.19109400
C	5.30151400	-0.49933200	-1.80558800
H	3.26139800	0.14563700	-1.66892900
C	-1.92758500	4.70513700	0.13257100
H	-1.07020100	5.19544700	-1.77101600
C	2.08135700	4.77643900	-1.82112900
C	0.48826500	3.48611000	-3.30475400
H	1.70197000	2.66570400	-1.74906500
H	-2.54799000	4.06287700	2.08341200
C	-1.88436600	1.32458300	2.99844300
C	-0.44250500	3.18571500	3.95221200
H	0.21616600	1.58625800	2.69833100
H	3.75138700	-5.00809800	0.25158100
H	3.73053500	-1.34533200	3.92670200
H	2.31558700	-1.42738300	4.99295000
H	2.96899700	-2.90444700	4.27189000
H	-0.24559000	-2.12559600	2.31685800
H	0.55977000	-3.40040600	3.24256400
H	0.01474400	-1.92816900	4.05800900
H	2.28228200	-1.56843000	-3.21595600
H	3.56914200	-0.60978800	-3.97118700
H	3.89181900	-2.26589900	-3.45678400
H	5.61769700	-0.05535100	-0.85505400
H	5.88834500	-1.41256300	-1.95600600

H	5.55746900	0.20113100	-2.60832300
H	-2.73801500	5.42138000	0.03141600
H	2.58374600	4.83289600	-0.84924000
H	2.85164200	4.69724200	-2.59640900
H	1.54743200	5.72139800	-1.97206900
H	-0.04562700	4.40308500	-3.57619900
H	1.27562100	3.33771300	-4.05202500
H	-0.21519700	2.65068300	-3.38150800
H	-2.00932900	0.60525000	2.17983900
H	-1.76311300	0.76090200	3.93048200
H	-2.81065100	1.90432600	3.07919500
H	0.44060400	3.81599500	3.80151000
H	-1.30203100	3.84736200	4.10606700
H	-0.29694400	2.61084600	4.87371600
C	-1.52263300	-3.14593900	-0.50255900
H	-0.49181200	-3.30341800	-0.17387900
H	-2.16890700	-3.82238500	0.06552500
C	-3.10029400	-1.18185100	-0.50717200
O	-1.81865000	-1.78183800	-0.07670000
H	-3.10155900	-0.26060500	0.08233400
C	-4.27741500	-2.04941000	-0.04188600
C	-5.60517600	-1.29350500	0.20742200
H	-3.97855100	-2.50722100	0.91012600
H	-4.45734300	-2.86950500	-0.75042500
C	-6.58090900	-2.21441900	0.95855500
H	-5.37856400	-0.43979400	0.86486500
H	-7.51237300	-1.68706800	1.19064800
H	-6.84011100	-3.09176000	0.35239900
H	-6.15357400	-2.57234600	1.90239900
C	-6.26645800	-0.75085800	-1.06925100
H	-5.65229900	-0.00231700	-1.57946500
H	-6.47358700	-1.56045900	-1.78079700
H	-7.22320600	-0.27523200	-0.82741000

TS35

Ni	-0.30563700	-0.64021000	-0.35280200
C	-1.29717900	-2.33037100	0.58308600
C	-0.26102900	-1.76177500	1.34515000
H	-1.48921700	-1.56708200	-0.75159200
H	0.70271800	-2.25583000	1.38045900
C	-0.85290200	0.41260600	-2.00822900
C	-1.90153200	-0.51317300	-1.87514300
H	-0.09513800	0.26458500	-2.77171800
H	-0.99326500	1.42805800	-1.65304400

H	-1.93454900	-1.34485600	-2.58156000
C	-3.23272300	-0.11082800	-1.25194500
H	-3.04871000	0.52066200	-0.37331400
H	-3.75241100	0.53362100	-1.97404100
C	1.26190000	0.40678600	0.04206000
N	2.54711900	-0.06118300	0.07221900
N	1.38200200	1.74398400	0.30627200
C	3.44581500	0.96693700	0.33842600
C	2.97003300	-1.43631800	-0.11369100
C	2.71545000	2.09456600	0.49890700
C	0.30797400	2.71429800	0.40171400
H	4.50859800	0.79443500	0.38643700
C	3.36153800	-2.17959700	1.02469800
C	3.03249300	-1.96080000	-1.42170200
H	3.00849600	3.10515900	0.73215800
C	0.10636000	3.60918500	-0.67470800
C	-0.44631200	2.77590100	1.59326800
C	3.77654600	-3.50109900	0.81657100
C	3.40849500	-1.58995700	2.43565000
C	3.45263100	-3.29037400	-1.56363300
C	2.75009400	-1.12797000	-2.66917300
C	-0.92418300	4.54934500	-0.54306400
C	0.98989400	3.62921800	-1.92300100
C	-1.46607800	3.73460600	1.66177700
C	-0.12763500	1.92182500	2.81810000
C	3.81256200	-4.05647800	-0.45972100
H	4.08352300	-4.10245200	1.66611500
C	4.86128300	-1.23947100	2.82738600
C	2.79493100	-2.51370400	3.50653000
H	2.83005100	-0.65932600	2.43883400
H	3.51644600	-3.72525100	-2.55620700
C	1.77049200	-1.82056400	-3.63536400
C	4.06843600	-0.77341400	-3.38932500
H	2.28779200	-0.18715600	-2.35628800
C	-1.70960000	4.60659700	0.60469900
H	-1.11026200	5.25213900	-1.34875600
C	2.02165300	4.77596900	-1.83726500
C	0.19239300	3.75232200	-3.23649700
H	1.54458200	2.68520900	-1.96522500
H	-2.06525100	3.81339000	2.56320300
C	-1.38285600	1.34070800	3.49428000
C	0.70331000	2.73646100	3.83349300
H	0.48907100	1.07806700	2.49467000
H	4.13903800	-5.08358900	-0.59501100

H	5.32579800	-0.54759900	2.11719600
H	4.88759000	-0.77372400	3.81882700
H	5.48279100	-2.14124000	2.86237700
H	1.76877800	-2.80803400	3.26351100
H	3.38087100	-3.42897300	3.64131400
H	2.77769000	-1.99756100	4.47263700
H	0.83513300	-2.09229100	-3.13212300
H	1.53127700	-1.15441000	-4.47244700
H	2.19383100	-2.73547900	-4.06313900
H	4.75275500	-0.23092500	-2.72785800
H	4.58488100	-1.67538000	-3.73622300
H	3.86960400	-0.14274900	-4.26338900
H	-2.50191400	5.34560000	0.68283900
H	2.64899100	4.70173200	-0.94318000
H	2.67981300	4.76312700	-2.71315300
H	1.51904500	5.74925300	-1.80764700
H	-0.57923800	2.98134500	-3.32858200
H	-0.29733200	4.72770800	-3.32673700
H	0.87127500	3.65419300	-4.09060300
H	-2.01737500	0.80339200	2.77951900
H	-1.09305100	0.64311400	4.28825200
H	-1.99643700	2.11823700	3.96102400
H	1.63650800	3.09980800	3.38962100
H	0.14171500	3.60704700	4.19055000
H	0.95914400	2.11976500	4.70264900
H	-1.07748500	-3.26023100	0.05434400
C	-2.77809900	-2.15787200	0.90129000
H	-2.96748200	-1.17475800	1.34928700
H	-3.06248800	-2.91799300	1.63963300
C	-4.18853900	-1.27444200	-0.91303000
O	-3.54125900	-2.38942700	-0.27071300
H	-0.49511300	-1.09376300	2.17045600
H	-4.51819300	-1.71741200	-1.85844100
C	-5.41415000	-0.78587200	-0.12897200
C	-6.48613400	-1.85788500	0.15517100
H	-5.86988400	0.04440700	-0.68858500
H	-5.07602000	-0.35348500	0.82459400
C	-7.55343100	-1.29303000	1.10506800
H	-5.98843700	-2.69729600	0.65968700
H	-8.30099100	-2.05503500	1.35133700
H	-7.11223000	-0.94144500	2.04577100
H	-8.08188700	-0.44688100	0.64710900
C	-7.13466800	-2.39468600	-1.13020300
H	-7.61122100	-1.58547600	-1.69924400

H	-6.41106900	-2.89055100	-1.78675300
H	-7.91049900	-3.13006800	-0.89077600

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C	0.25225700	-0.87417700	-1.84967000
C	1.24164900	-2.02838800	-1.96925400
C	2.73273100	-1.66031100	-1.92591900
C	3.17506200	-1.05830700	-0.59149100
H	-0.77671800	-1.22438600	-1.90560800
H	1.02776400	-2.78424500	-1.20121500
H	1.04699200	-2.52659200	-2.93316100
H	3.32161500	-2.56931600	-2.09725100
H	2.98555000	-0.96856000	-2.73812800
H	2.79207100	-1.67858900	0.22433200
H	0.41485000	-0.09582900	-2.60786500
O	2.44006000	0.21042700	-0.35979000
Ni	0.50807100	0.09058600	-0.22430800
C	-1.29835200	0.24721000	0.30079200
N	-2.34482500	-0.60292900	0.50450000
N	-1.74750200	1.45846000	0.74231400
C	-3.42006600	0.07142000	1.07389700
C	-2.36611700	-2.02574900	0.22487600
C	-3.04575900	1.36773700	1.22345200
C	-0.94480700	2.66334400	0.71774800
H	-4.33911800	-0.43579000	1.32051400
C	-1.75733200	-2.90340900	1.14462000
C	-3.03975400	-2.47504100	-0.93187600
H	-3.57172800	2.22183200	1.62037800
C	-1.06092100	3.52853100	-0.39143700
C	-0.08773300	2.92507800	1.80875400
C	-1.79936500	-4.27260800	0.84930300
C	-1.10662600	-2.43676000	2.44430300
C	-3.06022100	-3.85563500	-1.16515600
C	-3.76806200	-1.53273100	-1.88958200
C	-0.26008500	4.67727900	-0.39354200
C	-2.02466800	3.27149700	-1.54646800
C	0.69386700	4.08702300	1.74569500
C	-0.01021000	2.02863300	3.04255300
C	-2.43961800	-4.74555900	-0.29217400
H	-1.33809100	-4.97859600	1.53347500
C	-1.84175700	-3.01024900	3.67281500
C	0.39427600	-2.78039600	2.48721900
H	-1.18960800	-1.34695700	2.49950600
H	-3.57128100	-4.23952900	-2.04238500

C	-3.41421200	-1.78822800	-3.36741300
C	-5.29558700	-1.62048900	-1.68350900
H	-3.46153300	-0.50653600	-1.65864800
C	0.61196200	4.95262700	0.65771000
H	-0.32366900	5.36954800	-1.22766900
C	-3.14611800	4.33049200	-1.57582700
C	-1.29652100	3.20172500	-2.90249900
H	-2.49949300	2.29818900	-1.38712600
H	1.36272100	4.32420200	2.56769000
C	1.41058600	1.47261100	3.26219000
C	-0.51250200	2.76970800	4.29845300
H	-0.67423200	1.17211300	2.88809800
H	-2.46661200	-5.81214400	-0.49624500
H	-2.90460500	-2.74545100	3.66183800
H	-1.77116500	-4.10279700	3.71121700
H	-1.40248100	-2.61636800	4.59626800
H	0.92298900	-2.32542500	1.64123800
H	0.84545100	-2.40752100	3.41383300
H	0.56262300	-3.86224600	2.44718500
H	-2.33457800	-1.73258300	-3.54231600
H	-3.75910700	-2.77059600	-3.70753600
H	-3.89913300	-1.03710200	-4.00057800
H	-5.58300900	-1.39258100	-0.65114700
H	-5.81179600	-0.91323700	-2.34230600
H	-5.66467300	-2.62610900	-1.91447900
H	1.22040700	5.85229300	0.63437400
H	-3.69966300	4.35668300	-0.63062000
H	-2.74405900	5.33425700	-1.75334500
H	-3.85690000	4.10839400	-2.37941100
H	-0.52338800	2.42518800	-2.89790100
H	-2.00895800	2.96612900	-3.70081900
H	-0.81836500	4.15365700	-3.15821300
H	1.76589400	0.91147400	2.38887000
H	2.13202700	2.27388700	3.45771300
H	1.42426100	0.79793800	4.12538500
H	-1.53637500	3.13497700	4.16400600
H	-0.50181700	2.09866600	5.16444800
H	0.12036400	3.63177500	4.53682300
C	4.68517000	-0.88394100	-0.41471400
C	5.47938000	-2.20402000	-0.25262200
H	4.86334700	-0.27497500	0.48259300
H	5.09360100	-0.33259400	-1.27005000
C	6.98433800	-1.89186200	-0.24075900
H	5.28196700	-2.83989800	-1.12695200

H	7.57219700	-2.81246300	-0.16050900
H	7.29548400	-1.37459400	-1.15567500
H	7.24761400	-1.25432900	0.61290500
C	5.08237500	-2.98593800	1.00957100
H	5.22999200	-2.37604800	1.91041300
H	4.03725600	-3.31597200	0.99365200
H	5.70183900	-3.88310700	1.11389300
C	3.00688300	1.48609300	-0.80051200
H	2.34397800	2.22426200	-0.33731600
H	3.99559500	1.59633200	-0.34913400
C	3.06341500	1.68187400	-2.28629200
C	4.16855100	2.05314700	-2.93567300
H	2.12398100	1.57115300	-2.82504600
H	4.16365900	2.25302800	-4.00320100
H	5.11925000	2.18517000	-2.42293000

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Ni	0.07216300	-0.62250100	-0.88071900
C	-0.62971100	-2.76449100	-0.34980600
C	-0.37431200	-2.34257400	-1.78511600
H	-0.29145400	-1.98278800	0.40093600
H	0.65902300	-2.45726800	-2.13590800
C	-2.62534600	-0.59443300	-2.31212400
H	-2.84005300	0.19633100	-1.58029100
H	-3.17696600	-0.35373000	-3.22973100
C	-1.13173000	-0.56372300	-2.65433300
C	-0.37861400	0.60189800	-2.30430500
H	-0.85750500	-1.04377300	-3.59082200
H	0.48688600	0.87355800	-2.90518000
H	-0.89114200	1.43515000	-1.82910400
H	-1.06530500	-2.82595600	-2.46560500
H	0.04241900	-3.59658400	-0.10327100
C	1.08076100	0.55746300	0.25742800
N	2.35221600	0.23209800	0.63643600
N	0.86311100	1.78390400	0.81412600
C	2.91775500	1.23545600	1.41193400
C	3.01333800	-1.01233400	0.29835900
C	1.97948100	2.20755600	1.52859700
C	-0.35897500	2.56210200	0.74191800
H	3.91997700	1.16128400	1.80307500
C	2.99031300	-2.06314000	1.24284500
C	3.68154700	-1.11141700	-0.94089200
H	1.99444700	3.15116100	2.04967400
C	-0.43763300	3.61247600	-0.19863200

C	-1.38993300	2.28075300	1.66419500
C	3.63402200	-3.25596300	0.88977900
C	2.36502200	-1.91399500	2.62906700
C	4.30473700	-2.33090400	-1.23759600
C	3.80669500	0.06157200	-1.91018900
C	-1.61770700	4.36763400	-0.21750500
C	0.71736100	3.98046500	-1.12985400
C	-2.54537300	3.06965700	1.59404600
C	-1.24727700	1.22765800	2.76174400
C	4.27685100	-3.39338500	-0.33828000
H	3.64262100	-4.08506700	1.59008500
C	3.46261900	-1.67296700	3.68872400
C	1.49094300	-3.11526100	3.03518700
H	1.71712600	-1.03057700	2.61957300
H	4.83354600	-2.44400400	-2.17884600
C	3.43948700	-0.31884900	-3.35667100
C	5.22830000	0.65950600	-1.84707100
H	3.10878800	0.84332600	-1.59394900
C	-2.66225600	4.09738500	0.66194300
H	-1.71701700	5.18411700	-0.92528200
C	1.50874400	5.18001600	-0.56330800
C	0.26438600	4.28790000	-2.57024200
H	1.40073300	3.12509500	-1.17918700
H	-3.35989300	2.88672000	2.28706400
C	-2.53717200	0.42540300	3.00917700
C	-0.76688600	1.88295600	4.07529600
H	-0.47853100	0.51268800	2.44951600
H	4.77242100	-4.32722400	-0.58805300
H	4.06639700	-0.78956800	3.45502300
H	3.01438100	-1.52492800	4.67749000
H	4.14108900	-2.53127500	3.75013900
H	0.70822000	-3.31961200	2.29660600
H	2.08086300	-4.02973600	3.15820600
H	1.00454400	-2.91348500	3.99574000
H	2.43317000	-0.74936000	-3.41592100
H	3.46855700	0.56930500	-3.99775500
H	4.13915300	-1.04691100	-3.78089700
H	5.48189800	0.98509700	-0.83225500
H	5.97979400	-0.07449800	-2.15900600
H	5.30862700	1.52709100	-2.51165700
H	-3.56629800	4.69873800	0.62967300
H	1.90852800	4.97372900	0.43493500
H	2.35111600	5.42645000	-1.21931900
H	0.86931200	6.06671200	-0.48762400

H	-0.32625400	5.20846500	-2.62584200
H	1.14157700	4.43074200	-3.21078100
H	-0.33749100	3.47801200	-2.99521000
H	-2.93397800	-0.00254400	2.08215100
H	-2.33652900	-0.39551400	3.70657100
H	-3.32523700	1.04013500	3.45711700
H	0.19041100	2.39867700	3.94538100
H	-1.49646800	2.61811800	4.43332800
H	-0.63917200	1.12578100	4.85734500
C	-3.13650500	-2.06427100	-0.43933300
H	-2.87957300	-1.11750800	0.06247200
C	-4.54156600	-2.48988000	0.00818800
C	-5.67720800	-1.47418500	-0.26798800
H	-4.48145800	-2.67896000	1.08881800
H	-4.78575200	-3.45387500	-0.45914100
C	-6.77540600	-1.59803300	0.80083800
H	-5.25222600	-0.46044800	-0.19134200
H	-7.59062800	-0.89035100	0.61238300
H	-7.20767000	-2.60672700	0.80106400
H	-6.38507700	-1.40198400	1.80687200
C	-6.28262600	-1.63652400	-1.67196400
H	-5.51994300	-1.58084300	-2.45266200
H	-6.78079900	-2.61047500	-1.76254700
H	-7.03532800	-0.86310600	-1.86369300
O	-3.12802200	-1.83593000	-1.86221600
C	-2.09288700	-3.13196800	-0.06402800
H	-2.32930400	-4.04972400	-0.61724500
H	-2.20166000	-3.36996600	1.00065000

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Ni	0.15864400	-0.84437900	0.02826600
C	2.33459100	-3.18762900	-2.50809600
C	0.83669600	-2.94782800	-2.77261200
H	2.85057200	-3.07928500	-3.46965000
H	0.72315200	-1.93990200	-3.19083100
C	0.49239800	-3.57344300	-0.28498800
H	-0.26071400	-3.80649700	0.47387000
H	1.15454100	-4.43574000	-0.39365100
C	-0.15616200	-3.10541700	-1.57906900
C	-0.90664700	-1.80844100	-1.23217200
H	-0.90934800	-3.86025000	-1.85582100
H	-1.11542400	-1.17741900	-2.09961800
H	-1.82979500	-1.99676300	-0.67545100
H	0.52982700	-3.63307800	-3.57118000

H	2.51243400	-4.22754500	-2.20057500
C	-0.89722900	0.72946400	0.02578600
N	-0.39095800	1.97993400	-0.18385400
N	-2.21783800	0.93600800	0.30582600
C	-1.37352600	2.94802900	-0.03248700
C	1.00673800	2.27692400	-0.42669700
C	-2.52004700	2.29167800	0.27716300
C	-3.19570700	-0.07488300	0.66038400
H	-1.16177900	3.99914300	-0.14817900
C	1.82263700	2.58329000	0.68314800
C	1.47748200	2.29648600	-1.75740300
H	-3.51360600	2.65480800	0.48587800
C	-4.16364600	-0.44354000	-0.29929200
C	-3.16992700	-0.61059100	1.96466100
C	3.16816700	2.87996000	0.42522600
C	1.28907900	2.66608000	2.11243200
C	2.83100800	2.59909900	-1.95069600
C	0.55323200	2.08078100	-2.95321500
C	-5.10962600	-1.40356400	0.08071600
C	-4.23548900	0.17710800	-1.69361400
C	-4.13371500	-1.57760200	2.27988500
C	-2.18243300	-0.16320800	3.03985300
C	3.66906500	2.88163000	-0.87364200
H	3.82608400	3.12974500	1.25206300
C	1.30784900	4.12425000	2.61734600
C	2.04816300	1.74210200	3.08307900
H	0.24424400	2.33981600	2.11045600
H	3.23280300	2.62864800	-2.95828500
C	1.18206800	1.21518600	-4.05916000
C	0.09556000	3.43930500	-3.52772000
H	-0.33952700	1.55378100	-2.59970200
C	-5.09184900	-1.97307600	1.35135500
H	-5.87179400	-1.70853200	-0.62925800
C	-5.41258100	1.17114700	-1.79100300
C	-4.33589800	-0.87958200	-2.81096200
H	-3.31190400	0.74011500	-1.86639000
H	-4.14194700	-2.01424500	3.27399400
C	-1.28569900	-1.32366400	3.51351500
C	-2.91392100	0.49036200	4.23012900
H	-1.52512700	0.59882300	2.60948600
H	4.71377700	3.12129400	-1.05043700
H	0.73643500	4.78615300	1.95738300
H	0.87088100	4.18480100	3.62023200
H	2.33031200	4.51398600	2.67387800

H	2.00128200	0.69539000	2.76255000
H	3.10492200	2.01759200	3.16774800
H	1.61005400	1.80947000	4.08509500
H	1.54828000	0.26072600	-3.66575300
H	0.43614000	1.00130100	-4.83245000
H	2.02008300	1.71943400	-4.55261500
H	-0.41727800	4.04673100	-2.77407200
H	0.95159300	4.01666500	-3.89498000
H	-0.59395700	3.28730400	-4.36567800
H	-5.83451800	-2.71816400	1.62192400
H	-5.34211200	1.96391500	-1.03807900
H	-5.43314000	1.64387900	-2.77925600
H	-6.37074400	0.66054500	-1.64266400
H	-5.27878400	-1.43502400	-2.76532200
H	-4.29492400	-0.39045900	-3.79053100
H	-3.51652600	-1.60385900	-2.75711200
H	-0.72816500	-1.76342100	2.67753200
H	-0.56269100	-0.96713100	4.25624900
H	-1.87247200	-2.12263500	3.98018400
H	-3.52727200	1.33812000	3.90598900
H	-3.57237100	-0.22213800	4.73892100
H	-2.18917400	0.85606700	4.96617900
O	1.26284200	-2.45415000	0.25301300
C	3.00195500	-2.22837200	-1.50449200
H	2.73324600	-1.18915700	-1.74311800
H	4.08964500	-2.29977100	-1.62696700
C	2.70675400	-2.49134000	-0.02839700
H	3.01224100	-3.51075900	0.23430100
C	3.35633200	-1.49736400	0.93540300
C	4.90227000	-1.51083600	0.97414200
H	2.97715300	-1.71434000	1.94363100
H	3.01999300	-0.48267700	0.67365800
C	5.40516400	-0.41618400	1.92785500
H	5.27529300	-1.26704700	-0.03063700
H	6.50000900	-0.38329200	1.93929300
H	5.04148600	0.57310500	1.62699200
H	5.06779700	-0.60301200	2.95531500
C	5.47042200	-2.88091400	1.37761500
H	5.09101200	-3.19057600	2.35995900
H	5.22261200	-3.66928100	0.65768100
H	6.56281200	-2.83755800	1.44461200
TS40			
Ni	0.03953600	-0.79407000	-0.54085500

C	-0.04602200	-2.13475100	0.82646000
C	1.01620000	-1.89735400	-1.89136100
C	1.12006900	-2.55879500	0.09789000
H	0.08758900	-1.65269800	1.79291900
H	-0.95962500	-2.71739500	0.72561400
C	-1.20622400	0.48267100	0.17120000
C	1.38697900	-0.50666000	-2.37837800
H	1.82637100	-2.59634000	-2.06804600
H	0.08784100	-2.31122700	-2.30384600
C	2.49810400	-2.23864900	0.66802200
H	1.03382300	-3.53765100	-0.36848200
N	-0.97624700	1.77117700	0.56368200
N	-2.55624300	0.32253400	0.31091300
C	2.88028900	-0.18967300	-2.22963800
H	1.05110400	-0.39022600	-3.41748700
H	0.79515400	0.31454000	-1.86409600
C	3.65704300	-1.79153900	-0.25731800
H	2.37813600	-1.47525400	1.44713300
H	2.80989000	-3.15440400	1.19033100
C	-2.15888900	2.39874400	0.93544100
C	0.31315700	2.43282900	0.57846700
C	-3.15197300	1.49053000	0.76980400
C	-3.30787900	-0.87476200	-0.01003600
C	3.46464800	-0.34763200	-0.81316400
H	3.04975900	0.84130500	-2.56237800
H	3.43453300	-0.83113500	-2.92822900
C	4.97996800	-1.88771300	0.54535700
H	3.73084300	-2.49605900	-1.09687100
H	-2.17912900	3.42083700	1.27793500
C	0.69732400	3.18466800	-0.55327600
C	1.10208100	2.34630500	1.74566000
H	-4.21569900	1.56162000	0.93091500
C	-3.69891000	-1.72911000	1.04401100
C	-3.66033000	-1.10979000	-1.35571000
H	4.44464900	0.14098000	-0.83218300
H	2.86430100	0.24177100	-0.10443800
C	6.29096600	-1.81490900	-0.26738900
H	4.98175400	-1.08625800	1.29945700
H	4.99000100	-2.83185500	1.10863200
C	-0.21600000	3.37811600	-1.76314700
C	1.94105100	3.82759400	-0.50251300
C	0.61773700	1.64053200	3.01050600
C	2.33582600	3.00964200	1.73549600
C	-3.41091700	-1.42069600	2.51281800

C	-4.43210500	-2.87258000	0.70268000
C	-3.35088900	-0.12424100	-2.48057100
C	-4.39206200	-2.27197700	-1.63445900
C	7.48913000	-1.67877400	0.68610600
C	6.47611300	-3.03138200	-1.18865900
H	6.26934400	-0.91386000	-0.89848400
C	0.52062900	3.26989400	-3.11135400
C	-0.94913300	4.73465100	-1.67271000
H	-0.97756700	2.59034600	-1.74455500
C	2.75499600	3.73571100	0.62350700
H	2.27177100	4.41906700	-1.35020600
C	1.71387900	0.81563500	3.70842900
C	0.01417500	2.66463800	3.99688600
H	-0.18027500	0.94594100	2.72605900
H	2.97126800	2.96860200	2.61413000
C	-2.88497600	-2.63700900	3.29917700
C	-4.67129800	-0.85367900	3.20199200
H	-2.63535300	-0.64782400	2.55352100
C	-4.76757900	-3.14834300	-0.62052000
H	-4.75211200	-3.55393200	1.48450500
C	-2.70002500	-0.79703300	-3.70327400
C	-4.62801800	0.63699600	-2.89583100
H	-2.63905300	0.61675500	-2.10271600
H	-4.68585900	-2.48490500	-2.65764700
H	7.39997600	-0.78778400	1.31891300
H	7.56584600	-2.55175600	1.34682900
H	8.42945600	-1.60204200	0.12897300
H	5.67126300	-3.12648200	-1.92697100
H	6.50752700	-3.96149700	-0.60648100
H	7.41796500	-2.95758300	-1.74343700
H	1.22118700	4.09768200	-3.26388700
H	-0.20279600	3.30646100	-3.93320600
H	1.08549100	2.33557400	-3.19886300
H	-0.23385500	5.56470800	-1.68701000
H	-1.62905000	4.85963700	-2.52290300
H	-1.53848900	4.81917400	-0.75387000
H	3.71372500	4.24623400	0.64088700
H	2.49890500	1.45033300	4.13367200
H	1.27932200	0.24495000	4.53643900
H	2.19152400	0.10901200	3.02135100
H	-0.36366600	2.15718500	4.89160300
H	0.77049800	3.39126100	4.31448600
H	-0.81534300	3.22150600	3.54842400
H	-2.61080100	-2.33078400	4.31473700

H	-2.00084400	-3.07943100	2.82897300
H	-3.64223500	-3.42259500	3.39386300
H	-5.48304400	-1.58968600	3.19553400
H	-4.45491800	-0.59908800	4.24551800
H	-5.04002700	0.04901700	2.70328400
H	-5.33835100	-4.04114000	-0.85952500
H	-2.42720200	-0.04033200	-4.44747900
H	-1.79337200	-1.34652300	-3.42521500
H	-3.37828200	-1.50371800	-4.19291800
H	-4.39895700	1.37273700	-3.67506400
H	-5.38495100	-0.04869600	-3.29283900
H	-5.07235000	1.16825700	-2.04712100

TS41

Ni	0.18982800	-0.73309200	-0.87984400
C	0.10813000	0.33415700	-2.47886300
C	-0.22671300	-2.49565200	-1.68804900
C	-0.73087300	-0.77162700	-2.83616200
H	-0.36134800	1.27378600	-2.20147900
H	1.08408900	0.42672500	-2.95044600
C	1.07714600	0.53488500	0.26353200
C	-0.75615700	-2.77497800	-0.29414200
H	-0.79482000	-3.02947400	-2.44125700
H	0.84351700	-2.69334400	-1.83642400
C	-2.24320500	-0.60192100	-2.77282500
H	-0.36726800	-1.38207200	-3.65964300
N	0.66397100	1.68612300	0.86917800
N	2.38999400	0.41401800	0.62185900
C	-2.26011700	-3.08485500	-0.23920300
H	-0.18248700	-3.60370800	0.14149200
C	-3.13704300	-1.77914500	-2.33074700
H	-2.54194200	-0.31215500	-3.79130600
H	-2.47144400	0.26156600	-2.13551200
C	1.69919200	2.26304200	1.59748500
C	-0.68130300	2.22692700	0.84864800
C	2.78456500	1.46595000	1.43887900
C	3.25702600	-0.68966800	0.25694200
C	-3.24889700	-2.03389300	-0.79859700
H	-2.52049100	-3.27890900	0.80820300
H	-2.41936700	-4.03510500	-0.76895400
H	-2.85668900	-2.70399200	-2.85304900
H	-4.13845400	-1.54133300	-2.70323500
H	1.56171900	3.17334800	2.15838500
C	-1.60997100	1.74106600	1.79368800

C	-0.98576500	3.26339200	-0.06087500
H	3.78747500	1.54215600	1.82769500
C	4.00435700	-0.60135600	-0.93753300
C	3.35666100	-1.78467000	1.14291300
C	-4.68382000	-2.50109400	-0.43643200
H	-3.05509300	-1.08116200	-0.28299700
C	-1.23712900	0.72318300	2.87016200
C	-2.89611100	2.29631000	1.77433100
C	0.05829600	3.87860900	-0.99204100
C	-2.28882900	3.77688800	-0.03311500
C	3.97700500	0.63522900	-1.83207300
C	4.84356800	-1.67836300	-1.24947700
C	2.63374500	-1.82857100	2.48771700
C	4.21513100	-2.82978300	0.77744500
C	-5.82842300	-1.47575800	-0.58346000
H	-4.68818000	-2.85601000	0.60416800
H	-4.91702000	-3.38212100	-1.05288400
C	-2.28157800	-0.39515800	3.03637500
C	-0.99118200	1.43528400	4.21798800
H	-0.29696800	0.24411500	2.57800900
C	-3.23618500	3.29580800	0.86679800
H	-3.63661600	1.95325400	2.48972700
C	-0.48212800	4.18369800	-2.40220100
C	0.64489400	5.16564500	-0.37025100
H	0.87995200	3.16147600	-1.10207300
H	-2.56275700	4.57301700	-0.71743400
C	3.97118000	0.29606600	-3.33430100
C	5.16288700	1.56730800	-1.50051600
H	3.05531800	1.18655700	-1.61738100
C	4.94523500	-2.78245300	-0.40672800
H	5.43530300	-1.64790100	-2.15842200
C	1.95208900	-3.18137100	2.76400000
C	3.60550700	-1.47430400	3.63414800
H	1.84702700	-1.06641100	2.47880500
H	4.32315100	-3.68670600	1.43480100
C	-5.70680100	-0.31296400	0.41373600
C	-7.18348600	-2.18345300	-0.41940000
H	-5.80344500	-1.05207200	-1.59814900
H	-2.48764800	-0.90043900	2.08677800
H	-1.91706900	-1.14197800	3.75064300
H	-3.23269700	-0.01553700	3.42440200
H	-1.89884200	1.94141900	4.56557400
H	-0.69430200	0.71089600	4.98495700
H	-0.19940100	2.18804000	4.13857000

H	-4.23878800	3.71373400	0.87232200
H	-1.21526600	4.99731000	-2.39057200
H	0.33943900	4.50095800	-3.05343100
H	-0.96076600	3.31214200	-2.86152900
H	1.41746700	5.58726700	-1.02301700
H	-0.13523200	5.92351500	-0.23675700
H	1.09685800	4.97873400	0.60919300
H	3.81486500	1.20709000	-3.92240400
H	3.17930500	-0.41743100	-3.58980400
H	4.92308100	-0.13623600	-3.66093600
H	6.11845400	1.06431900	-1.68707200
H	5.12808700	2.46834000	-2.12338000
H	5.15038200	1.88177900	-0.45146100
H	5.60759300	-3.60299200	-0.66762100
H	1.26866000	-3.46345000	1.95567900
H	1.37426900	-3.12563500	3.69312600
H	2.67857600	-3.99190600	2.88392700
H	3.07828600	-1.46806600	4.59474500
H	4.41805600	-2.20658300	3.70016900
H	4.05894800	-0.48765600	3.49069700
H	-4.77806800	0.25484600	0.28613300
H	-5.73530200	-0.68284900	1.44738300
H	-6.53909900	0.38991300	0.29266500
H	-8.01365300	-1.47887400	-0.54169200
H	-7.27400900	-2.63328700	0.57769300
H	-7.31014000	-2.98307400	-1.15849800
H	-0.52352500	-1.93670900	0.43446200

styrene

C	0.51528500	-0.22083400	0.00006600
C	0.00914400	1.09256200	0.00017700
C	-1.36214400	1.33005500	0.00001900
C	-2.26572400	0.26215500	-0.00015400
C	-1.78144500	-1.04621400	-0.00010200
C	-0.40671800	-1.28180300	0.00011300
H	0.69466700	1.93510600	0.00059000
H	-1.73019200	2.35282400	0.00012800
H	-3.33580100	0.45105200	-0.00023800
H	-2.47278100	-1.88487300	-0.00013500
H	-0.03541600	-2.30432300	0.00020100
C	1.95498400	-0.52959300	0.00005800
H	2.18689700	-1.59489600	0.00027500
C	2.97774200	0.33513600	-0.00021000
H	4.00483400	-0.01690300	-0.00003000

H	2.84103500	1.41323000	-0.00059300
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2,3-diphenyl-1-butene

C	-0.48405100	0.34802000	-0.71923100
C	-0.09547200	0.16782700	-1.99081700
H	-0.78450200	-0.16365600	-2.76161100
H	0.92768600	0.35516300	-2.30350600
C	0.49128800	0.92836100	0.32406500
C	1.84938900	0.22872800	0.28704500
C	1.97000800	-1.04590000	0.86393300
C	2.98717100	0.79454800	-0.30139400
C	3.18113900	-1.73414500	0.85021300
H	1.09774100	-1.50191300	1.32760400
C	4.20505300	0.10695600	-0.31916300
H	2.93561600	1.78357700	-0.74609500
C	4.30775700	-1.15875000	0.25532600
H	3.24795900	-2.71821900	1.30722500
H	5.07436200	0.56840000	-0.78095500
H	5.25497400	-1.69137000	0.24476700
C	-1.87230200	0.02653000	-0.28571300
C	-2.52052800	0.75040200	0.73168100
C	-2.58114800	-1.03248200	-0.88455000
C	-3.82752700	0.44729100	1.11440000
H	-2.00989500	1.57368500	1.22158900
C	-3.88576500	-1.33749200	-0.50254000
H	-2.08867400	-1.63888400	-1.63879000
C	-4.51867600	-0.59657600	0.49818200
H	-4.30583200	1.03138300	1.89643500
H	-4.40469600	-2.16560000	-0.97855300
H	-5.53441500	-0.83668900	0.80045600
H	0.06873300	0.71526000	1.31334400
C	0.58158500	2.46182300	0.18689100
H	0.94488800	2.75182300	-0.80428300
H	-0.40498000	2.92030800	0.31056100
H	1.25351300	2.88589800	0.94185100

TS-S1

Ni	-0.15304300	-0.09157300	-1.19475800
C	-4.15603000	-0.90995800	-2.56169200
C	-2.82706500	-0.44377800	-3.16307400
H	-4.99244000	-0.36968600	-3.01676000
H	-2.83706700	-0.60595500	-4.24927900
C	-4.33364100	-2.42959600	-2.77633200
H	-4.89790200	-2.87769600	-1.94496000

H	-4.87644300	-2.63411600	-3.70301600
O	-3.08065300	-3.10891000	-2.92892900
C	-2.07770500	-2.61643100	-2.06170200
H	-1.24533600	-3.32478200	-2.09327400
H	-2.43568200	-2.55829400	-1.02543100
C	-1.65555700	-1.25394400	-2.61740900
C	-0.36334100	-1.00335800	-3.04922400
H	-1.54510700	-0.46737200	-0.86395300
H	0.38136600	-1.79562100	-3.00007400
H	-0.19905000	-0.23646100	-3.80244500
H	-2.67274000	0.62693100	-3.00845000
H	-4.17054600	-0.66482100	-1.49369200
C	1.54059700	1.09505900	-2.10427300
C	2.17485700	0.14452100	-1.37279400
H	1.20842200	2.02911700	-1.66428100
H	1.50060300	1.02757900	-3.18720000
H	2.36063900	0.30513900	-0.31463900
C	2.86898900	-1.06095000	-1.95681900
H	2.33345300	-1.99039400	-1.69612300
H	2.89500600	-0.99338500	-3.05706500
O	4.16925500	-1.07909400	-1.40993300
C	4.99976300	-2.09973000	-1.97590100
H	4.54200400	-3.09025600	-1.82796400
H	5.08322500	-1.92796300	-3.06287600
C	6.34765700	-2.03426900	-1.32543100
C	6.94674000	-3.07624900	-0.74924500
H	6.84282300	-1.06522400	-1.36790900
H	7.94116600	-2.99652300	-0.31971500
H	6.47304900	-4.05455700	-0.69791400
C	-0.23564600	0.53938000	0.65032900
N	-0.12591200	1.81751600	1.12995100
N	-0.41709700	-0.22699100	1.77105900
C	-0.22779500	1.83893400	2.51746800
C	0.05890000	3.03885400	0.36749100
C	-0.39733900	0.55857000	2.91809200
C	-0.69136300	-1.65259900	1.83589500
H	-0.16580800	2.75845500	3.07618200
C	1.32412000	3.66748500	0.39944400
C	-1.05222500	3.59335100	-0.30812700
H	-0.50709600	0.12990000	3.90049000
C	-2.03206500	-2.06463600	2.01294200
C	0.38867800	-2.56199000	1.82649000
C	1.46428700	4.86543000	-0.31511400
C	2.51237400	3.13180500	1.19917800

C	-0.84378200	4.78551100	-1.01235300
C	-2.45369000	2.99119400	-0.21569200
C	-2.27323800	-3.44154100	2.11275800
C	-3.19322100	-1.08372600	2.17741800
C	0.08210300	-3.92547100	1.92543500
C	1.84566500	-2.10587300	1.80677500
C	0.39938900	5.41367800	-1.02199900
H	2.42239300	5.37482300	-0.31435500
C	2.72567700	3.96685300	2.48121200
C	3.81897800	3.08760000	0.38211900
H	2.28590400	2.10519600	1.50834600
H	-1.66985200	5.23923800	-1.54873100
C	-3.29368200	3.19493300	-1.48905900
C	-3.20189800	3.56392600	1.00891100
H	-2.35197700	1.91149500	-0.06842200
C	-1.23253200	-4.36350100	2.05722100
H	-3.28991900	-3.79590600	2.24782400
C	-3.53897300	-0.89514400	3.67170200
C	-4.46103600	-1.50775700	1.41362900
H	-2.88170400	-0.11186400	1.77873800
H	0.88535900	-4.65405200	1.91493200
C	2.78653900	-3.08582200	1.08319100
C	2.35600900	-1.85786600	3.24402900
H	1.89252100	-1.15097600	1.27385600
H	0.53301600	6.34102900	-1.57155800
H	1.83316500	3.98761300	3.11558200
H	3.55038600	3.55312300	3.07195400
H	2.97700900	5.00419900	2.23330300
H	3.70210100	2.52955600	-0.55165600
H	4.17564500	4.09230900	0.13161000
H	4.60606700	2.60234700	0.96936700
H	-2.75433000	2.87924200	-2.38934200
H	-4.21771600	2.61044400	-1.41984300
H	-3.58860600	4.24094800	-1.62692900
H	-2.66878700	3.36256900	1.94395700
H	-3.32174400	4.64947700	0.91789900
H	-4.20093300	3.11993900	1.08811800
H	-1.44451700	-5.42592200	2.13640100
H	-2.68641700	-0.53131000	4.25297300
H	-4.35591900	-0.17374500	3.78566900
H	-3.86183400	-1.84325600	4.11619100
H	-4.24795000	-1.73800200	0.36588600
H	-4.93251500	-2.39045100	1.85894000
H	-5.20062600	-0.70012400	1.44314200

H	2.37446000	-3.40971100	0.12094900
H	3.75075200	-2.60453700	0.89532700
H	2.97578100	-3.98342300	1.68229800
H	1.76986400	-1.09191000	3.76213000
H	2.30435300	-2.77851100	3.83611600
H	3.40047600	-1.52683300	3.22377200

int-S2

Ni	-0.19767000	-0.09319800	-1.16823800
C	-4.14996400	-1.17982500	-2.49353600
C	-2.88314500	-0.63719700	-3.16165500
H	-5.03935800	-0.69456000	-2.90816100
H	-2.93681600	-0.80595700	-4.24615400
C	-4.24472800	-2.70915600	-2.69399800
H	-4.73352500	-3.18601100	-1.83145000
H	-4.82450400	-2.95222600	-3.58842300
O	-2.96329700	-3.31126500	-2.91501300
C	-1.94219700	-2.75470800	-2.10905400
H	-1.07027900	-3.40894200	-2.19597100
H	-2.23649800	-2.72021500	-1.05146000
C	-1.64190700	-1.36897500	-2.67562900
C	-0.38213200	-0.99003200	-3.07714700
H	-1.54675500	-0.50506900	-0.75277200
H	0.43519200	-1.70719200	-3.03910700
H	-0.27568700	-0.17008700	-3.78343900
H	-2.78440000	0.44186600	-3.01848300
H	-4.12493700	-0.92924500	-1.42700200
C	1.46224400	1.16606800	-2.10658100
C	2.14303300	0.23576500	-1.39432300
H	1.09595700	2.08046100	-1.65286600
H	1.40755100	1.10646100	-3.18941900
H	2.33220700	0.39110400	-0.33605800
C	2.87359800	-0.93745000	-1.99797500
H	2.39293500	-1.88951700	-1.71103200
H	2.85576000	-0.87738400	-3.09892400
O	4.19219200	-0.88702900	-1.50031900
C	5.04307400	-1.89149500	-2.06470200
H	4.64628100	-2.89490000	-1.84528200
H	5.05956100	-1.76939100	-3.16143800
C	6.41907500	-1.72673400	-1.49536200
C	7.09923200	-2.70562800	-0.89891600
H	6.86197100	-0.73921200	-1.61639100
H	8.10978300	-2.55555000	-0.53013100
H	6.67812800	-3.70052900	-0.76894200

C	-0.25111200	0.53763200	0.66494300
N	-0.22428300	1.82526000	1.12986500
N	-0.34339900	-0.22990700	1.79511800
C	-0.28891500	1.85201000	2.51968100
C	-0.14748800	3.04889500	0.35249500
C	-0.35145100	0.56645800	2.93486900
C	-0.50585400	-1.67176100	1.87617700
H	-0.27935600	2.77920700	3.06896000
C	1.06927900	3.76786900	0.34973200
C	-1.31102400	3.51376200	-0.30205300
H	-0.40046600	0.14030500	3.92331400
C	-1.81229200	-2.18599200	2.04252900
C	0.64298500	-2.49193900	1.89289000
C	1.10584200	4.96469900	-0.37926000
C	2.31021900	3.32874400	1.12802700
C	-1.20547100	4.71001500	-1.02218800
C	-2.66191600	2.81234800	-0.17006900
C	-1.94456000	-3.57602100	2.15845900
C	-3.04750500	-1.29594800	2.18085800
C	0.44425100	-3.87412100	2.00941200
C	2.06090200	-1.92561000	1.88409900
C	-0.01165600	5.42633600	-1.06651100
H	2.02376400	5.54296600	-0.40499900
C	2.49401200	4.19734300	2.39221100
C	3.59716900	3.36221700	0.28007100
H	2.16317700	2.29396700	1.45716300
H	-2.07374600	5.09725100	-1.54374100
C	-3.55115300	2.95111100	-1.41836800
C	-3.41386200	3.33144100	1.07587600
H	-2.47767800	1.74328300	-0.02688800
C	-0.83300700	-4.41297400	2.13048700
H	-2.93134400	-4.00901000	2.28458600
C	-3.39547100	-1.07441000	3.67008400
C	-4.28425100	-1.85235700	1.45153000
H	-2.81873000	-0.31990400	1.73847700
H	1.30272600	-4.53682700	2.02047300
C	3.07201800	-2.81857300	1.14201100
C	2.55027200	-1.66825500	3.32679300
H	2.03650200	-0.95864800	1.37141600
H	0.04202300	6.35486600	-1.62759300
H	1.61602100	4.16873600	3.04633600
H	3.35735500	3.85021300	2.97060600
H	2.66918300	5.24504700	2.12321800
H	3.50132600	2.77248600	-0.63643600

H	3.87025000	4.38411000	-0.00400800
H	4.43236000	2.95316500	0.85887500
H	-3.01605300	2.67550400	-2.33419300
H	-4.42566400	2.29832700	-1.32238500
H	-3.92858800	3.97146200	-1.54635800
H	-2.83985700	3.17169500	1.99459000
H	-3.61582000	4.40503300	0.98824900
H	-4.37467200	2.81528200	1.18481600
H	-0.96150600	-5.48767400	2.22270400
H	-2.57178400	-0.61724500	4.22604700
H	-4.26840500	-0.41858600	3.76369300
H	-3.63540300	-2.02707800	4.15550800
H	-4.06247000	-2.11504000	0.41318100
H	-4.68168700	-2.74651400	1.94370000
H	-5.08452200	-1.10421500	1.45239200
H	2.68187100	-3.15743400	0.17607900
H	3.99653400	-2.26391700	0.95710700
H	3.33111800	-3.70860800	1.72613000
H	1.90640600	-0.95994800	3.85833400
H	2.56885000	-2.60134500	3.90105600
H	3.56622300	-1.25767200	3.31549500

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Ni	-0.29909400	-0.47292800	0.22165400
C	1.18704600	0.29627900	-0.66407400
C	-1.54063900	0.91136500	-0.27479900
C	1.93688300	-0.93327600	-0.22598900
H	1.47559800	1.23416900	-0.19843600
H	1.01744700	0.39899800	-1.73484600
N	-1.41299500	2.24534700	-0.08001000
N	-2.71777700	0.69211300	-0.90734700
C	3.14144100	-0.69352800	0.77369700
C	2.28759400	-1.89784300	-1.35145600
C	-2.63723700	2.98721800	-0.46729900
C	-0.37662300	2.97033400	0.61624000
C	-3.39008200	1.95391800	-1.29928200
C	-3.27262400	-0.55360200	-1.38004200
C	2.68591800	-0.00474900	2.06946500
C	4.32728600	-0.00010300	0.11372400
H	3.47580600	-1.70155500	1.04704300
C	2.08673700	-3.27683400	-1.20174600
C	2.87318400	-1.43448900	-2.53881100
H	-2.38161900	3.88856200	-1.02548100
H	-3.18371100	3.28358900	0.43625800

C	-0.38557800	3.01264900	2.02829500
C	0.55200000	3.72148600	-0.14546500
H	-4.45647400	1.90937800	-1.07368500
H	-3.26998700	2.10856700	-2.37819900
C	-2.80068000	-1.11913900	-2.58644700
C	-4.35786900	-1.11790900	-0.66433400
H	3.53305000	0.09262300	2.75599400
H	1.91448000	-0.59851800	2.57273200
H	2.28397900	0.99898800	1.90070200
C	4.39951800	1.39479900	-0.02450500
C	5.40124800	-0.76725300	-0.36058800
C	2.43958700	-4.17097000	-2.21422500
H	1.65913800	-3.65921400	-0.27776300
C	3.23077700	-2.32555200	-3.55146300
H	3.06432100	-0.37333100	-2.66703400
C	-1.47511500	2.35643800	2.87173000
C	0.61461200	3.75766600	2.66826900
C	0.49868400	3.81187800	-1.67058000
C	1.52381000	4.45367700	0.54807300
C	-1.74909100	-0.44907500	-3.46637600
C	-3.39147200	-2.31411000	-3.01982000
C	-4.96525300	-0.46572300	0.57718500
C	-4.91340000	-2.30753000	-1.15104900
C	5.50330200	1.99824400	-0.63077200
H	3.60333600	2.02665700	0.35816500
C	6.50765500	-0.16740800	-0.96390000
H	5.37115300	-1.84885500	-0.25458000
C	3.01082100	-3.69575600	-3.39563600
H	2.26996600	-5.23555400	-2.07861500
H	3.68690400	-1.94754600	-4.46215200
C	-0.89983600	1.44411800	3.96926500
C	-2.40271900	3.42415700	3.49059400
H	-2.08636100	1.72813900	2.21506100
C	1.56744100	4.46263800	1.94019100
H	0.63420700	3.80268000	3.75294300
C	1.85765700	3.54293700	-2.34636000
C	-0.03320200	5.19330000	-2.11517700
H	-0.20028700	3.04786900	-2.02903000
H	2.25140100	5.03476100	-0.01022300
C	-0.62404400	-1.41035600	-3.89004200
C	-2.41265000	0.18036100	-4.71131500
H	-1.28741700	0.36085100	-2.89225100
C	-4.42874500	-2.90945900	-2.30901400
H	-3.04520800	-2.77474300	-3.93969600

C	-5.05091700	-1.42492900	1.78069500
C	-6.36429600	0.11011300	0.26610700
H	-4.31696500	0.36672200	0.87347700
H	-5.74164500	-2.76585100	-0.61921700
C	6.56080700	1.21986100	-1.10491400
H	5.54135400	3.08056700	-0.72175200
H	7.32834200	-0.78465000	-1.31871800
H	3.28769300	-4.38759500	-4.18583700
H	-0.32753900	2.01083000	4.71151000
H	-1.71337500	0.93940900	4.50446600
H	-0.23561200	0.68420200	3.54634500
H	-1.85431500	4.06612200	4.18902400
H	-3.21951000	2.94782500	4.04511200
H	-2.84310600	4.07299800	2.72546800
H	2.33084600	5.03743700	2.45670600
H	2.58698900	4.32654100	-2.11342800
H	1.73483600	3.53096400	-3.43522900
H	2.28925500	2.58570200	-2.04071700
H	0.66049800	5.98949600	-1.82241400
H	-0.14179200	5.22881400	-3.20508700
H	-1.00502400	5.43072800	-1.66846000
H	0.14746200	-0.86491200	-4.44431800
H	-0.99497900	-2.20272700	-4.54913700
H	-0.14628800	-1.88508200	-3.02792700
H	-3.19683800	0.89628500	-4.44007900
H	-1.66616600	0.70604400	-5.31759200
H	-2.87418800	-0.58864100	-5.34090300
H	-4.87375700	-3.83299300	-2.66827900
H	-5.73836500	-2.25605700	1.58953400
H	-5.42542100	-0.88941900	2.66036100
H	-4.07633800	-1.85504900	2.03243400
H	-7.06792700	-0.68880100	0.00681300
H	-6.76460700	0.63724300	1.13950300
H	-6.34512600	0.81157100	-0.57545300
H	7.42182500	1.69110000	-1.57038300
C	-1.33818400	-2.37229100	0.85701000
C	-1.10417400	-2.09195400	2.17024900
H	-0.77802600	-3.13470400	0.32068500
H	-2.24787300	-2.02831400	0.37852200
C	-0.09420300	-2.69231100	3.05087000
H	-1.77203800	-1.38430000	2.66049600
C	0.03156300	-2.21292000	4.36822500
C	0.72280600	-3.76873900	2.65050400
C	0.96047500	-2.76662800	5.24774800

H	-0.60911600	-1.40269900	4.70382500
C	1.65074100	-4.32041900	3.52740900
H	0.61018300	-4.19688700	1.65932800
C	1.77770900	-3.81700500	4.82738200
H	1.04139600	-2.38298900	6.26040300
H	2.26778600	-5.15407400	3.20513900
H	2.50013200	-4.25338100	5.51081800
H	1.21565600	-1.52769300	0.44859100

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Ni	-0.05679500	0.23166700	-0.61665000
C	-3.19514600	0.28944300	2.24346900
C	-2.60354700	-1.08213200	2.54867600
H	-3.00635800	1.01947400	3.03935800
H	-2.39708500	-1.24058400	3.60750000
H	-3.24033200	-1.90036400	2.19406600
H	-4.26788200	0.25802100	2.05224900
N	-1.34490400	-1.06352000	1.76336800
N	-2.44980100	0.68142600	1.02197900
C	-1.33706700	-0.08180900	0.83208900
C	2.24774500	0.55542400	-0.73863400
C	1.62669400	0.28278100	0.49995700
H	1.68277600	-0.70889200	0.93346200
H	1.48369300	1.09881500	1.20168300
C	-1.47712600	0.02638000	-2.26043500
C	-0.44060200	0.89546200	-2.62510100
H	-2.32272000	0.46360800	-1.74551100
C	-2.74225500	1.96724800	0.42283300
C	-1.97545100	3.10135900	0.79113800
C	-3.86695900	2.09146400	-0.43283700
C	-2.28364400	4.32852800	0.18882700
C	-4.13135800	3.34653000	-0.99608000
C	-3.33765000	4.45190500	-0.70959400
H	-1.70347100	5.20793100	0.44903500
H	-4.98127100	3.46224100	-1.66087100
H	-3.55964900	5.41452400	-1.16133700
C	-0.31422000	-2.02515700	2.09405300
C	-0.27877900	-3.27999900	1.44428900
C	0.56493200	-1.72208300	3.16603700
C	0.71393900	-4.19125700	1.83248200
C	1.53536700	-2.67176600	3.50851200
C	1.62127900	-3.89054500	2.84235200
H	0.76606300	-5.15894900	1.34497900
H	2.22334500	-2.45964700	4.32108800

H	2.37991700	-4.61450900	3.12606900
C	2.98327000	-0.56176500	-1.51948000
C	4.45442400	-0.59794000	-1.09284100
C	4.83563500	-1.02729500	0.18655100
C	5.45422900	-0.21734300	-1.99640200
C	6.18195000	-1.07690400	0.54910100
H	4.08225400	-1.33230600	0.90819100
C	6.80232700	-0.26764600	-1.63708200
H	5.17743500	0.12057800	-2.99225200
C	7.17039500	-0.69722100	-0.36181300
H	6.45954400	-1.41619600	1.54337100
H	7.56240600	0.02811100	-2.35473200
H	8.21847400	-0.73800100	-0.07948400
H	0.91935000	0.62246700	-1.75174400
C	2.74973800	1.94659400	-1.03265900
C	3.40170900	2.67625000	-0.02599300
C	2.68373700	2.50267700	-2.32067200
C	3.94982700	3.93141700	-0.29373900
H	3.50680100	2.24672600	0.96527400
C	3.22156400	3.76079000	-2.58745000
H	2.20798300	1.95188000	-3.12759000
C	3.85522400	4.48122700	-1.57235900
H	4.45850600	4.47432000	0.49764600
H	3.15040100	4.17574700	-3.58880700
H	4.28086300	5.45843200	-1.78069600
H	-0.55384000	1.95817300	-2.42016700
C	2.32792600	-1.94688000	-1.42512000
H	2.35010500	-2.35495900	-0.41078800
H	1.28244300	-1.91400600	-1.75267400
H	2.86589100	-2.64832100	-2.07082400
H	2.97606300	-0.26288800	-2.57436500
H	0.17699600	0.66600600	-3.49044900
C	-1.70451500	-1.30130800	-2.86095200
C	-0.81107700	-1.88863800	-3.77872700
C	-2.91436300	-1.97232300	-2.59863400
C	-1.12837700	-3.08056200	-4.42478100
H	0.13254200	-1.40423900	-4.01155000
C	-3.23541300	-3.16253400	-3.24885800
H	-3.61985500	-1.54003500	-1.89587100
C	-2.34545900	-3.71947100	-4.16977400
H	-0.42936600	-3.50723600	-5.13829100
H	-4.18455200	-3.64980600	-3.04412800
H	-2.59696100	-4.64128300	-4.68593200
C	-1.31733300	-3.70868800	0.41272800

C	-2.39902400	-4.59188900	1.07555900
C	-0.70654100	-4.45543100	-0.78600300
H	-1.80634800	-2.80888200	0.02530900
H	-2.87513400	-4.09761400	1.92936200
H	-3.18012200	-4.84624300	0.34986800
H	-1.96407700	-5.52886000	1.44208200
H	0.09550300	-3.88033500	-1.25712300
H	-0.29885600	-5.42944500	-0.49427900
H	-1.47661500	-4.63850800	-1.54016800
C	-4.84968200	0.95156300	-0.70230300
C	-5.22064000	0.79942400	-2.19172900
C	-6.14426500	1.15020000	0.12030400
H	-4.38146500	0.01579700	-0.37340200
H	-4.34192300	0.70486300	-2.83678200
H	-5.84107200	-0.09258800	-2.33312300
H	-5.80439100	1.65403200	-2.54899500
H	-5.94718100	1.26248700	1.19163100
H	-6.67315400	2.05208900	-0.20739500
H	-6.81957300	0.29781700	-0.01568900
C	0.45888200	-0.45028100	4.00790600
C	1.80529000	0.27896500	4.18960600
C	-0.13937500	-0.76643600	5.39767700
H	-0.22080700	0.24146600	3.49935100
H	2.29236600	0.49251200	3.23360700
H	1.64693200	1.22914500	4.71214400
H	2.50489100	-0.30779300	4.79455800
H	-1.10710000	-1.27498300	5.32978400
H	0.53001500	-1.41909800	5.96911800
H	-0.27939500	0.15556100	5.97351100
C	-0.92207200	3.07850900	1.89650000
C	-1.50721300	3.66656900	3.20043800
C	0.36871200	3.82590600	1.51977200
H	-0.65030600	2.03736800	2.09335600
H	-2.41720200	3.14503700	3.51608800
H	-0.77520300	3.59834600	4.01363200
H	-1.76485100	4.72353300	3.06911200
H	0.78593300	3.46906800	0.57440300
H	0.20323600	4.90467500	1.42709900
H	1.12473600	3.68585200	2.30100100

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C	-0.73764500	0.71906700	0.34861300
N	-0.18590300	1.77243400	0.99367800
N	-2.08816800	0.83436800	0.46224700

C	-1.18916100	2.59894900	1.70946100
C	1.20304800	2.16270700	1.06768300
C	-2.49940000	2.10962100	1.10199000
C	-3.09427800	0.05223000	-0.22354600
H	-1.00462600	3.66145900	1.54437300
H	-1.12491800	2.39984000	2.78493600
C	2.02830400	1.65050400	2.09588900
C	1.67326200	3.15165700	0.16577300
H	-3.27688200	1.93964600	1.84619600
H	-2.89298500	2.79214100	0.34023800
C	-3.35449300	0.29529400	-1.59659400
C	-3.88948000	-0.85707000	0.52228600
C	1.51175600	0.71399300	3.18438100
C	3.35786700	2.09254500	2.15065700
C	0.78020100	3.83996100	-0.86645400
C	3.01072700	3.55465300	0.26991600
C	-2.68211200	1.40852600	-2.39844800
C	-4.34965300	-0.46634300	-2.22427400
C	-3.78742600	-1.00897300	2.03999400
C	-4.87003100	-1.58787300	-0.16090600
C	2.48298700	-0.43889300	3.49393400
C	1.21590100	1.50764100	4.47738100
H	0.57460800	0.26686300	2.83581300
C	3.85146600	3.02465200	1.24309100
H	4.01195000	1.71572400	2.93013400
C	1.38656000	3.84689200	-2.28404000
C	0.46279500	5.28906000	-0.43331800
H	-0.16745600	3.29245100	-0.91718500
H	3.39577600	4.30402600	-0.41455700
C	-2.20853200	0.95074000	-3.79195700
C	-3.63657100	2.61493300	-2.54891700
H	-1.80225600	1.74939800	-1.84355500
C	-5.09042100	-1.41091800	-1.52318700
H	-4.56113700	-0.30137000	-3.27587500
C	-3.88520100	-2.47152800	2.52111600
C	-4.89798900	-0.19122900	2.74160500
H	-2.81562800	-0.61139100	2.35540300
H	-5.48314200	-2.29683400	0.38580300
H	2.02618400	-1.12619800	4.21336300
H	3.41506100	-0.07866800	3.94264500
H	2.73261400	-1.00986000	2.59444300
H	2.13559200	1.94385700	4.88381900
H	0.78995000	0.84892600	5.24288800
H	0.51301600	2.33027600	4.30751700

H	4.88467900	3.35380400	1.30809200
H	2.28542500	4.47058700	-2.33631600
H	0.66514400	4.26147000	-2.99721100
H	1.66061500	2.84243600	-2.62025700
H	1.37443600	5.89622500	-0.40464100
H	-0.22901300	5.75749500	-1.14253400
H	0.01039100	5.33522800	0.56326200
H	-3.05295800	0.74748500	-4.45881200
H	-1.61008700	1.73770700	-4.26476800
H	-1.60192000	0.04199800	-3.73768500
H	-4.52465300	2.33753700	-3.12787300
H	-3.13650200	3.43628500	-3.07500000
H	-3.98285300	2.99117100	-1.58051300
H	-5.85745800	-1.98906900	-2.03052900
H	-4.89943300	-2.86693800	2.40278400
H	-3.64785500	-2.52844700	3.58956300
H	-3.20703200	-3.14045100	1.98372900
H	-5.88525000	-0.59517200	2.49064200
H	-4.78141600	-0.24254400	3.83017500
H	-4.89814200	0.86328100	2.44910200
C	0.90028700	0.05310000	-2.37555400
C	2.01780800	-0.03450800	-1.56539200
H	0.78477800	-0.57841100	-3.25119300
H	0.30166100	0.95587600	-2.36351600
C	3.16916300	-0.92984300	-1.70600900
H	2.14171800	0.73478300	-0.80817400
C	4.13434500	-0.94288700	-0.67980200
C	3.38544600	-1.73496000	-2.84294500
C	5.26306900	-1.75445300	-0.77115800
H	3.99288100	-0.30487200	0.18888900
C	4.51431300	-2.54398700	-2.93357600
H	2.68321400	-1.70666800	-3.67099100
C	5.45307700	-2.56160700	-1.89542200
H	5.99819000	-1.75166500	0.02832700
H	4.67244500	-3.15193200	-3.81950600
H	6.33579700	-3.18966300	-1.97279500
C	0.27778400	-2.64305400	-1.46593800
C	-1.04530300	-2.83237500	-2.18299900
C	0.45714800	-2.99441000	-0.07592800
H	1.14893900	-2.83871600	-2.08763700
Ni	0.10933800	-0.85564700	-0.65343000
H	-1.89973500	-2.37924500	-1.66792500
H	-1.26969400	-3.90453700	-2.28753400
H	-1.00435200	-2.40715600	-3.19038600

C	1.70883200	-3.47419500	0.41610100
C	-0.56289300	-2.68703900	0.86683600
C	1.89118900	-3.71109000	1.76195800
H	2.49803600	-3.69671000	-0.29547700
C	-0.33775400	-2.89285700	2.24426400
H	-1.56398700	-2.44431900	0.52616600
C	0.86321200	-3.41994200	2.68494800
H	2.82922600	-4.12938900	2.11573100
H	-1.13201000	-2.68491400	2.95287700
H	1.01488000	-3.62248600	3.74102200

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Ni	0.13816500	-0.13408900	-0.54468500
C	-1.44276300	0.36687500	0.63839000
C	1.37058000	1.14005500	0.29318200
C	-2.11034500	-0.63451500	-0.08579300
H	-1.58924200	1.40887400	0.38145400
H	-1.13019100	0.16234600	1.65847100
N	1.21390700	2.48408700	0.38437300
N	2.54589300	0.82321100	0.89045500
C	-3.06109200	-0.28639500	-1.25835700
C	-2.40228500	-1.95268500	0.57720200
C	2.40844400	3.15351900	0.95462800
C	0.16822000	3.31378700	-0.16743900
C	3.15770200	1.98373900	1.58098500
C	3.14265600	-0.47838500	1.07812400
C	-2.64427800	0.93682200	-2.08699900
C	-4.49045000	-0.14760800	-0.72433200
H	-3.06365000	-1.15634200	-1.92502400
C	-2.87491500	-1.96219100	1.89990200
C	-2.33104700	-3.16987400	-0.11645800
H	2.11716100	3.91686400	1.67667700
H	2.97624700	3.63589800	0.14987600
C	0.20481000	3.67322500	-1.53503400
C	-0.80618700	3.84887000	0.71328400
H	4.23341600	2.01717800	1.40766300
H	2.98212600	1.89924600	2.66046200
C	2.66964100	-1.32592800	2.10605700
C	4.27802100	-0.82079000	0.29858900
H	-3.31398200	1.03888100	-2.94673900
H	-1.61907300	0.83259000	-2.46016400
H	-2.69829800	1.86924700	-1.51891900
C	-4.86700600	0.93450400	0.08403600
C	-5.45832700	-1.10338500	-1.05655300

C	-3.24509600	-3.15776400	2.51615800
H	-2.98652700	-1.02579500	2.43755400
C	-2.68777600	-4.36654800	0.50337500
H	-1.97560900	-3.19139900	-1.14125300
C	1.34386100	3.27632200	-2.47175400
C	-0.81015100	4.50892600	-2.02112100
C	-0.77750500	3.61925500	2.22511500
C	-1.79334300	4.68104400	0.17088300
C	1.57331800	-0.91626800	3.08615300
C	3.30422400	-2.56445100	2.27975800
C	4.92478200	0.13474500	-0.70636400
C	4.87120600	-2.06953400	0.51930400
C	-6.17783900	1.05653800	0.54594500
H	-4.13866200	1.69560100	0.35161600
C	-6.77133200	-0.98297000	-0.59783700
H	-5.18343600	-1.95095300	-1.67977900
C	-3.14528800	-4.36471600	1.82284700
H	-3.61938300	-3.14276800	3.53577000
H	-2.60601500	-5.29919100	-0.04708100
C	0.85164000	2.70100000	-3.81379000
C	2.27462300	4.48262000	-2.72831700
H	1.93823300	2.50060400	-1.97832500
C	-1.80783900	4.99838400	-1.18477900
H	-0.80712000	4.79663900	-3.06787500
C	-2.13694900	3.19044300	2.81231400
C	-0.28804100	4.89109200	2.95511900
H	-0.06357900	2.81387000	2.43104400
H	-2.55342500	5.10063300	0.82285100
C	0.48837600	-1.99530400	3.25041800
C	2.18509300	-0.55931300	4.45889300
H	1.08554300	-0.01610500	2.69827000
C	4.38545000	-2.94117100	1.49005400
H	2.95865000	-3.23323400	3.06185200
C	5.20428200	-0.50798500	-2.08013400
C	6.24460300	0.70415700	-0.13638500
H	4.23669700	0.97203900	-0.86980600
H	5.73696800	-2.35883500	-0.06816200
C	-7.13481300	0.09759400	0.20651400
H	-6.45310800	1.90338000	1.16872600
H	-7.50805200	-1.73340300	-0.87037000
H	-3.43076100	-5.29602700	2.30347400
H	0.15686700	1.86657900	-3.67038100
H	0.33637000	3.45756900	-4.41505300
H	1.70158400	2.34328100	-4.40635700

H	1.74040000	5.28544300	-3.24861600
H	3.12461600	4.18540600	-3.35322900
H	2.66709200	4.90166300	-1.79532400
H	-2.58246100	5.64730300	-1.58339100
H	-2.88750100	3.98273500	2.71845600
H	-2.02790700	2.97630100	3.88144400
H	-2.53413700	2.29334700	2.32801600
H	-1.00266900	5.71179900	2.82606800
H	-0.18764600	4.70120500	4.02975100
H	0.67906600	5.24281600	2.57980800
H	0.88576000	-2.90225500	3.71913200
H	-0.31545300	-1.62601600	3.89679000
H	0.04662900	-2.27831800	2.29049300
H	2.66908900	-1.43186600	4.91185500
H	1.40496900	-0.21440000	5.14733900
H	2.94098500	0.22987500	4.37801300
H	4.86606600	-3.90277800	1.64684900
H	5.94970100	-1.30720800	-2.00884200
H	5.60423100	0.24621300	-2.76694600
H	4.30412000	-0.93278100	-2.53447000
H	6.98871500	-0.09086600	-0.01439000
H	6.66441300	1.45310300	-0.81740700
H	6.10968700	1.17294400	0.84436400
H	-8.15574300	0.19395300	0.56466600
C	0.47182700	-1.50211800	-2.31668500
C	1.48770700	-0.59356300	-1.98932200
C	0.56629900	-2.96855000	-2.09909400
H	-0.21272100	-1.21085800	-3.11287200
H	2.38856400	-0.95771700	-1.51229200
H	1.57592600	0.32659700	-2.55727600
C	1.30309400	-3.53193400	-1.04508100
C	-0.06717200	-3.82067900	-3.01739600
C	1.40641400	-4.91525700	-0.92137600
H	1.78599400	-2.89201900	-0.31284000
C	0.04357700	-5.20660500	-2.89561700
H	-0.63684200	-3.39675600	-3.84166100
C	0.77973700	-5.75728700	-1.84531500
H	1.97775300	-5.33750300	-0.09980200
H	-0.44244500	-5.85230700	-3.62120900
H	0.86612800	-6.83544400	-1.74646400
H	-0.83142600	-1.14392000	-1.18449100

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C	0.05437300	-1.18937400	0.03574800
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N	-1.01955000	-1.97934500	-0.16357200
N	1.07967200	-1.96867100	0.45175900
C	-0.70290700	-3.41895900	0.00057900
C	-2.33685700	-1.59164400	-0.60842100
Ni	0.12371300	0.78006900	-0.20173600
C	0.65108700	-3.36701800	0.70749100
C	2.38805500	-1.53793900	0.88222600
H	-1.47667800	-3.92128600	0.58299900
H	-0.64892600	-3.89413800	-0.98641500
C	-2.58991100	-1.42874900	-1.98990100
C	-3.37099100	-1.50303100	0.35448300
C	1.45019000	0.54161300	-1.73758600
H	1.37448400	-4.07708600	0.30589700
H	0.56886500	-3.53010500	1.78897900
C	2.53949700	-0.88296900	2.12744900
C	3.50650300	-1.86485600	0.07424000
C	-1.52858600	-1.65000900	-3.06391100
C	-3.89813000	-1.11512800	-2.38219100
C	-3.15036900	-1.78470300	1.83986700
C	-4.65972800	-1.19531400	-0.09715500
C	1.39849400	1.92518200	-1.81819600
H	2.32166500	0.04918400	-1.32346600
H	0.85396700	-0.04259400	-2.43013300
C	1.38362100	-0.65303200	3.09874000
C	3.83228500	-0.50299700	2.51413500
C	3.39612200	-2.67981800	-1.21548800
C	4.77387300	-1.46445400	0.51605500
C	-1.40204700	-0.44910100	-4.02201600
C	-1.81155700	-2.94247400	-3.85965300
H	-0.56184300	-1.78005100	-2.56609500
C	-4.92335800	-0.99587900	-1.44893000
H	-4.12096400	-0.98572800	-3.43711500
C	-3.65879200	-0.64773100	2.74733600
C	-3.81025300	-3.11961600	2.25003400
H	-2.07202300	-1.87861600	2.01058900
H	-5.47060700	-1.11658200	0.62033900
C	2.42948300	2.87551100	-1.38078400
H	0.62743400	2.35391700	-2.45494600
C	1.33747500	0.78765400	3.64292100
C	1.45158300	-1.66073400	4.26727700
H	0.44347200	-0.82911500	2.56686000
C	4.93840200	-0.78058200	1.71744100
H	3.97709300	-0.00013800	3.46518400
C	4.12805300	-2.03623000	-2.41072200

C	3.92999100	-4.11402600	-0.99905200
H	2.33557100	-2.74853400	-1.48311400
H	5.64651400	-1.70101600	-0.08490800
H	-1.22111700	0.48518800	-3.47778300
H	-0.57450300	-0.60527400	-4.72367200
H	-2.31035300	-0.31092100	-4.61808200
H	-1.87563000	-3.81671800	-3.20225400
H	-1.01644900	-3.12392300	-4.59187300
H	-2.75891100	-2.87105200	-4.40544300
H	-5.93244800	-0.76273900	-1.77683200
H	-4.74795100	-0.54422000	2.69367200
H	-3.40308300	-0.86017900	3.79170400
H	-3.22638900	0.31979800	2.47544000
H	-3.59425000	-3.34663900	3.30017500
H	-3.45875000	-3.96007200	1.64088200
H	-4.89890000	-3.06874500	2.13676700
C	3.53916100	2.49761500	-0.59990700
C	2.32118700	4.21353800	-1.79963200
H	1.34504900	1.52594600	2.83356200
H	0.43050800	0.93529200	4.24049500
H	2.18999600	1.00562700	4.29485800
H	1.44601700	-2.69685800	3.91126500
H	0.59688700	-1.52705000	4.94027300
H	2.36635900	-1.51920500	4.85363500
H	5.93139700	-0.48317500	2.04260000
H	5.21101900	-1.99962000	-2.25143500
H	3.95405600	-2.62948900	-3.31519900
H	3.78551600	-1.01547700	-2.60784400
H	5.00301100	-4.09905900	-0.77771300
H	3.78324900	-4.71711100	-1.90203600
H	3.43465500	-4.62253700	-0.16461500
C	4.50893800	3.43449900	-0.25892600
H	3.64517700	1.47304700	-0.25591000
C	3.29780800	5.14947400	-1.46141100
H	1.47190500	4.51697000	-2.40738600
C	4.39308100	4.76197200	-0.68871400
H	5.36137800	3.13099800	0.34181600
H	3.20316100	6.17652700	-1.80086000
H	5.15572200	5.48782200	-0.42218800
C	-0.10613300	2.67831200	0.19606800
C	-1.14100300	2.09324800	1.09592400
H	-0.47628000	3.36603900	-0.56092700
H	0.81034500	3.02566300	0.67208300
C	-2.56561300	2.54906000	0.85653300

H	-0.85642000	2.17579000	2.14915500
H	-1.14416400	0.91970900	0.98203000
C	-3.24386200	2.25050100	-0.33112300
C	-3.19895500	3.33853900	1.82464400
C	-4.52895900	2.74671800	-0.55266200
H	-2.77529100	1.61600900	-1.07989400
C	-4.48515400	3.83405400	1.60281900
H	-2.68224900	3.57656300	2.75148000
C	-5.15184400	3.54175000	0.41197900
H	-5.04578300	2.50523000	-1.47699500
H	-4.96272500	4.44910100	2.36008800
H	-6.15211800	3.92757700	0.23796000

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Ni	0.57475600	-0.38502900	-0.03897200
H	2.32578700	-0.69929500	-0.37333200
C	1.04990000	-1.52678500	1.96085600
C	0.63298500	-2.37522200	0.98590300
H	0.32887200	-1.06464700	2.63237800
H	-0.41125600	-2.63602300	0.86628200
C	-1.22025800	0.29003900	0.01928200
N	-2.38198500	-0.40411500	-0.18743500
N	-1.63421600	1.57173100	0.27049100
C	-3.48881100	0.42864100	-0.06844300
C	-2.52464400	-1.81875400	-0.47364000
C	-3.02119200	1.66257300	0.22995000
C	-0.80659400	2.72930800	0.55505600
H	-4.49238100	0.05948200	-0.20480500
C	-2.31835800	-2.27107300	-1.79346800
C	-2.94018400	-2.67426300	0.57259200
H	-3.53357500	2.59201800	0.41750200
C	-0.30883400	2.90136800	1.86498800
C	-0.60584700	3.68167000	-0.46936500
C	-2.48622800	-3.64109300	-2.03560700
C	-2.01698800	-1.32803100	-2.95520000
C	-3.09846200	-4.03190500	0.26547600
C	-3.26333400	-2.17688200	1.98229300
C	0.46652400	4.04154100	2.11340800
C	-0.67409500	1.96065700	3.01149000
C	0.16925900	4.80605400	-0.15585400
C	-1.24166900	3.56747500	-1.85562500
C	-2.86389600	-4.51410100	-1.01955100
H	-2.33683900	-4.02659300	-3.03897300
C	-3.29235200	-1.08580500	-3.79113300

C	-0.86826400	-1.82764800	-3.85047900
H	-1.70978100	-0.36287700	-2.54121600
H	-3.41486300	-4.72027000	1.04271900
C	-2.58464100	-3.00856500	3.08857800
C	-4.79033900	-2.14498900	2.20986300
H	-2.89425900	-1.14976100	2.07793900
C	0.71055700	4.98027800	1.11429100
H	0.86851800	4.20926200	3.10696100
C	-1.91764100	2.49048400	3.75933800
C	0.48006200	1.72448300	4.00166700
H	-0.94037800	0.98878100	2.58247100
H	0.34620600	5.55951500	-0.91660800
C	-0.25919000	3.86341800	-3.00569900
C	-2.46591700	4.50335200	-1.96656100
H	-1.59585100	2.53923700	-1.98701600
H	-2.99240700	-5.57127200	-1.23321700
H	-4.10135600	-0.67015600	-3.18034100
H	-3.08731200	-0.38255700	-4.60634200
H	-3.65582000	-2.01920600	-4.23541400
H	0.03820200	-2.02848900	-3.26866700
H	-1.13200500	-2.74729400	-4.38339000
H	-0.63000400	-1.07373900	-4.60926600
H	-1.49891700	-3.06080000	2.95713900
H	-2.78734200	-2.55874400	4.06690300
H	-2.96561500	-4.03477400	3.12058400
H	-5.30315900	-1.52341800	1.46817900
H	-5.21608900	-3.15266500	2.14683000
H	-5.01987500	-1.74440100	3.20352600
H	1.30918000	5.86009500	1.33231700
H	-2.77833200	2.59460100	3.09032100
H	-2.19957100	1.80709400	4.56859600
H	-1.71625200	3.47278300	4.20127400
H	1.40022500	1.42104900	3.49002700
H	0.70691000	2.61998600	4.58975800
H	0.20579400	0.93862000	4.71456900
H	0.63472800	3.23391400	-2.95640300
H	-0.75033500	3.67759200	-3.96713500
H	0.06557000	4.90937300	-3.00735500
H	-3.21672300	4.29515300	-1.19717100
H	-2.16555300	5.55165100	-1.85892300
H	-2.94558000	4.38950500	-2.94508800
C	2.49637500	-1.33777400	2.34010800
H	2.64494700	-1.81678800	3.32527700
H	2.72952700	-0.26726900	2.48021400

C	4.70860500	-1.99967700	1.74355100
H	5.08618000	-0.97782200	1.92231800
H	4.80755100	-2.56244300	2.68329700
C	5.46579700	-2.66493900	0.63447800
C	6.26466900	-3.71609300	0.81779200
H	5.33756400	-2.22625300	-0.35443800
H	6.82393300	-4.15463900	-0.00359900
H	6.40075000	-4.17346700	1.79580800
O	3.32489400	-1.92088300	1.36718200
H	1.36069400	-2.93817700	0.40779400
C	2.43309400	0.02453800	-1.26454700
C	1.11475800	0.68476100	-1.50088100
H	1.04815400	1.74604000	-1.28112000
H	0.59470000	0.41520600	-2.42157100
C	3.68525200	0.89326800	-0.86416100
C	4.71541800	0.45576600	-1.92843700
H	4.64843100	1.10650800	-2.81647500
H	5.74656900	0.45898500	-1.56837500
O	4.37493200	-0.88305900	-2.27305400
C	2.96722800	-0.88969900	-2.40751500
H	2.66768800	-0.47042800	-3.38132200
H	2.62197800	-1.92459800	-2.34643700
C	3.49107900	2.40710500	-0.80054200
H	4.44178100	2.89300300	-0.55221200
H	3.15416700	2.81399500	-1.76090000
H	2.76596700	2.70000800	-0.03381500
H	4.03952900	0.54355500	0.11122800

TS-S9

Ni	0.41942300	-0.59590400	-0.12199900
C	1.92083800	-0.62959500	-1.77852100
C	0.88443100	0.31328100	-1.85847200
H	1.72257500	-1.40328500	-0.35977200
H	1.08815600	1.35216100	-1.62536700
H	0.04376400	0.13089000	-2.52299200
C	0.05848300	-1.77079600	1.49197600
C	1.30302200	-2.23491400	1.04976300
H	-0.84181700	-2.31080500	1.22218700
H	-0.00030800	-1.14313000	2.37766100
H	1.33718900	-3.14673900	0.45288000
C	2.55141600	-1.98228500	1.86614700
H	2.53268800	-0.97213200	2.30516400
H	2.53448700	-2.70039700	2.70533400
O	3.69991900	-2.18543400	1.07908300

C	4.91014900	-2.20220900	1.84527900
H	5.09960700	-1.21012900	2.28409200
H	4.79311000	-2.91812200	2.67652000
C	6.04272900	-2.62046700	0.95748500
C	7.15531800	-1.90586600	0.78364700
H	5.92198200	-3.58534800	0.46678100
H	7.97262000	-2.26386500	0.16419500
H	7.30030900	-0.94314400	1.26988700
C	-1.19014600	0.46619200	0.13311900
N	-2.49782300	0.06002200	0.09391200
N	-1.26579000	1.81085800	0.38513100
C	-3.36060500	1.13012300	0.31132200
C	-2.99610200	-1.28353500	-0.13766300
C	-2.58931000	2.22365500	0.50554000
C	-0.15819900	2.73953200	0.51431100
H	-4.43113200	1.00591500	0.30486800
C	-3.10623400	-1.74680000	-1.46599200
C	-3.43193900	-2.04351500	0.97252300
H	-2.84717800	3.24839600	0.71685300
C	0.52476300	2.81258500	1.74793900
C	0.14131400	3.59052500	-0.57443100
C	-3.60164400	-3.04343500	-1.65716400
C	-2.81162700	-0.86202300	-2.67467600
C	-3.92346300	-3.33016700	0.71628300
C	-3.45209700	-1.49774700	2.40124000
C	1.58485300	3.72356000	1.84403700
C	0.07732800	2.02642200	2.97869000
C	1.21004300	4.48318800	-0.41531300
C	-0.68660000	3.62747800	-1.86051500
C	-3.99515100	-3.83219200	-0.58028900
H	-3.69862400	-3.43412900	-2.66485100
C	-4.12508700	-0.27664400	-3.23833500
C	-2.03021400	-1.58925200	-3.78421400
H	-2.19904500	-0.01985200	-2.33860600
H	-4.26302100	-3.94510400	1.54339700
C	-2.93908700	-2.50217700	3.45165400
C	-4.87713700	-1.03726100	2.78181200
H	-2.79840500	-0.61914200	2.44108500
C	1.93322000	4.54126200	0.77253400
H	2.13500900	3.80828400	2.77529800
C	-0.90194100	2.87193300	3.82290400
C	1.24564000	1.53856200	3.85315300
H	-0.46703100	1.14099400	2.63594800
H	1.47255400	5.15060100	-1.22968100

C	0.16441400	3.71310300	-3.14284700
C	-1.67875000	4.81207000	-1.82668000
H	-1.27361600	2.70384900	-1.91693400
H	-4.37865300	-4.83361400	-0.75327300
H	-4.66600800	0.30278900	-2.48232600
H	-3.91637500	0.38484200	-4.08692300
H	-4.79090800	-1.07374700	-3.58777400
H	-1.11752100	-2.05732900	-3.39903800
H	-2.62846400	-2.37327000	-4.26011200
H	-1.74804300	-0.88030000	-4.57077800
H	-1.94452400	-2.88809900	3.20662400
H	-2.88145300	-2.01439800	4.43093200
H	-3.61237300	-3.35905800	3.56001800
H	-5.26475100	-0.28035300	2.09246300
H	-5.57409800	-1.88271500	2.77036200
H	-4.88303300	-0.60922900	3.79048800
H	2.75717500	5.24221200	0.87146500
H	-1.78546300	3.16466600	3.24602400
H	-1.24197500	2.30503700	4.69714300
H	-0.41697600	3.78704400	4.18081200
H	2.00014300	1.00593700	3.26363500
H	1.74767500	2.36522900	4.36704400
H	0.87358100	0.86069500	4.62947300
H	0.91418200	2.91795400	-3.20044700
H	-0.48458900	3.62867900	-4.02129300
H	0.68691500	4.67227600	-3.22213100
H	-2.34635600	4.76964000	-0.96035300
H	-1.14152000	5.76608400	-1.78269400
H	-2.29888900	4.81575600	-2.73003600
C	3.41257500	-0.29446300	-1.53387000
C	4.11072400	-1.50822200	-2.20788100
H	4.44365700	-1.23981500	-3.22386500
H	4.96212600	-1.87870600	-1.63641800
O	3.14050400	-2.55352200	-2.27840900
C	1.92556100	-1.92079800	-2.60574800
H	1.89112000	-1.64669700	-3.67578800
H	1.09836700	-2.60386000	-2.39823700
C	3.85228600	1.05536000	-2.11030900
H	4.93766600	1.16774900	-2.00844800
H	3.60570000	1.13940200	-3.17512200
H	3.38610100	1.89415200	-1.58256100
H	3.63910500	-0.32073500	-0.46618700

int-S10

Ni	0.33475300	-0.55276200	-0.12532000
C	2.18742700	-0.23720600	-2.08096600
C	1.09592700	0.55522400	-1.94074900
H	1.74617200	-1.67414300	-0.10951800
H	1.17182200	1.51912500	-1.44699200
H	0.19933900	0.37250100	-2.52915800
C	0.10555700	-1.74963200	1.32150700
C	1.41935000	-2.26609900	0.83135100
H	-0.75341300	-2.39864700	1.17062600
H	0.10568100	-1.26309600	2.29792200
H	1.36071600	-3.27925900	0.42037400
C	2.60001200	-2.12044600	1.79031700
H	2.57811100	-1.12847500	2.27142700
H	2.50991600	-2.87607400	2.58727200
O	3.79164900	-2.29837200	1.05815100
C	4.96410800	-2.34685500	1.87588300
H	5.11386400	-1.38457600	2.39076800
H	4.82825900	-3.12126400	2.64986900
C	6.14134200	-2.67854200	1.00902100
C	7.24731100	-1.93668500	0.93684500
H	6.05689800	-3.60260800	0.43867900
H	8.09502100	-2.23342400	0.32585800
H	7.35627200	-1.01370100	1.50304000
C	-1.27648700	0.42480700	0.14822000
N	-2.56428300	-0.03247800	0.08579900
N	-1.40169800	1.75146100	0.46518000
C	-3.46762700	0.99126700	0.34931900
C	-3.00386600	-1.37970800	-0.22668700
C	-2.74016600	2.10495500	0.59846200
C	-0.32590900	2.70839400	0.64548900
H	-4.53247800	0.82557800	0.33202400
C	-3.06247500	-1.77574700	-1.57931500
C	-3.43233500	-2.21202000	0.83195600
H	-3.03928700	3.10758300	0.85638100
C	0.35474800	2.73553200	1.88222100
C	-0.05309900	3.62334000	-0.39755800
C	-3.51566200	-3.07339300	-1.85113100
C	-2.74482400	-0.82866700	-2.73361800
C	-3.88074300	-3.49565400	0.49598200
C	-3.48094500	-1.75039900	2.28899500
C	1.38524400	3.67355200	2.02775500
C	-0.06440800	1.86939200	3.06814500
C	0.98562200	4.54082600	-0.18870600
C	-0.87846800	3.69708100	-1.68359800

C	-3.91297500	-3.92794900	-0.82718000
H	-3.57492200	-3.41320300	-2.88025700
C	-4.04833000	-0.29942500	-3.36955800
C	-1.84253900	-1.46878900	-3.80443100
H	-2.20762200	0.03504800	-2.32873200
H	-4.21626000	-4.16505800	1.28156300
C	-2.92318200	-2.79252500	3.27816200
C	-4.92453700	-1.37471200	2.69099000
H	-2.86447400	-0.84945900	2.38281800
C	1.70626000	4.55869000	1.00224300
H	1.93279200	3.72496700	2.96295200
C	-1.04316400	2.64918200	3.97368000
C	1.12425000	1.34559200	3.89299800
H	-0.60029500	0.99774100	2.68074600
H	1.22666600	5.25842000	-0.96612500
C	-0.02772600	3.88416000	-2.95525300
C	-1.91665900	4.83816600	-1.59182300
H	-1.42770700	2.75498000	-1.79322700
H	-4.26474600	-4.92848000	-1.06179200
H	-4.67486700	0.21557200	-2.63324000
H	-3.82177600	0.40715400	-4.17619400
H	-4.63883400	-1.11840200	-3.79531800
H	-0.93070300	-1.88863700	-3.36488700
H	-2.35124700	-2.27610800	-4.34185200
H	-1.55366800	-0.71937500	-4.55025300
H	-1.91073200	-3.11264800	3.01263100
H	-2.88997900	-2.36406200	4.28593200
H	-3.55464700	-3.68583800	3.32962700
H	-5.34315200	-0.59449300	2.04678100
H	-5.58560600	-2.24619600	2.62589300
H	-4.95022300	-1.00874100	3.72350900
H	2.50638200	5.28037100	1.14023500
H	-1.93664300	2.96555000	3.42486000
H	-1.36686000	2.02495700	4.81442200
H	-0.56634700	3.54693700	4.38298600
H	1.86623500	0.84425200	3.26150800
H	1.63488300	2.14810100	4.43606400
H	0.77120600	0.62813800	4.64208400
H	0.75369500	3.12402700	-3.04969200
H	-0.67051600	3.81970300	-3.83996000
H	0.45504800	4.86682400	-2.98217400
H	-2.58395700	4.72428500	-0.73176700
H	-1.41725400	5.80875400	-1.49553200
H	-2.53415600	4.86507100	-2.49652600

C	3.58601700	-0.00009600	-1.52557900
C	4.39736900	-1.09814500	-2.25485400
H	4.82390700	-0.70624100	-3.19323100
H	5.19598100	-1.51846200	-1.64243300
O	3.46121800	-2.13857800	-2.53331900
C	2.26794600	-1.49368600	-2.92986600
H	2.30530400	-1.19866600	-3.99527900
H	1.42905400	-2.18340300	-2.80120000
C	4.11862500	1.42529700	-1.71315900
H	5.15030100	1.49226400	-1.35114800
H	4.11212900	1.71570500	-2.76969200
H	3.52421900	2.15592600	-1.15442700
H	3.59238400	-0.25120200	-0.45784100

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Ni	0.20574400	-0.65351800	-0.71653300
H	0.92361900	-1.66991600	-1.65399900
C	-0.18543100	-2.39249800	0.40285100
C	0.16177400	-2.82119400	-0.88187700
H	-1.23449100	-2.28334800	0.65010800
H	-0.62089200	-3.00741900	-1.61468200
C	-0.82504100	0.63002600	0.31256200
N	-2.18305400	0.57474700	0.50678500
N	-0.45579800	1.80253200	0.92204600
C	-2.63836200	1.68340200	1.21138500
C	-3.09541900	-0.45030400	0.03701800
C	-1.55456000	2.44491800	1.48304600
C	0.86840700	2.39392800	0.99472400
H	-3.68150900	1.81978600	1.44505000
C	-3.49911600	-0.43279200	-1.31566400
C	-3.61301000	-1.37590300	0.97297500
H	-1.45421100	3.37528300	2.01762700
C	1.73338100	1.99779000	2.03576100
C	1.20056900	3.41946400	0.07834600
C	-4.40220100	-1.42013000	-1.73171500
C	-3.07553300	0.66288500	-2.29143500
C	-4.51733900	-2.33427700	0.49713900
C	-3.27524600	-1.33461700	2.46445900
C	2.99641500	2.60329000	2.09031600
C	1.30510600	1.03766700	3.14234900
C	2.47584700	3.98847000	0.18573800
C	0.21427000	3.96788800	-0.95421000
C	-4.90056300	-2.36603400	-0.84065600
H	-4.73631600	-1.43585900	-2.76409300

C	-4.19254800	1.72110500	-2.42115500
C	-2.68354200	0.11841200	-3.67667100
H	-2.19462700	1.16420500	-1.88052200
H	-4.93344100	-3.06212800	1.18636500
C	-2.94889900	-2.72052200	3.05591800
C	-4.43009800	-0.69317400	3.26532500
H	-2.38788600	-0.70549000	2.59723400
C	3.37090800	3.57704900	1.16993900
H	3.68933100	2.32315700	2.87684900
C	0.86397700	1.83217600	4.39126600
C	2.39481700	0.01600300	3.50911200
H	0.43499300	0.47485700	2.78778500
H	2.76836600	4.77289500	-0.50432900
C	0.85067500	4.24227100	-2.33094000
C	-0.45029100	5.26166800	-0.43158900
H	-0.57678800	3.22344400	-1.09965400
H	-5.60376700	-3.11865800	-1.18552600
H	-4.44062400	2.16497300	-1.45088800
H	-3.87955400	2.52844500	-3.09305600
H	-5.10774200	1.27805300	-2.82986900
H	-1.92031100	-0.66419300	-3.59921300
H	-3.53986400	-0.30470600	-4.21229700
H	-2.28407700	0.92728400	-4.29900200
H	-2.16299700	-3.23806600	2.49591600
H	-2.60999000	-2.60989900	4.09177100
H	-3.82700300	-3.37472100	3.07339800
H	-4.66548400	0.31670800	2.91439300
H	-5.34254700	-1.29348900	3.17808200
H	-4.16896400	-0.62878400	4.32751600
H	4.35409000	4.03458500	1.23382000
H	0.04676500	2.52493900	4.16297000
H	0.51977700	1.15007700	5.17705400
H	1.69602800	2.41975200	4.79545500
H	2.71744100	-0.55012900	2.63023900
H	3.27411100	0.49391500	3.95376300
H	2.00756900	-0.68943300	4.25365100
H	1.38601800	3.37187800	-2.72268900
H	0.07019500	4.51348300	-3.05033400
H	1.55562500	5.07977000	-2.29427700
H	-0.97528900	5.10362500	0.51551800
H	0.29949900	6.04393800	-0.26856400
H	-1.17724700	5.63782900	-1.16017400
C	0.76108900	-2.61641100	1.55772700
H	0.54981900	-3.61480800	1.97978600

H	0.58943300	-1.88745400	2.36175200
C	3.01666700	-3.35418700	1.86210700
H	2.95076700	-3.06605200	2.92309800
H	2.74118300	-4.41630000	1.78292400
C	4.40455900	-3.12409400	1.34536600
C	5.18062400	-4.08695800	0.84610600
H	4.77649500	-2.10276300	1.42121900
H	6.19547500	-3.88828900	0.51334000
H	4.83770400	-5.11662600	0.76841700
O	2.09981300	-2.55845000	1.09560900
H	1.08684000	-3.37500300	-1.02515100
C	1.61926900	-0.53581600	-2.44585600
C	1.00630100	0.66034800	-2.03007900
H	1.56806200	1.37283600	-1.43761000
H	0.18916700	1.07233600	-2.61864200
C	3.06988500	-0.94497200	-2.09579600
C	3.35506100	-2.03502700	-3.16855300
H	3.97920700	-1.62181100	-3.97622100
H	3.84461300	-2.92412600	-2.76631900
O	2.08684800	-2.43719700	-3.69617100
C	1.31409700	-1.25498900	-3.76460000
H	1.63967400	-0.61274600	-4.60163100
H	0.26661100	-1.52177300	-3.91859400
C	4.07021400	0.21669300	-2.14190000
H	5.08850300	-0.16082400	-1.99514500
H	4.04091100	0.73334100	-3.10815800
H	3.87504700	0.95124400	-1.35378400
H	3.10023200	-1.39442400	-1.09807800

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Ni	0.14793900	-0.82364500	-0.46115400
H	0.63078700	-2.56647900	-1.05330100
C	-0.43714800	-2.11410100	0.80536400
C	-0.04191600	-3.06804900	-0.28905300
H	-1.50112500	-2.07821600	1.02196200
H	-0.88859800	-3.46303100	-0.85370200
C	-0.86321100	0.69193100	0.11252700
N	-2.23330300	0.74820800	0.16380200
N	-0.46759800	1.96622300	0.43558400
C	-2.67109500	2.02215900	0.50196500
C	-3.17341000	-0.32152800	-0.11148400
C	-1.56607400	2.78102500	0.68399300
C	0.88572100	2.48368500	0.53609400
H	-3.71960100	2.26085100	0.57524500

C	-3.46340200	-0.64565100	-1.45291900
C	-3.82664400	-0.93962500	0.97959000
H	-1.45184900	3.81358700	0.96999500
C	1.58159100	2.31480800	1.75161300
C	1.41054000	3.22919000	-0.54601200
C	-4.40172700	-1.66138200	-1.68200300
C	-2.86721200	0.10362200	-2.64181100
C	-4.75974900	-1.94178600	0.68625900
C	-3.59261700	-0.53003500	2.43439700
C	2.87619400	2.84505100	1.83122800
C	0.93999900	1.68840100	2.98707300
C	2.70919000	3.73586300	-0.40452800
C	0.60211000	3.56266100	-1.80140400
C	-5.03922200	-2.30800400	-0.62784500
H	-4.65111100	-1.93531500	-2.70251800
C	-3.93417300	0.99416000	-3.31265600
C	-2.21986200	-0.84495000	-3.66772400
H	-2.07861600	0.76579300	-2.27133200
H	-5.28003000	-2.43844900	1.49901400
C	-3.37108200	-1.73176800	3.37424400
C	-4.76686800	0.32717600	2.95529500
H	-2.68686800	0.08513000	2.47524200
C	3.44090900	3.53514900	0.76292400
H	3.44305900	2.73326000	2.74951900
C	0.40400400	2.79393200	3.92311800
C	1.89110400	0.75101800	3.75024800
H	0.08442500	1.08811300	2.66015800
H	3.14894500	4.30700800	-1.21527700
C	1.42350800	3.49339000	-3.10415200
C	-0.03102500	4.96769800	-1.67977900
H	-0.21358100	2.83498500	-1.88544500
H	-5.76777800	-3.08777300	-0.83038700
H	-4.36416300	1.70725700	-2.60087600
H	-3.49283200	1.56297000	-4.13898600
H	-4.75524100	0.39378100	-3.71988200
H	-1.45580600	-1.47434700	-3.19655700
H	-2.95518900	-1.50856200	-4.13514500
H	-1.74645700	-0.26817100	-4.47087600
H	-2.56214600	-2.38360900	3.02814400
H	-3.11267500	-1.37475000	4.37725300
H	-4.27266300	-2.34555700	3.47291600
H	-4.92438100	1.22380000	2.34674400
H	-5.70098900	-0.24567000	2.94685800
H	-4.57797800	0.64784100	3.98585800

H	4.44520500	3.94020900	0.84899300
H	-0.32393600	3.43796100	3.41791900
H	-0.08670800	2.35045000	4.79705400
H	1.22057600	3.43082800	4.28168000
H	2.29489500	-0.01963900	3.08774500
H	2.72848300	1.29316400	4.20242800
H	1.35203600	0.25950400	4.56830800
H	1.95457700	2.54315600	-3.21386500
H	0.75700300	3.61242600	-3.96541600
H	2.16313300	4.29929300	-3.16049800
H	-0.68008400	5.05853000	-0.80378200
H	0.74712700	5.73481500	-1.59742500
H	-0.63241100	5.19152100	-2.56799400
C	0.41489700	-2.18587700	2.05197500
H	0.20484200	-3.14077500	2.56761100
H	0.16961700	-1.37825900	2.75583800
C	2.65975900	-2.81081700	2.60682200
H	2.49945000	-2.41073900	3.62079400
H	2.41874000	-3.88419600	2.62848500
C	4.08239900	-2.59527000	2.18634300
C	4.92985400	-3.58344800	1.89447600
H	4.41792500	-1.55891700	2.15914500
H	5.96721900	-3.38979600	1.63613900
H	4.62483900	-4.62745100	1.92556300
O	1.79065700	-2.13557500	1.68727500
H	0.61718600	-3.87318600	0.05228600
C	2.11413800	-1.04662700	-2.33712600
C	1.38879200	0.08401400	-2.17223700
H	1.73765700	0.87349700	-1.51353200
H	0.57687900	0.32969700	-2.85361400
C	3.34927800	-1.47320200	-1.55508000
C	3.73364000	-2.79066300	-2.27153700
H	4.48415300	-2.60214600	-3.05628000
H	4.11237300	-3.55962600	-1.59592400
O	2.52250400	-3.27484100	-2.85697900
C	1.86754500	-2.12740700	-3.37141400
H	2.31673000	-1.81210200	-4.33149200
H	0.81568900	-2.36288100	-3.55187700
C	4.46895200	-0.42545500	-1.50473400
H	5.33703500	-0.82837400	-0.97169000
H	4.79272900	-0.14017600	-2.51193700
H	4.14769200	0.47986700	-0.97956300
H	3.04442600	-1.71244800	-0.52777900