

Supporting Information

Investigation of the Activation Mode of Vinylarene in Giri's Ni-catalyzed Vinylarene Intermolecular 1,2-Alkylarylation Cross-coupling: A Theoretical Study

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1. The calculated structure and free energy for Ni(0)-catalysts.

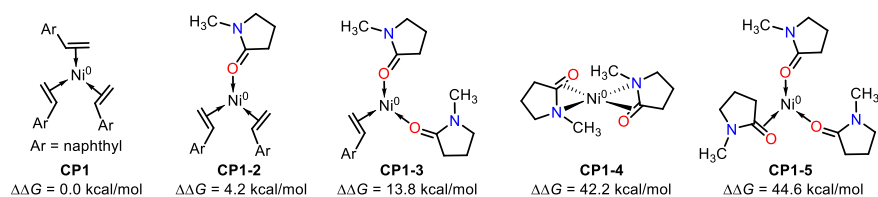


Figure S1. The calculated structure and free energy for Ni(0)-catalysts.

The calculated structure and free energy for other Ni(0)-catalysts, which is stabilized by solvent or olefin, are shown in **Figure S1**. The calculated results shown that the three olefin stabilized Ni(0)-catalyst **CP1** has the lowest free energy compared to the other Ni(0)-catalysts. So, in our theoretical study, **CP1** was set to be the active catalyst for the mechanistic study, and its free energy was set to be the baseline for the catalytic cycle.

2. The calculated free energy profiles of S_N2 type C-I bond activation of cyclohexyl iodide.

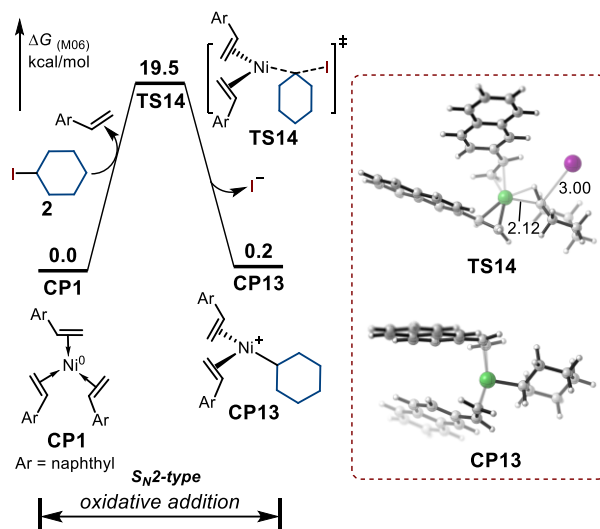


Figure S2. Free energy profiles and structural information of S_N2 type C-I bond activation of cyclohexyl iodide.

The calculated free energy profiles and structural information of S_N2 type C-I bond activation of cyclohexyl iodide are shown in Figure S2. As shown in Figure S2, the S_N2 type C-I bond oxidation addition onto Ni(0) center occurs via **TS14** with an activation barrier of 19.5 kcal/mol, which is 0.8 kcal/mol higher than that of SET transition state **TS1**. The calculated results indicated that the S_N2 type C-I bond activation of cyclohexyl iodide pathway is unfavorable.

3. The free energy profiles and structural information of concerted alkene-coupled radical transfer pathway from CP2.

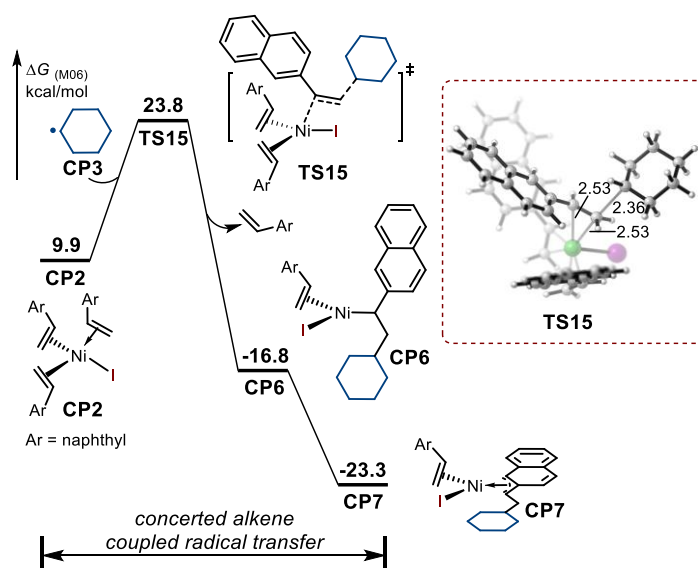


Figure S3. Free energy profiles and structural information of concerted alkene-coupled radical transfer pathway from CP2.

The concerted alkene-coupled radical transfer process from cyclohexyl radical, vinylarene, and **CP2** has also been calculated. As shown in Figure S3, the concerted alkene-coupled radical transfer process need overcome activation barrier of 13.9 kcal/mol to give alkyl-Ni(II) intermediate **CP6**. The calculated results also showed that the pathway was unfavorable due to the high free energy of **TS15**.

4. The calculated free energy profiles for Paths I and II using *t*BuI as electrophile.

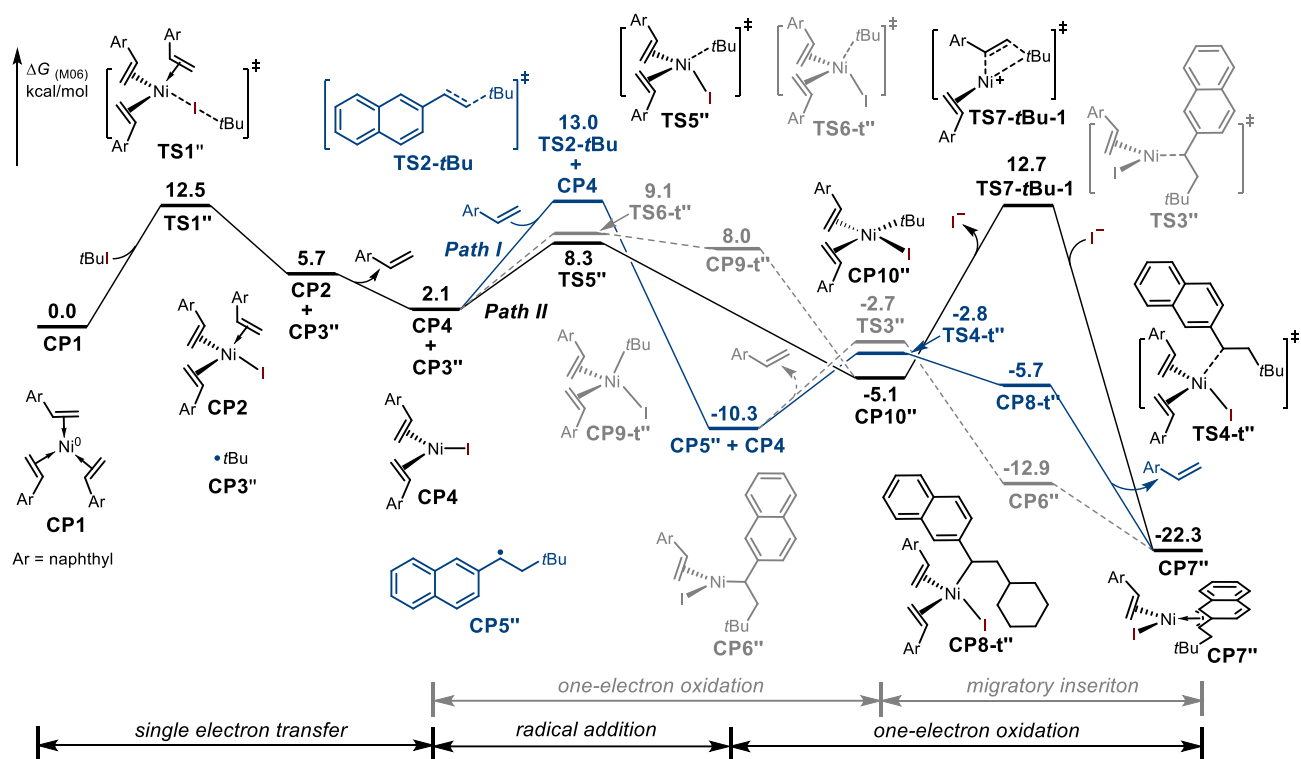


Figure S4. Free energy profiles and structural information for Paths I and II using *t*BuI as electrophile.

The whole free energy profiles for this 1,2-alkylarylation cross-coupling using *tert*-butyl iodide as electrophile are shown in Figure S4. As shown in Figure S4, when using NiBr₂ as catalyst, the energies of the **TS2''** and **TS7''** are similar, which indicated that Path I and Path II may occur simultaneously. So, in this case, there would be more side reactions occur, which led to low yields.

5. The free energy profiles and structural information of concerted alkene-coupled radical transfer pathway from **CP2'**.

As shown in Figure S5, the concerted alkene-coupled radical transfer process from cyclohexyl radical, vinylarene, and **CP2'** occurred via transition state **TS15'** yielding alkyl-Ni(II) intermediate **CP6'**. In **TS15'**, the bond lengths of forming C-C and C-Ni were 2.31 and 2.16 Å, respectively. The coordination of the C=C bond of naphthol onto the Ni(II) center in **CP6'** generated the allyl-Ni(II) intermediate **CP7'**. The free energy of **TS15'** is 7.4 kcal/mol higher than that of **TS2**. The calculated results showed that the pathway was unfavorable due to the high free energy of **TS15'**.

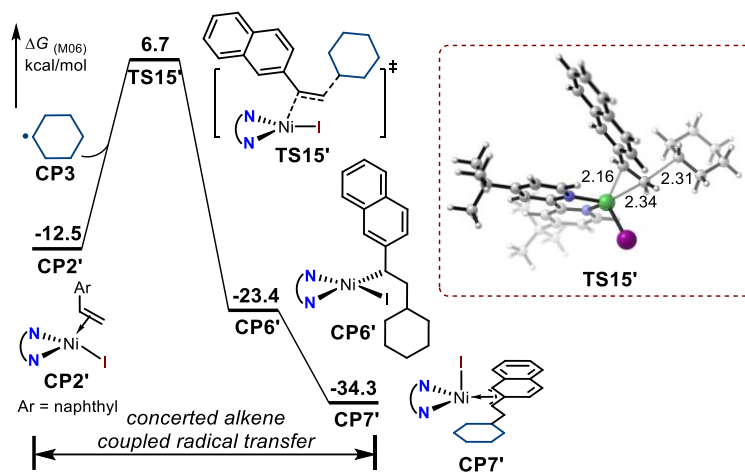


Figure S5. Free energy profiles and structural information of concerted alkene-coupled radical transfer pathway from **CP2'**.

6. The calculated free energy for the triplet migratory insertion of vinylarene from **CP9'-t**.

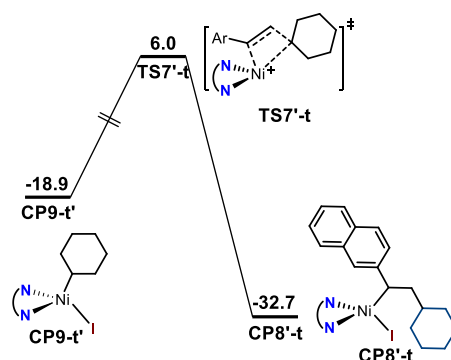


Figure S6. The calculated free energy for the triplet migratory insertion of vinylarene.

The calculated free energy for the triplet migratory insertion of vinylarene from **CP9'-t** is shown in **Figure S6**. The free energy of transition state **TS7'-t** is 6.7 kcal/mol higher than that of **TS2**, which indicated that the triplet migratory insertion of vinylarene from **CP9'-t** process is also unfavorable.

7. Complete reference for Gaussian 16

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S.

Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

8. B3-LYP and M06-L absolute calculation energies, enthalpies, and free energies.

Table S1. B3-LYP and M06-L absolute calculation energies, enthalpies, and free energies.

Geometry	$E_{(\text{elec-B3-LYP})}^1$	$H_{(\text{corr-B3-LYP})}^2$	$G_{(\text{corr-B3-LYP})}^3$	$E_{(\text{solv-M06-L})}^4$	IF ⁵
CP1	-1559.224330	0.579407	0.480364	-1559.489121	-
2	-246.662222	0.169310	0.128140	-246.682089	-
TS1	-1805.855227	0.748566	0.623145	-1806.156076	-117.7
CP2	-1570.651486	0.583447	0.474036	-1570.906955	-
CP3	-235.209762	0.163298	0.126560	-235.240515	-
CP4	-1107.369403	0.390022	0.304944	-1107.541254	-
naphthyl	-463.283461	0.190989	0.146060	-463.348451	-
TS2	-698.487899	0.355741	0.291656	-698.589238	-230.4
CP5	-698.543045	0.359213	0.298374	-698.641934	-
TS3	-1342.618856	0.557144	0.456357	-1342.821285	-28.9
CP6	-1342.631877	0.559778	0.462050	-1342.849102	-
CP7	-1342.641906	0.559815	0.465036	-1342.862419	-
TS4-t	-1805.909232	0.751053	0.627958	-1806.195370	-118.0
CP8-t	-1805.915627	0.752044	0.622222	-1806.195829	-
TS5	-1342.577259	0.554948	0.454690	-1342.793767	-36.3
TS6-t	-1342.577247	0.554769	0.452591	-1342.792385	-45.1
CP9-t	-1342.589902	0.556806	0.452850	-1342.799573	-
CP10	-1342.593864	0.557900	0.461136	-1342.825804	-
TS7	-1330.954567	0.554724	0.466750	-1331.235202	-172.3
I	-11.474445	0.002360	-0.016848	-11.556306	-
PhZnI	-308.664966	0.099707	0.053276	-308.267025	-
TS8	-1651.305798	0.660491	0.540088	-1651.136103	-59.9
CP11	-1562.834368	0.652135	0.549881	-1563.095491	-

ZnI ₂	-88.469679	0.007284	-0.029984	-88.046873	-
TS9	-1562.814009	0.650713	0.552558	-1563.084068	-271.6
3	-930.229276	0.458668	0.386452	-930.363677	-
TS10	-1342.553182	0.556144	0.460998	-1342.786036	-176.5
TS11	-1342.575381	0.555091	0.452582	-1342.781989	-224.6
TS2-<i>t</i>Bu	-621.073362	0.316764	0.254696	-621.167034	-309.9
TS7-<i>t</i>Bu-1	-1253.529420	0.515691	0.430282	-1253.803927	-206.6
TS7-<i>t</i>Bu-2	-1826.546957	0.616293	0.514234	-1826.859062	-215.4
TS12	-1651.257540	0.659011	0.536481	-1651.089415	-28.4
CP12	-1562.781510	0.650206	0.545572	-1563.046550	-
TS13	-1562.756620	0.647873	0.547196	-1563.028550	-254.9
4	-466.921530	0.263551	0.216119	-466.986230	-
CP1'	-1789.137524	0.813963	0.695209	-1789.444043	-
bipyridyl	-809.873859	0.404941	0.335919	-810.003492	-
TS1'	-1689.193402	0.768924	0.643910	-1689.463988	-150.3
CP2'	-1454.002165	0.604326	0.497365	-1454.240984	-
TS3'	-1689.250184	0.771843	0.649073	-1689.516798	-66.1
CP6'	-1689.257124	0.774675	0.656562	-1689.531394	-
CP7'	-1689.258116	0.774800	0.656383	-1689.548537	-
TS4'-<i>t</i>	-1689.252633	0.771887	0.647769	-1689.520683	-53.7
CP8'-<i>t</i>	-1689.269582	0.773589	0.650873	-1689.540578	-
CP4'	-990.707461	0.411707	0.329713	-990.858073	-
TS5'	-1225.918097	0.576084	0.471652	-1226.107954	-31.6
TS6'-<i>t</i>	-1225.918532	0.575912	0.470282	-1226.108160	-106.4
CP9'-<i>t</i>	-1225.946495	0.578203	0.478558	-1226.143851	-
CP10'	-1225.942401	0.579533	0.485540	-1226.144994	-
TS7'	-1677.589745	0.770352	0.660658	-1677.909407	-269.6
TS12'	-1534.612609	0.680385	0.562385	-1534.429065	-70.9
CP12'	-1446.131547	0.671896	0.569972	-1446.376887	-
TS13'	-1446.083783	0.669529	0.570265	-1446.337496	-288.5

CP1-2	-1421.880592	0.535355	0.440079	-1422.131863	-
CP1-3	-1284.527497	0.491997	0.399823	-1284.765886	-
CP1-4	-821.181961	0.298438	0.236039	-821.354451	-
CP1-5	-1147.150463	0.448226	0.362437	-1147.369003	-
TS14	-1342.549463	0.554956	0.458508	-1342.787614	-176.6
CP13	-1330.975440	0.555226	0.464095	-1331.250938	-
TS15	-1805.853020	0.748650	0.620697	-1806.142004	-296.7
<i>t</i> BuI	-169.240784	0.130116	0.090766	-169.251377	-
TS1''	-1728.440175	0.709621	0.584859	-1728.734380	-159.3
CP3''	-157.795396	0.124605	0.087764	-157.815114	-
CP5''	-621.120698	0.320115	0.261149	-621.210700	-
TS3''	-1265.196352	0.518062	0.419288	-1265.390695	-32.4
CP6''	-1265.206701	0.519759	0.428371	-1265.416011	-
CP7''	-1265.218112	0.520636	0.427442	-1265.429995	-
TS4-t''	-1728.485483	0.711646	0.589388	-1728.763254	-133.4
CP8-t''	-1728.491442	0.712995	0.585995	-1728.764501	-
TS5''	-1265.162372	0.516319	0.417541	-1265.371298	-25.6
TS6-t''	-1265.162256	0.516185	0.415317	-1265.367727	-61.7
CP9-t''	-1265.170045	0.517799	0.415552	-1265.369728	-
CP10''	-801.888260	0.325093	0.253142	-802.025851	-
TS15'	-1689.197652	0.769320	0.643414	-1689.470412	-481.9
TS7'-t	-1689.175469	0.770242	0.648237	-1689.453633	-303.8

¹The electronic energy calculated by B3-LYP. ²The thermal correction to enthalpy calculated by B3-LYP. ³The thermal correction to Gibbs free energy calculated by B3-LYP. ⁴The electronic energy calculated by M06-L in N,N-dimethylacetamide solvent. ⁵The B3-LYP calculated imaginary frequencies for the transition states.

9. B3-LYP geometries for all the optimized compounds and transition states.

CP1				C	-5.78279500	-3.76857700	0.29105300
Ni	0.86726100	0.22255900	-0.47049400	H	-1.51916800	-3.04357800	-1.94691100
C	-5.35747600	-4.07272500	-1.02544000	H	-6.04677800	-4.55312400	-1.71466400
C	-4.07860600	-3.76322600	-1.43381300	H	-3.75211500	-3.99678500	-2.44464900
C	-3.16235500	-3.13384000	-0.54740700	C	-1.83897100	-2.79628500	-0.93586600
C	-3.59329300	-2.82994000	0.78500800	C	-2.66704400	-2.20291000	1.66465500
C	-4.91732800	-3.16095800	1.17541700	H	-5.23738700	-2.92970100	2.18900400

H	-6.79371500	-4.01858500	0.60122200
C	-1.39478600	-1.88835400	1.25548500
C	-0.94624200	-2.18180600	-0.06938900
H	-2.98598800	-1.96709100	2.67746100
H	-0.71928000	-1.39822900	1.94974700
C	0.41869100	-1.85376300	-0.52684600
H	0.63343500	-2.14341700	-1.55567300
C	1.49527100	-1.57381200	0.31014900
H	1.39158600	-1.60974800	1.39196100
H	2.51196900	-1.68427200	-0.05557900
C	-5.92668600	2.42364100	1.34628500
C	-5.04627900	1.55574000	0.73872200
C	-3.85515100	2.03823700	0.12996800
C	-3.58372800	3.44471000	0.15859900
C	-4.51109500	4.31208100	0.79143000
C	-5.65750600	3.81433900	1.37312900
H	-3.14506500	0.10648800	-0.52324000
H	-6.83411800	2.04387100	1.80818100
H	-5.24801000	0.48739100	0.71639100
C	-2.93001000	1.17190500	-0.50494600
C	-2.39069000	3.91432800	-0.45931900
H	-4.30249100	5.37939800	0.81027700
H	-6.36047800	4.48847800	1.85508700
C	-1.51286300	3.04883500	-1.06347900
C	-1.76477800	1.64283400	-1.09452000
H	-2.18474900	4.98236400	-0.45276800
H	-0.61869400	3.44159900	-1.53711600
C	-0.86074100	0.68115800	-1.74575500
H	-1.29883000	-0.30035600	-1.89507200
C	0.35238300	0.95099700	-2.35221600
H	0.72060800	1.96357800	-2.48167700
H	0.79669700	0.20813000	-3.01139300
C	8.07296600	-1.16199200	1.48688400
C	6.77190800	-0.87440400	1.83685000
C	5.90853700	-0.19307800	0.93613400
C	6.41755800	0.19182300	-0.34642500
C	7.76182900	-0.11908600	-0.67741600
C	8.57404100	-0.78142600	0.21782100
H	4.19039400	-0.17058900	2.24471700
H	8.72147900	-1.68357100	2.18578000
H	6.38652300	-1.16626000	2.81116800
C	4.56375600	0.11966600	1.26424000
C	5.54494800	0.87397200	-1.23942200
H	8.14239200	0.17533100	-1.65296000
H	9.60212000	-1.01373200	-0.04647000
C	4.24862500	1.16139700	-0.88993900
C	3.72467900	0.78909200	0.38638100
H	5.92304200	1.16760000	-2.21627800
H	3.60690000	1.67668600	-1.59806700
C	2.33857000	1.09851400	0.78905900
H	2.08434600	0.77644700	1.79700900
C	1.50464400	2.03144500	0.17182800
H	1.87192700	2.65902500	-0.63624300
H	0.66023700	2.43980700	0.72320000

2

I	0.32919800	-1.68434000	0.00000000
C	-1.02085300	3.17692900	0.00000000
C	-0.35897800	2.61475600	1.26645500
C	-0.35897800	1.07114900	1.27066600
C	0.30654000	0.55077300	0.00000000
C	-0.35897800	1.07114900	-1.27066600
C	-0.35897800	2.61475600	-1.26645500

H	0.15726100	0.69158000	2.15848000
H	0.67690900	2.97828100	1.32966700
H	-0.87263200	2.97812700	2.16523400
H	-2.08815500	2.91181800	0.00000000
H	-0.97008500	4.27287700	0.00000000
H	1.37428700	0.78301800	0.00000000
H	0.15726100	0.69158000	-2.15848000
H	-1.39262100	0.70461600	-1.31642400
H	0.67690900	2.97828100	-1.32966700
H	-0.87263200	2.97812700	-2.16523400
H	-1.39262100	0.70461600	1.31642400

TS1

Ni	0.78732000	0.28122900	0.67971600
C	-4.17047400	-5.88243800	-0.30641600
C	-2.92023400	-5.30329700	-0.28661600
C	-2.67706100	-4.12525500	0.47082600
C	-3.75570000	-3.54596100	1.21383500
C	-5.03110800	-4.16512600	1.17179900
C	-5.23576100	-5.30879100	0.42989900
H	-0.58132800	-3.96283400	-0.03133800
H	-4.34285200	-6.78526400	-0.88619000
H	-2.09933100	-5.74435100	-0.84744400
C	-1.40120100	-3.50731900	0.52089100
C	-3.50110400	-2.36569900	1.96761900
H	-5.84817400	-3.72022800	1.73463900
H	-6.21696000	-5.77511100	0.40715800
C	-2.25253700	-1.79797100	2.00248200
C	-1.16353000	-2.37046500	1.27832300
H	-4.32048400	-1.91472100	2.52218300
H	-2.09169000	-0.89689800	2.58689000
C	0.21547400	-1.87213200	1.37769500
H	0.93912800	-2.38540400	0.74860700
C	0.71728200	-1.05749000	2.36821500
H	0.07594300	-0.67369400	3.15801500
H	1.78188400	-1.06686700	2.56964900
C	-6.24683700	-1.90384500	-2.09617100
C	-4.87321300	-2.00221100	-2.11946700
C	-4.06054900	-0.96073900	-1.59496100
C	-4.69545800	0.19557600	-1.03616400
C	-6.11288400	0.26624900	-1.02568600
C	-6.87339300	-0.75866900	-1.54587400
H	-2.17183500	-1.90620100	-2.04348600
H	-6.85625500	-2.70816700	-2.49908000
H	-4.39122000	-2.88506100	-2.53163500
C	-2.64347400	-1.02796200	-1.61009100
C	-3.87256200	1.23074600	-0.51323200
H	-6.59036900	1.14698700	-0.60203500
H	-7.95807500	-0.69201400	-1.53553500
C	-2.50320100	1.13906100	-0.54989600
C	-1.85557700	-0.00301700	-1.11205600
H	-4.34597700	2.10988900	-0.08179400
H	-1.90617700	1.94901800	-0.14335900
C	-0.38777000	-0.08097300	-1.24650400
H	0.01437900	-1.04826300	-1.53947700
C	0.43370100	1.02073000	-1.32271100
H	0.02013200	2.02325800	-1.28943600
H	1.44538600	0.91901700	-1.69860400
C	-1.39612900	7.41174500	-1.27097400
C	-0.43753100	6.42807700	-1.16696400
C	-0.51880000	5.43952900	-0.14894800
C	-1.61648100	5.48315700	0.77046800
C	-2.58735100	6.50912700	0.63719100

C	-2.48099800	7.45342900	-0.36111800
H	1.28661000	4.39298700	-0.70892300
H	-1.32310200	8.16167500	-2.05377400
H	0.39609000	6.39458200	-1.86432500
C	0.45046800	4.41224500	-0.01260100
C	-1.68587500	4.48905500	1.78644300
H	-3.41850200	6.53911000	1.33793000
H	-3.22993900	8.23508200	-0.45377400
C	-0.72913100	3.50964800	1.89310000
C	0.37320900	3.45204500	0.98570300
H	-2.51574800	4.51722400	2.48889300
H	-0.81361900	2.76840400	2.68211500
C	1.44017000	2.44124300	1.09651800
H	2.23011100	2.51134800	0.35257600
C	1.65243700	1.60770500	2.16998100
H	1.02031200	1.64500200	3.05238400
H	2.61096200	1.11430000	2.27990600
I	3.37678600	-0.68803300	-0.12688900
C	8.91056700	-1.33067900	-0.52222700
C	8.16228000	-2.54077300	0.06010300
C	6.66928200	-2.20185600	0.32254600
C	6.04575500	-1.64856300	-0.92485500
C	6.73634400	-0.46094900	-1.52791900
C	8.22947900	-0.79704100	-1.79286600
H	6.13163700	-3.08691700	0.68006400
H	8.22367100	-3.38114000	-0.64605400
H	8.63801900	-2.87480000	0.99219300
H	8.94256100	-0.53020600	0.23217200
H	9.95346500	-1.59908000	-0.73692100
H	5.58342200	-2.35724300	-1.60835800
H	6.24508300	-0.13963500	-2.45290700
H	6.69450100	0.38837900	-0.82995400
H	8.29429900	-1.55493000	-2.58661700
H	8.75227800	0.09519900	-2.16343000
H	6.62403300	-1.45198300	1.12622600

CP2

Ni	0.83296700	-1.72748400	0.32663100
C	-6.90603600	-0.18693700	-0.88132700
C	-5.78840100	-0.99232800	-0.85711200
C	-4.73601100	-0.74566000	0.06638900
C	-4.85345400	0.35715700	0.97312000
C	-6.01697600	1.16690800	0.92358500
C	-7.02209300	0.90151800	0.01787400
H	-3.49932400	-2.40766400	-0.55161400
H	-7.70545400	-0.38641500	-1.58963600
H	-5.69794400	-1.83141400	-1.54286100
C	-3.57549800	-1.55853800	0.12479400
C	-3.79158400	0.59771600	1.89060200
H	-6.10209500	2.00446100	1.61149700
H	-7.90955500	1.52789700	-0.00943400
C	-2.68248100	-0.20855400	1.92342000
C	-2.55587000	-1.31968300	1.03528100
H	-3.87400900	1.43948500	2.57366100
H	-1.89273500	-0.00077000	2.63890600
C	-1.44814700	-2.27766100	1.10324500
H	-1.51412700	-3.11101900	0.40657200
C	-0.45698600	-2.34404100	2.04602900
H	-0.39071600	-1.62634500	2.86043400
H	0.09543700	-3.26928300	2.16057900
C	-4.08714000	4.27455700	-1.03518500
C	-3.63124900	3.01554400	-1.35864100
C	-2.33029000	2.59249700	-0.97221800

C	-1.49967300	3.49817000	-0.23563000
C	-1.99994300	4.78678700	0.08534900
C	-3.26465700	5.16906900	-0.30702500
H	-2.46566600	0.62658200	-1.85581900
H	-5.08318900	4.58604300	-1.33770300
H	-4.26439800	2.32525200	-1.90993100
C	-1.82793100	1.30578900	-1.29588300
C	-0.19908000	3.06519200	0.14380300
H	-1.36549700	5.47123500	0.64389400
H	-3.63563900	6.16006600	-0.05959500
C	0.26397600	1.81857900	-0.19722500
C	-0.54975800	0.90776200	-0.93787400
H	0.43632100	3.74400600	0.70813000
H	1.26550100	1.52511500	0.10140900
C	-0.04207200	-0.40132200	-1.39014400
H	-0.78601700	-1.09348600	-1.77958100
C	1.28487700	-0.69884000	-1.57253200
H	2.05514000	0.04641700	-1.40047600
H	1.57408300	-1.59224100	-2.11454600
C	6.46161700	3.39593100	-1.39351900
C	5.94717900	2.11882200	-1.35246900
C	5.08678000	1.71728300	-0.29497400
C	4.76228200	2.66306000	-0.73094500
C	5.30864800	3.97016500	0.66057200
C	6.13997200	4.32994100	-0.37847900
H	4.79749800	-0.30565900	-0.99819700
H	7.11820900	3.69200500	-2.20684500
H	6.19289300	1.39969500	-2.13004100
C	4.53903800	0.41075100	-0.22091200
C	3.90203500	2.24787300	1.78662400
H	5.06153800	4.68534200	1.44159300
H	6.55314800	5.33380400	-0.42240800
C	3.39067100	0.97449700	1.83140900
C	3.70331800	0.01907200	0.81549800
H	3.65784700	2.96004200	2.57146800
H	2.74452300	0.68946800	2.65621100
C	3.21191000	-1.36622400	0.84820900
H	3.55196800	-2.00391500	0.03464500
C	2.50796300	-1.96439000	1.85484500
H	2.24256100	-1.43661000	2.76685100
H	2.40239800	-3.04304400	1.86080300
I	1.12537000	-4.24872100	-0.74257200

CP3

C	0.00000000	-1.41092000	0.27230300
C	-1.26811800	-0.71332500	-0.24307800
C	-1.29158800	0.77822800	0.15585400
C	0.00000000	1.46466500	-0.16550000
C	1.29158800	0.77822800	0.15585400
C	1.26811800	-0.71332500	-0.24307800
H	-2.13559300	1.29005800	-0.32401200
H	-1.29975100	-0.79190600	-1.33881400
H	-2.16568100	-1.21694900	0.13809000
H	0.00000000	-1.40095400	1.37310400
H	0.00000000	-2.46613900	-0.03022100
H	0.00000000	2.53102200	-0.37891600
H	2.13559300	1.29005800	-0.32401200
H	1.48720900	0.83617900	1.24568500
H	1.29975100	-0.79190600	-1.33881400
H	2.16568100	-1.21694900	0.13809000
H	-1.48720900	0.83617900	1.24568500

CP4

Ni	-1.97094000	-0.90409400	0.54519400
C	5.46460700	-2.16572200	0.53923700
C	4.22853500	-2.47646000	1.06155000
C	3.05032400	-2.32034300	0.28125500
C	3.16865900	-1.83719900	-1.06281700
C	4.45649900	-1.52513800	-1.57085900
C	5.58017700	-1.68470300	-0.78840400
H	1.67732900	-2.98933100	1.80982300
H	6.35794800	-2.28928800	1.14512800
H	4.13791300	-2.84633400	2.08019700
C	1.75979900	-2.61884600	0.78934100
C	1.98370900	-1.68471600	-1.83602400
H	4.54228300	-1.15772100	-2.59058300
H	6.56109900	-1.44388100	-1.18863500
C	0.74910400	-1.98823100	-1.31846100
C	0.61504500	-2.46529400	0.02122300
H	2.06809500	-1.31327000	-2.85422700
H	-0.13628200	-1.84641000	-1.93052000
C	-0.69336400	-2.79250200	0.61158800
H	-0.67043400	-3.04597200	1.67090300
C	-1.87702100	-2.96544400	-0.06017700
H	-1.94668100	-2.90515900	-1.14163700
H	-2.74754300	-3.36775300	0.44947400
C	3.58203900	3.70734600	-0.57244700
C	3.07863300	2.57170300	0.02215900
C	1.71582900	2.50706900	0.42274100
C	0.86963300	3.64071500	0.19420600
C	1.41963200	4.79519500	-0.42009200
C	2.74579700	4.82930800	-0.79437700
H	1.81175200	0.49780900	1.20750300
H	4.62477400	3.74699300	-0.87547200
H	3.71533500	1.70605800	0.18841100
C	1.16574000	1.35657000	1.03947600
C	-0.49450600	3.56168000	0.59208100
H	0.77570200	5.65406100	-0.59324400
H	3.15536400	5.71913800	-1.26465700
C	-1.00072800	2.43284300	1.18517100
C	-0.16668700	1.29818900	1.42531800
H	-1.14147800	4.41696200	0.41399100
H	-2.04820200	2.40149800	1.46527800
C	-0.65936300	0.07356900	2.07474300
H	0.11189600	-0.66391800	2.28274900
C	-1.92701100	-0.16354000	2.55637200
H	-2.70707300	0.59136800	2.54387800
H	-2.12197200	-1.03830100	3.17091900
I	-3.84384900	0.01833500	-0.89833100

naphthyl

C	3.07238300	-1.03573200	-0.00000300
C	1.78004300	-1.51278500	-0.00000200
C	0.67454400	-0.61941900	-0.00000300
C	0.92640000	0.79049900	-0.00000500
C	2.26856100	1.25059500	-0.00000600
C	3.31972900	0.35891500	-0.00000500
H	-0.85127800	-2.14841700	0.00000000
H	3.90884000	-1.72943900	-0.00000200
H	1.58773900	-2.58323600	0.00000000
C	-0.66880500	-1.07533800	-0.00000200
C	-0.18813600	1.67583000	-0.00000600
H	2.45508300	2.32211700	-0.00000800
H	4.34351800	0.72312100	-0.00000600
C	-1.47532600	1.20075400	-0.00000500
C	-1.74513600	-0.20191900	-0.00000100

H	-0.00281600	2.74761600	-0.00000900
H	-2.30282200	1.90355000	-0.00000800
C	-3.11079000	-0.74554000	0.00000300
H	-3.16207100	-1.83447400	-0.00001800
C	-4.26238100	-0.06062700	0.00002900
H	-4.30540800	1.02501800	0.00005200
H	-5.21730100	-0.57724900	0.00002800

TS2

C	5.38597500	1.16237300	-0.51457000
C	4.20847100	1.49658500	0.11766400
C	3.14638400	0.55698500	0.22574400
C	3.32369000	-0.74903900	-0.33733400
C	4.54719700	-1.06227700	-0.98189500
C	5.55859100	-0.12894700	-1.07018100
H	1.79713800	1.86218600	1.29153800
H	6.18904000	1.89081700	-0.58927000
H	4.07490300	2.48788000	0.54484900
C	1.92213100	0.86727800	0.86793000
C	2.25392500	-1.68199000	-0.22449400
H	4.67587300	-2.05513200	-1.40726500
H	6.49189000	-0.38101200	-1.56636800
C	1.08149600	-1.35065600	0.40517400
C	0.88408700	-0.05241500	0.97538000
H	2.38121800	-2.67461300	-0.65106700
H	0.28669700	-2.08747300	0.47076100
C	-0.34938600	0.32810900	1.65350100
H	-0.38102200	1.35944000	2.00363000
C	-1.45473700	-0.44247200	1.84320600
H	-1.46073000	-1.50767900	1.63561100
H	-2.27274600	-0.07783400	2.45549900
C	-5.69101500	0.54640100	-0.82268800
C	-4.49134100	1.45053700	-1.15040700
C	-3.33440000	1.22736600	-0.14165700
C	-2.98399600	-0.23106300	-0.06800600
C	-4.12555500	-1.15551100	0.24855500
C	-5.28861500	-0.93587400	-0.75602500
H	-2.46254900	1.83215800	-0.41597800
H	-4.13288000	1.22726200	-2.16522300
H	-4.79436000	2.50614200	-1.14662700
H	-6.11579700	0.84850400	0.14656200
H	-6.48485800	0.68729700	-1.56765300
H	-2.23884500	-0.59118300	-0.77596000
H	-3.80972600	-2.20592400	0.23710600
H	-4.50856400	-0.94738300	1.26074900
H	-4.96963000	-1.27189100	-1.75271600
H	-6.14985000	-1.55578900	-0.47292800
H	-3.67260500	1.58189600	0.84537500

CP5

C	-5.35739800	-0.93110400	-0.54932200
C	-4.16385800	-1.43759100	-0.08110500
C	-3.03831600	-0.58913800	0.12038500
C	-3.17303100	0.80955800	-0.17516600
C	-4.40975000	1.29750700	-0.65414300
C	-5.48480700	0.44779700	-0.83940700
H	-1.70956100	-2.13678900	0.81961000
H	-6.20719700	-1.59218200	-0.69752700
H	-4.06526100	-2.49744500	0.14216500
C	-1.80260500	-1.07539700	0.59806700
C	-2.03921800	1.65612200	0.03021600
H	-4.50440500	2.35821800	-0.87615100
H	-6.43005600	0.83656700	-1.20802600

C	-0.85210400	1.16503900	0.49505800	H	-1.68872200	3.39088400	2.78848100
C	-0.68350400	-0.23693400	0.80157400	H	-2.95925900	5.19548700	1.66205000
H	-2.13849500	2.71612700	-0.19387500	C	1.25108800	1.19656800	1.00279400
H	-0.01391100	1.84036500	0.63508600	C	1.55265000	1.49438700	-0.37997900
C	0.52935000	-0.77180400	1.28595400	H	0.07097300	1.63180600	2.71898600
H	0.55072000	-1.84525900	1.46440700	H	1.79301300	0.40178600	1.50322500
C	1.79562400	-0.00916200	1.53582700	C	2.52808900	0.78456100	-1.12012900
H	1.56915000	1.00312800	1.89776400	H	2.65787600	1.09290200	-2.15694500
H	2.35709700	-0.50263300	2.34201800	C	3.50916000	-0.21126300	-0.57874300
C	5.36972100	-0.20752400	-1.07244400	H	3.05285500	-0.82382200	0.20738800
C	4.17482900	-1.11320800	-1.40609700	H	3.79203800	-0.90797200	-1.38007300
C	3.21642900	-1.24937300	-0.21187800	C	7.78345300	0.70026200	0.14454300
C	2.73669000	0.11949800	0.30481900	C	6.91218000	1.78465600	-0.50690500
C	3.94163700	1.02157000	0.63090100	C	5.60832800	1.19944400	-1.07367000
C	4.90111200	1.16334200	-0.56151200	C	4.81140200	0.42325700	-0.00883400
H	2.35408700	-1.86792500	-0.49014900	C	5.69519400	-0.65799500	0.64137400
H	3.62754400	-0.68903800	-2.26099800	C	6.99749400	-0.07503000	1.21250300
H	4.52431600	-2.10462600	-1.72209800	H	4.99181500	2.00262300	-1.49725400
H	5.98476500	-0.69067400	-0.29842900	H	6.66673800	2.55041800	0.24393800
H	6.01415500	-0.08611500	-1.95264200	H	7.47010600	2.29656300	-1.30168400
H	2.16119800	0.59973800	-0.50220200	H	8.12824700	-0.00053800	-0.63049100
H	3.59124000	2.01158000	0.95375900	H	8.68418200	1.14827500	0.58354400
H	4.48705100	0.59157400	1.48553100	H	4.51414000	1.13640800	0.77629300
H	4.38861800	1.69640300	-1.37608700	H	5.13285900	-1.17517600	1.42976200
H	5.76342500	1.78125700	-0.27943100	H	5.93964600	-1.41954300	-0.11521200
H	3.73072800	-1.77745900	0.60691100	H	6.75623200	0.60135100	2.04597100
				H	7.61518600	-0.87875600	1.63327300
				H	5.84856000	0.51674200	-1.90419700

TS3

Ni	-0.07398700	-1.48932300	-0.79033000
C	-6.59176800	1.03406100	1.26129600
C	-5.32442500	1.24246100	0.76412600
C	-4.68760000	0.25207100	-0.03244200
C	-5.38286100	-0.96939300	-0.31102500
C	-6.68705000	-1.15263200	0.21577800
C	-7.27912900	-0.17343100	0.98452700
H	-2.86178500	1.36339100	-0.34194400
H	-7.07042500	1.79613600	1.87015600
H	-4.78962400	2.16555600	0.97468600
C	-3.38532200	0.43512500	-0.55902700
C	-4.73375900	-1.95339500	-1.10905600
H	-7.21298100	-2.08059700	0.00459500
H	-8.27825400	-0.32547700	1.38352800
C	-3.47167800	-1.74785000	-1.60699100
C	-2.76809000	-0.53443400	-1.33713300
H	-5.25749100	-2.88209800	-1.32195200
H	-3.00480600	-2.51898600	-2.21236000
C	-1.41684100	-0.26645900	-1.85328500
H	-1.04268900	0.73568600	-1.64489300
C	-0.66728200	-1.06029400	-2.71117400
H	-1.05347900	-1.97863600	-3.14664200
H	0.21242900	-0.64186200	-3.19487900
I	0.69766200	-3.08419700	0.95288200
C	-1.90969000	4.98183300	-0.22555500
C	-0.93090300	4.30439500	-0.92099400
C	-0.18433400	3.26070100	-0.30237300
C	-0.46954100	2.93093500	1.06665600
C	-1.47940300	3.64473800	1.75193500
C	-2.18954400	4.65120300	1.12194700
H	1.03119000	2.79777900	-2.02398000
H	-2.47021000	5.77573400	-0.71157500
H	-0.71500800	4.55907100	-1.95600100
C	0.81616300	2.53760500	-0.98902900
C	0.28438300	1.88363700	1.68288900

CP6

Ni	-0.27597800	-1.45430100	-0.15742200
I	-0.21675400	-2.78797300	1.99128300
C	1.46165100	3.69456300	3.32833400
C	0.74546200	2.55241500	3.04548700
C	0.19935000	2.34212200	1.74966300
C	0.40611200	3.33716700	0.73940900
C	1.14480400	4.50269000	1.06276100
C	1.66179500	4.67836800	2.32944800
H	-0.70773300	0.43569100	2.20631100
H	1.87680300	3.84494800	4.32089800
H	0.59011400	1.79302300	3.80747600
C	-0.54930500	1.18206200	1.43240100
C	-0.14920600	3.11362800	-0.55302900
H	1.29802600	5.25823700	0.29567600
H	2.22703000	5.57569500	2.56598900
C	-0.85695800	1.97293200	-0.83764700
C	-1.08192300	0.96783800	0.15985900
H	-0.00999600	3.87366700	-1.31879700
H	-1.27783800	1.84306200	-1.82985600
C	-1.82712200	-0.27838700	-0.11594100
H	-2.25286300	-0.70280900	0.79485400
C	-2.80749100	-0.34571800	-1.27380500
H	-2.32162000	-0.07047400	-2.21915700
H	-3.13966600	-1.38559600	-1.38804300
C	-7.03018200	0.96645700	-1.07078400
C	-6.20629700	0.97948800	0.22496700
C	-4.93613800	0.12195000	0.10103300
C	-4.06795400	0.54369200	-1.10068700
C	-4.90738000	0.53205100	-2.39390800
C	-6.17531500	1.39184700	-2.27370800
H	-4.35922800	0.18407800	1.03160600
H	-5.92018600	2.01520600	0.46111600
H	-6.81389600	0.62544500	1.06734100

H	-7.41807600	-0.04851900	-1.24342000
H	-7.90440800	1.62277900	-0.97371300
H	-3.73341300	1.57812300	-0.92697500
H	-4.29607600	0.87827600	-3.23892200
H	-5.19415900	-0.50614300	-2.62265000
H	-5.88657800	2.44703800	-2.15732800
H	-6.75994700	1.32927100	-3.20053800
H	-5.22092700	-0.93485100	-0.01991600
C	5.96813400	1.80735100	-1.39990700
C	4.62149000	1.68671700	-1.65872300
C	3.97522200	0.42262400	-1.57245600
C	4.74986700	-0.72767600	-1.20905900
C	6.13587900	-0.56946000	-0.94894000
C	6.73279800	0.66895000	-1.04209900
H	2.00837900	1.14087400	-2.09955100
H	6.45111600	2.77827300	-1.46798800
H	4.03123300	2.55842000	-1.93078900
C	2.59335600	0.26317400	-1.83426200
C	4.09514500	-1.98710200	-1.12626300
H	6.72021900	-1.44378200	-0.67257000
H	7.79473100	0.77794000	-0.83969600
C	2.75345000	-2.11282100	-1.38890100
C	1.96749500	-0.97524200	-1.75327700
H	4.67760100	-2.86258500	-0.85029500
H	2.28894200	-3.09084100	-1.31836800
C	0.52552300	-1.06744100	-2.03293500
H	0.07900500	-0.16346700	-2.43767200
C	-0.24010000	-2.23347200	-2.01935400
H	0.20659600	-3.21381600	-1.87167600
H	-1.23081800	-2.23873600	-2.45958400

CP7

Ni	0.20177700	0.46799400	-1.21009600
I	0.30532700	-1.67688700	-2.58940600
C	-0.54511200	5.73516000	-0.42509200
C	0.13505400	4.63559100	-0.91936900
C	0.38565500	3.51284800	-0.09821700
C	-0.06252100	3.53118600	1.25658800
C	-0.75415500	4.66568200	1.73681000
C	-0.99417400	5.74988200	0.91054200
H	1.60917800	2.44599300	-1.53697400
H	-0.73082200	6.59167300	-1.06692000
H	0.49022000	4.62683800	-1.94729900
C	1.09613400	2.35940300	-0.57946400
C	0.21730900	2.39401200	2.09079500
H	-1.09423500	4.67704500	2.76960700
H	-1.52686200	6.61644100	1.29175200
C	0.90215100	1.30918500	1.62927500
C	1.42016600	1.27446000	0.27807100
H	-0.13050400	2.41664700	3.12124000
H	1.09686400	0.46782500	2.28531200
C	2.00389300	0.12412200	-0.35153000
H	2.65433900	0.34364300	-1.19858200
C	2.34776400	-1.13988300	0.40355600
H	1.51561900	-1.42836000	1.05844000
H	2.45213000	-1.95482400	-0.32060800
C	6.35350700	-2.01968600	2.06895800
C	6.17919200	-0.73696200	1.24263900
C	4.89727500	-0.77751900	0.39497400
C	3.64381100	-1.04737800	1.24971200
C	3.83357500	-2.33325900	2.07857700
C	5.11218200	-2.29629600	2.93000000
H	4.78876400	0.16651600	-0.15365700

H	6.13482300	0.12698400	1.92279900
H	7.05150500	-0.57838200	0.59558300
H	6.51808600	-2.86845200	1.38855500
H	7.24802500	-1.94784900	2.70111300
H	3.53665600	-0.20737900	1.95611400
H	2.95660000	-2.49619000	2.71995900
H	3.87833900	-3.19263200	1.39242900
H	5.01771800	-1.50775300	3.69178800
H	5.22821700	-3.24215100	3.47476300
H	4.98647100	-1.57041200	-0.36361100
C	-4.99139600	-1.88970500	3.46624900
C	-4.19113100	-0.91325100	2.91591000
C	-3.85905700	-0.93897600	1.53387600
C	-4.37104000	-1.99889900	0.71685300
C	-5.19307700	-2.98904400	1.31389300
C	-5.49668300	-2.93732100	2.65758300
H	-2.65494500	0.85446000	1.55634500
H	-5.23859900	-1.86031600	4.52392900
H	-3.80167000	-0.10680300	3.53311400
C	-3.04073400	0.04978400	0.93376800
C	-4.03526700	-2.01342200	-0.66622200
H	-5.57980500	-3.79329400	0.69260800
H	-6.12649700	-3.70273400	3.10278700
C	-3.23887400	-1.04263400	-1.21829500
C	-2.72050000	0.01911000	-0.41662100
H	-4.42077000	-2.81711100	-1.28861400
H	-2.99026400	-1.08848400	-2.27203300
C	-1.90249400	1.10984100	-0.96630200
H	-1.73738300	1.93287800	-0.27432400
C	-1.48612200	1.27803900	-2.26688300
H	-1.74782600	0.58443900	-3.05670800
H	-1.08744700	2.23852800	-2.58150600

TS4-t

Ni	0.59990000	-0.40539700	-0.42533300
C	-5.66533700	4.05775700	0.19002600
C	-4.29869800	3.89331100	0.13848100
C	-3.72355000	2.80247700	-0.56956200
C	-4.59017100	1.87342000	-1.23256200
C	-5.99380000	2.07099500	-1.16073100
C	-6.52146500	3.13854500	-0.46532400
H	-1.66702600	3.32309600	-0.15687300
H	-6.09255600	4.89604300	0.73354200
H	-3.63963600	4.59916200	0.63877000
C	-2.32113800	2.60309900	-0.64594100
C	-4.00522300	0.77995800	-1.93151100
H	-6.64789900	1.36351500	-1.66454100
H	-7.59776600	3.28045700	-0.41957800
C	-2.64420400	0.61343600	-1.98820600
C	-1.76789100	1.54184500	-1.34806400
H	-4.65953800	0.06190200	-2.41942900
H	-2.22938700	-0.24346100	-2.50931200
C	-0.30304100	1.45073600	-1.45569400
H	0.24675900	2.20603800	-0.89254800
C	0.40321100	0.68111000	-2.34423600
H	-0.08258200	0.00823100	-3.04107200
H	1.45253300	0.87461500	-2.53196300
C	-7.05588000	-1.68213900	1.37105500
C	-5.93339100	-0.88405300	1.39481700
C	-4.63389700	-1.46135400	1.40958800
C	-4.50670700	-2.88856400	1.39654400
C	-5.68261500	-3.68146200	1.37138300
C	-6.92940800	-3.09296100	1.35986100

H	-3.55961200	0.41105400	1.44610800	C	-2.92910600	6.21359200	0.49994200
H	-8.04471100	-1.23160400	1.36048000	C	-2.53025800	7.03299400	1.53435500
H	-6.02585100	0.19900600	1.39561500	H	1.12135800	4.00134900	0.45635500
C	-3.45820900	-0.67160200	1.43818400	H	-0.93451100	7.55159100	2.90965100
C	-3.20089300	-3.45594500	1.40751800	H	0.62974600	5.84360100	2.04010900
H	-5.58431600	-4.76432300	1.36006200	C	0.12621400	4.09825100	0.02638100
H	-7.82246400	-3.71188800	1.34079400	C	-2.42468800	4.36077800	-1.08885900
C	-2.08032700	-2.66647400	1.43878200	H	-3.92142600	6.31599000	0.06725100
C	-2.19232000	-1.24220600	1.46054300	H	-3.20862700	7.78707000	1.92372400
H	-3.10112600	-4.53820900	1.38338300	C	-1.55767900	3.41299600	-1.57280500
H	-1.09965900	-3.12761700	1.42486600	C	-0.25069500	3.25959300	-1.01328800
C	-1.03124800	-0.35999800	1.56997700	H	-3.41286600	4.47020300	-1.52955700
H	-1.27033900	0.70244000	1.58522400	H	-1.86303400	2.78075200	-2.40107500
C	0.27548800	-0.71628500	1.75585300	C	0.70855400	2.26406800	-1.50287600
H	0.58117700	-1.75074000	1.87710100	H	1.69657200	2.31500800	-1.04871700
H	0.98997400	0.04471900	2.05518800	C	0.50199600	1.31844100	-2.44782300
I	0.38086900	-2.77309500	-1.56855400	H	-0.43297100	1.20767800	-2.98814800
C	3.14163100	6.06976800	-0.44376300	H	1.32653400	0.70267200	-2.79482500
C	3.07403300	4.78329400	-0.93257800	C	-7.58262900	-1.67344400	0.28620500
C	3.09581400	3.66623200	-0.04996100	C	-6.51326900	-0.83533400	0.06075400
C	3.19609800	3.90710900	1.36107100	C	-5.23440200	-1.12803500	0.60728500
C	3.26478400	5.23999700	1.83113300	C	-5.07128600	-2.31134700	1.39851700
C	3.23714100	6.30277300	0.94948500	C	-6.19161000	-3.15347400	1.61228900
H	2.98078700	2.16960100	-1.59206100	C	-7.42022200	-2.84242900	1.06900200
H	3.12344400	6.91275200	-1.12910400	H	-4.23917500	0.60609600	-0.20960600
H	3.00281700	4.60360800	-2.00276500	H	-8.55564800	-1.44185200	-0.13798300
C	3.02632700	2.33423600	-0.51793600	H	-6.63238000	0.06156600	-0.54230600
C	3.23446600	2.77938400	2.23377800	C	-4.11322900	-0.28933700	0.39525400
H	3.34148000	5.41557000	2.90170000	C	-3.78519100	-2.59673100	1.93998000
H	3.29101300	7.32177000	1.32230900	H	-6.06576900	-4.05243900	2.21080800
C	3.16354300	1.49830500	1.75437100	H	-8.27086700	-3.49681800	1.23855800
C	3.04132700	1.22312700	0.34465400	C	-2.71966100	-1.76323800	1.72014600
H	3.33271900	2.95343200	3.30305400	C	-2.86801500	-0.57904300	0.93526000
H	3.21857300	0.66900900	2.45206200	H	-3.65816600	-3.49800400	2.53458500
C	2.94543300	-0.12039600	-0.17452600	H	-1.75050600	-2.01244700	2.14011500
H	3.03074700	-0.19805700	-1.25706400	C	-1.77463600	0.36308200	0.70958400
C	3.45242300	-1.32492400	0.58307900	H	-2.03404900	1.22874700	0.10118600
H	3.10500900	-1.31033500	1.62395400	C	-0.50759200	0.31200500	1.22066500
H	3.03292800	-2.23061700	0.13114000	H	-0.20850500	-0.45345800	1.92892600
C	7.53752800	-2.97583900	0.14545000	H	0.14361700	1.17684400	1.14238500
C	7.12194800	-1.82094500	-0.77717900	I	-1.13641700	-2.18683000	-2.33391800
C	5.59529300	-1.64057400	-0.80858200	C	6.13557700	3.14633000	-1.15825900
C	5.00346400	-1.45037700	0.60075200	C	5.31391500	2.08943100	-1.48237100
C	5.43326600	-2.61055300	1.51982800	C	4.49640200	1.46995000	-0.49518500
C	6.95955700	-2.79082900	1.55614300	C	4.54933200	1.96821200	0.84897000
H	5.33878500	-0.78629100	-1.44738700	C	5.40630400	3.05717500	1.15038300
H	7.58905500	-0.88971400	-0.42289700	C	6.18359800	3.63710800	0.16999900
H	7.49889600	-1.99050100	-1.79397900	H	3.62616900	0.00183800	-1.81417600
H	7.17071700	-3.92422800	-0.27429100	H	6.75355600	3.60827200	-1.92358100
H	8.63145700	-3.05522900	0.18920100	H	5.27937800	1.71180000	-2.50177300
H	5.41526800	-0.51780500	1.01876400	C	3.63986500	0.38126200	-0.79343100
H	5.04961600	-2.44332900	2.53585300	C	3.73786400	1.33168700	1.82993500
H	4.96617100	-3.54000300	1.16003000	H	5.44307400	3.42715700	2.17277800
H	7.41775100	-1.90510700	2.02122400	H	6.83740700	4.47025500	0.41285400
H	7.22087600	-3.64667600	2.19196500	C	2.91720500	0.27925800	1.50647500
H	5.13251300	-2.52575600	-1.27083100	C	2.83123600	-0.22894300	0.16761500
				H	3.78411300	1.68942200	2.85659000
				H	2.32315900	-0.18662500	2.28674400
				C	1.91756300	-1.32699500	-0.19987600
				H	2.16501000	-1.71320900	-1.19620100
				C	1.70136400	-2.47204700	0.78875500
				H	1.30780800	-2.09115900	1.74211600
				H	0.92674000	-3.13891600	0.38725300
				C	4.41637500	-5.92535200	1.34432000
CP8-t							
Ni	0.11301000	-0.54680500	-0.77229700				
C	-1.23669100	6.89898100	2.09529700				
C	-0.36450100	5.94832800	1.61258900				
C	-0.74585300	5.08779300	0.54779300				
C	-2.05475100	5.22444800	-0.01866500				

C	4.72972100	-4.93077400	0.21692400
C	3.51168200	-4.05700500	-0.12494400
C	2.95961500	-3.31991000	1.11011100
C	2.65722100	-4.32731500	2.23703700
C	3.87283200	-5.20097000	2.58482000
H	3.78228400	-3.33723600	-0.90691200
H	5.56278200	-4.28300900	0.52864200
H	5.07040800	-5.46571600	-0.67904700
H	3.66638200	-6.64851100	0.99056600
H	5.31209900	-6.50496600	1.60302500
H	3.74385000	-2.63632700	1.47266900
H	2.31055000	-3.79198400	3.13227700
H	1.82475700	-4.97509800	1.92070200
H	4.66518400	-4.56552600	3.00797500
H	3.60543100	-5.92615900	3.36464600
H	2.71550700	-4.69017400	-0.54619800

TS5

Ni	-0.44063400	-1.21621700	-0.29953000
C	6.90169500	-0.41654000	1.52682900
C	5.77573000	-1.20459300	1.43374300
C	4.81984100	-0.98584900	0.40501600
C	5.04647500	0.06891100	-0.53757700
C	6.21595500	0.86224000	-0.41504800
C	7.12431200	0.62624100	0.59457200
H	3.48739400	-2.58079800	0.99409300
H	7.62510800	-0.59279200	2.31808200
H	5.60311000	-2.00608000	2.14818800
C	3.64753400	-1.77479300	0.27987800
C	4.08293800	0.27844000	-1.56465800
H	6.38476900	1.66198000	-1.13220300
H	8.01645200	1.24048200	0.67909200
C	2.95897800	-0.50378500	-1.66094900
C	2.71792800	-1.55882400	-0.72700600
H	4.25212800	1.07605900	-2.28419300
H	2.24339800	-0.31504900	-2.45497700
C	1.53414000	-2.42789800	-0.80539300
H	1.49013600	-3.20315100	-0.04199700
C	0.59292200	-2.44824900	-1.79948600
H	0.64522400	-1.79789600	-2.66548500
H	-0.13136300	-3.25312300	-1.86324200
C	-0.90692600	6.39779200	-0.27345600
C	-0.18471500	5.22629500	-0.32971000
C	-0.63925100	4.05950100	0.34257500
C	-1.86473300	4.11914400	1.08190400
C	-2.58532800	5.33996900	1.12033900
C	-2.11814700	6.45540600	0.45828600
H	1.01039500	2.79814500	-0.25369600
H	-0.55032400	7.28317800	-0.79269000
H	0.74458400	5.17757000	-0.89242300
C	0.08080300	2.83981500	0.31040500
C	-2.31088100	2.94486400	1.75155600
H	-3.51664700	5.38183400	1.68023700
H	-2.68005500	7.38476800	0.49422500
C	-1.58996200	1.77966900	1.70188500
C	-0.36431600	1.70626800	0.97362500
H	-3.24429700	2.98437100	2.30785400
H	-1.96100700	0.90105700	2.22000300
C	0.47206100	0.50113600	0.94110700
H	1.41542000	0.62225200	0.41205000
C	0.28558100	-0.67029700	1.64405700
H	-0.54638700	-0.78782800	2.33210700
H	1.11607500	-1.35644700	1.77455500

I	-2.26183300	-0.30128600	-1.87305500
C	-4.21054500	-3.27871700	2.00270200
C	-2.94864000	-2.76270800	2.71041000
C	-1.69339800	-3.50548900	2.21766600
C	-1.58529300	-3.53994000	0.71832200
C	-2.83181000	-3.85429800	-0.06157600
C	-4.08435900	-3.14023300	0.47875300
H	-0.78451800	-3.09305700	2.67189100
H	-2.83922500	-1.68812000	2.50581400
H	-3.04078700	-2.87270500	3.79820400
H	-4.36804500	-4.33505900	2.26987600
H	-5.09235100	-2.73162900	2.35908400
H	-0.64884600	-3.92601200	0.31590900
H	-2.69811200	-3.62744600	-1.12522300
H	-2.99581400	-4.94931300	0.00073400
H	-4.02466700	-2.07896200	0.20973900
H	-4.97566700	-3.54298000	-0.01755700
H	-1.75269800	-4.55185500	2.57809500

TS6-t

Ni	-0.46499800	-1.14090300	-0.32729200
C	6.95854600	-0.41951200	1.53581500
C	5.83319800	-1.20464000	1.41444000
C	4.87785000	-0.95045100	0.39360600
C	5.10355500	0.13731400	-0.51085000
C	6.27203300	0.92711500	-0.35959000
C	7.18032800	0.65586700	0.64127900
H	3.54734100	-2.56739400	0.92455300
H	7.68207400	-0.62316400	2.32029700
H	5.66111100	-2.03110100	2.09990800
C	3.70717100	-1.73672200	0.23925100
C	4.14029000	0.38225600	-1.53055600
H	6.44047600	1.75185100	-1.04791300
H	8.07200700	1.26738400	0.74756300
C	3.01880400	-0.39895600	-1.65672300
C	2.78008500	-1.48823400	-0.76221500
H	4.30818600	1.20610300	-2.22018300
H	2.30264200	-0.18398000	-2.44357500
C	1.60255800	-2.35969500	-0.87745900
H	1.54580900	-3.14948900	-0.12974000
C	0.66468600	-2.34766500	-1.86773000
H	0.71215600	-1.67020700	-2.71309600
H	-0.07186100	-3.14069900	-1.94430100
C	-0.99748700	6.36308900	-0.19878300
C	-0.25580100	5.20431700	-0.26294700
C	-0.69741600	4.02198400	0.39051900
C	-1.92986700	4.05285500	1.12006900
C	-2.67033600	5.26153100	1.16755800
C	-2.21576200	6.39220700	0.52304800
H	0.97504700	2.79460700	-0.21120700
H	-0.65105600	7.26039700	-0.70422000
H	0.67872200	5.17757100	-0.81840200
C	0.04062300	2.81342400	0.34605300
C	-2.36275200	2.86351000	1.77115400
H	-3.60681000	5.28128700	1.71993700
H	-2.79299000	7.31184700	0.56513200
C	-1.62452400	1.70949200	1.71005700
C	-0.39393100	1.66408900	0.98818900
H	-3.30019200	2.88152600	2.32170600
H	-1.98617000	0.81843500	2.21353900
C	0.45396600	0.46489900	0.93459100
H	1.40001200	0.60583700	0.41488800
C	0.27847700	-0.71547200	1.62826800

H	-0.54936000	-0.85017100	2.31766300
H	1.11047400	-1.40265700	1.74005100
I	-2.27879600	-0.33871100	-1.96292900
C	-4.16362200	-3.30648700	2.12284600
C	-2.86934200	-2.85081700	2.81327100
C	-1.64247500	-3.58250900	2.23714400
C	-1.59194100	-3.53653600	0.73574600
C	-2.86720900	-3.80472900	-0.01259000
C	-4.08579200	-3.09352100	0.60387200
H	-0.71354000	-3.20046400	2.67830000
H	-2.74934600	-1.76814100	2.66378200
H	-2.92708800	-3.01797400	3.89622400
H	-4.33286300	-4.37233700	2.34039100
H	-5.02242900	-2.76341300	2.53728800
H	-0.66708700	-3.87998200	0.27196500
H	-2.76608300	-3.53107400	-1.06844300
H	-3.05092200	-4.89834600	0.00838500
H	-4.01191200	-2.02119100	0.38456200
H	-5.00246300	-3.45202200	0.11993500
H	-1.70125100	-4.64409100	2.55044100

CP9-t

Ni	1.89425600	-0.85057400	-0.20199400
C	-5.92316000	-2.90992900	-1.13942100
C	-4.61574500	-3.26383400	-1.38980700
C	-3.58511300	-2.93427900	-0.46800900
C	-3.92670000	-2.22746800	0.73108300
C	-5.28269600	-1.87692200	0.95905700
C	-6.25977500	-2.20999900	0.04515700
H	-1.97395900	-3.81960000	-1.60374000
H	-6.70274000	-3.16733800	-1.85100800
H	-4.35451900	-3.80172600	-2.29811900
C	-2.22762300	-3.27830800	-0.69383900
C	-2.88680100	-1.90008100	1.64726200
H	-5.53946700	-1.34265000	1.87067300
H	-7.29490200	-1.93745000	0.23152800
C	-1.58283100	-2.24973900	1.40342900
C	-1.22673000	-2.95720600	0.21367500
H	-3.14040100	-1.35481500	2.55293000
H	-0.81191100	-1.96444100	2.11133300
C	0.15364500	-3.35121700	-0.08384900
H	0.29463100	-3.82066900	-1.05784100
C	1.24009400	-3.20824800	0.70795000
H	1.18477700	-2.80863200	1.71587900
H	2.19949100	-3.60986500	0.39871900
C	-2.05589000	6.05238100	-0.11196300
C	-1.08048600	5.22549600	-0.62338600
C	-1.30470000	3.82718100	-0.74288500
C	-2.56271100	3.28594900	-0.32149300
C	-3.54670100	4.16416400	0.19917400
C	-3.29990300	5.51680900	0.30213300
H	0.63120200	3.36210200	-1.57953700
H	-1.87381600	7.11966000	-0.02235700
H	-0.12261600	5.63126200	-0.93956100
C	-0.32483200	2.94838200	-1.26584500
C	-2.77610700	1.88311800	-0.44355400
H	-4.50095000	3.75246600	0.51895500
H	-4.06140500	6.17915600	0.70475700
C	-1.80792900	1.05737900	-0.95312300
C	-0.54951900	1.58352900	-1.37780300
H	-3.72888700	1.46813500	-0.12408800
H	-2.00381200	-0.00650800	-1.03348500
C	0.49916800	0.74845800	-1.95826200

H	1.37580000	1.29417200	-2.30696100
C	0.48914700	-0.60073400	-2.13304900
H	-0.37428800	-1.20347800	-1.86887300
H	1.25692800	-1.08034600	-2.73034900
I	1.68572600	0.62136200	1.91319700
C	5.90761200	0.25420100	-0.65999600
C	4.76587700	0.72901800	-1.57174500
C	4.05020900	-0.46604800	-2.22466600
C	3.52350100	-1.47269200	-1.19340000
C	4.64978200	-1.91733800	-0.24586600
C	5.40210700	-0.73909500	0.39731900
H	3.24850600	-0.10943700	-2.88681600
H	4.04632500	1.30811800	-0.97519700
H	5.15389500	1.40319400	-2.34713700
H	6.68007100	-0.22995300	-1.27736700
H	6.38821800	1.11277200	-0.17363200
H	3.11180700	-2.35479800	-1.71356800
H	4.26950800	-2.58380700	0.54097600
H	5.37787800	-2.51932300	-0.82081600
H	4.73343000	-0.21702000	1.09314400
H	6.24389600	-1.11894600	0.99129400
H	4.77351700	-0.97392300	-2.88901600

CP10

Ni	1.42943600	-0.50270700	0.14151900
I	1.81257200	1.53620800	1.75527300
C	5.74161100	-1.40561900	-1.91647400
C	5.39755700	0.01984600	-1.46703900
C	3.86839900	0.20736100	-1.30063700
C	3.32003700	-0.83058800	-0.32969000
C	3.61851000	-2.25613100	-0.78451300
C	5.14809900	-2.44510400	-0.95744200
H	3.65763300	1.21784700	-0.93946500
H	5.89138200	0.23424200	-0.50922700
H	5.77504400	0.75626300	-2.18805000
H	5.34360500	-1.57508500	-2.92819900
H	6.82981800	-1.53221800	-1.98371300
H	3.73415000	-0.65375100	0.66763900
H	3.25437200	-2.99854700	-0.06682500
H	3.13132700	-2.47291700	-1.74450100
H	5.63289400	-2.35436600	0.02479900
H	5.34755000	-3.46376600	-1.31492000
H	3.40348900	0.09859900	-2.29066100
C	-5.03311400	-4.15533400	-1.07075400
C	-3.65643500	-4.16141100	-1.04136200
C	-2.94518700	-3.33295600	-0.13013200
C	-3.68625000	-2.49012700	0.76217500
C	-5.10432600	-2.50760100	0.70641600
C	-5.76437700	-3.32083600	-0.18937900
H	-0.97244700	-3.96185200	-0.74553600
H	-5.56524600	-4.79264000	-1.77159200
H	-3.09348900	-4.80186800	-1.71633200
C	-1.52890500	-3.31133800	-0.07285400
C	-2.96563100	-1.66615400	1.67109400
H	-5.66294000	-1.86833000	1.38596700
H	-6.85034000	-3.32620000	-0.22243400
C	-1.59340200	-1.66893700	1.70574600
C	-0.83955400	-2.50511500	0.82470800
H	-3.52230900	-1.02107700	2.34635000
H	-1.07736000	-1.01762000	2.40352200
C	0.62954600	-2.55297400	0.85342100
H	1.08143900	-3.24222400	0.14489600
C	1.43007100	-1.94137000	1.78957600

H	1.02099600	-1.39333100	2.62974600
H	2.47949500	-2.19897200	1.87211100
C	-2.61611600	5.71416200	-0.61612500
C	-1.50465300	4.94431000	-0.87593900
C	-1.60529800	3.52842200	-0.96165800
C	-2.88462700	2.91144500	-0.76933100
C	-4.01081100	3.73298600	-0.50529900
C	-3.88109100	5.10308600	-0.43049700
H	0.48673600	3.18230900	-1.36330900
H	-2.52705100	6.79501500	-0.55006300
H	-0.53115400	5.40820600	-1.01401400
C	-0.48287600	2.70915500	-1.23062600
C	-2.97216300	1.49435500	-0.85458400
H	-4.98076500	3.26263600	-0.36112200
H	-4.75088800	5.72169200	-0.22629800
C	-1.86497800	0.72651400	-1.11634200
C	-0.58463400	1.32722700	-1.31165400
H	-3.93964600	1.01876900	-0.71236300
H	-1.97235000	-0.35094800	-1.18011800
C	0.61616600	0.54694400	-1.64843000
H	1.47152900	1.14458700	-1.94659200
C	0.67404000	-0.82293000	-1.82931600
H	-0.21288500	-1.44358400	-1.74850200
H	1.50923400	-1.26181800	-2.36153100

TS7

Ni	-0.39794700	-1.58764000	0.81065900
C	-4.39190400	-3.01905600	-1.10358800
C	-3.93875500	-1.85267300	-0.21453800
C	-2.56677600	-2.18341600	0.43367100
C	-1.53251600	-2.43923500	-0.66975200
C	-1.94507800	-3.65213200	-1.49960700
C	-3.32584700	-3.38248800	-2.14432700
H	-2.32798900	-1.31614100	1.09435300
H	-3.84687800	-0.93213500	-0.80476200
H	-4.66837500	-1.65570900	0.57851400
H	-4.60515300	-3.89311500	-0.47287500
H	-5.33192400	-2.75738800	-1.60260000
H	-1.41669300	-1.56143000	-1.32046500
H	-1.21599200	-3.86978900	-2.28630100
H	-2.00801300	-4.54003900	-0.85650900
H	-3.22661200	-2.56684600	-2.87365500
H	-3.62814600	-4.27163000	-2.70888600
H	-2.66694600	-3.06929700	1.07187300
C	6.52224200	1.09338000	0.51059600
C	5.59640700	0.18499200	0.97339100
C	4.43753200	-0.11784400	0.20800000
C	4.24678900	0.53523000	-1.05455200
C	5.21873600	1.46490300	-1.50254300
C	6.33223300	1.73798900	-0.73650800
H	3.62227400	-1.54855300	1.60382100
H	7.40578100	1.31801300	1.10056600
H	5.74249800	-0.31350600	1.92826600
C	3.46406800	-1.04774800	0.65042500
C	3.08467100	0.21967400	-1.81424600
H	5.07546700	1.95701400	-2.46102100
H	7.07262800	2.44988400	-1.08912900
C	2.16019100	-0.68897300	-1.36104200
C	2.33802600	-1.34975100	-0.10597400
H	2.94070400	0.70857800	-2.77451400
H	1.28714300	-0.90751500	-1.96978000
C	1.37250000	-2.33220700	0.41222800
H	1.67243900	-2.81300800	1.34381900

C	0.45585600	-3.07319800	-0.41228400
H	0.57477700	-2.98056500	-1.48680500
H	0.20421900	-4.07670300	-0.08100300
C	-2.35581400	4.79184800	-1.60306600
C	-1.39869500	3.89202600	-1.18995300
C	-1.66252400	3.00127300	-0.11375200
C	-2.93984700	3.05280300	0.53784600
C	-3.90218300	3.99132300	0.08929300
C	-3.61632600	4.84142900	-0.95867500
H	0.26923100	2.03228400	-0.14822400
H	-2.14664300	5.47135800	-2.42380400
H	-0.42822000	3.85500000	-1.67821600
C	-0.70191200	2.06671700	0.34174000
C	-3.18869300	2.16618000	1.62523800
H	-4.86798200	4.03496200	0.58567800
H	-4.36001700	5.55854300	-1.29336800
C	-2.23992600	1.26825900	2.04537800
C	-0.96686900	1.19810400	1.39677900
H	-4.14572700	2.22530600	2.13713200
H	-2.44587500	0.63432600	2.90296400
C	0.08154700	0.25871000	1.80653800
H	1.07426100	0.48142200	1.42132300
C	-0.03341000	-0.78741100	2.70383500
H	-0.94404500	-0.96291900	3.27264400
H	0.85998200	-1.26873100	3.08919200

I-

I	0.00000000	0.00000000	0.00000000
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PhZnI

Zn	-0.05341300	-0.00008600	-0.00000600
C	1.94667900	-0.00007800	0.00016300
C	2.66933200	1.20648000	0.00023500
C	2.66950000	-1.20653000	0.00023500
C	4.06684200	1.20779100	0.00037300
H	2.15004700	2.16305400	0.00018100
C	4.06701000	-1.20764300	0.00037400
H	2.15034600	-2.16317500	0.00018100
C	4.76714300	0.00012300	0.00044400
H	4.60708200	2.15132200	0.00042700
H	4.60738100	-2.15109900	0.00042700
H	5.85404000	0.00019800	0.00055300
I	-2.62048200	0.00002700	-0.00023700

TS8

Ni	-0.13722700	0.15052900	-0.84924400
I	-0.35377500	-2.04597400	0.99831100
C	-2.55335100	4.38237800	-3.61014200
C	-1.47906500	3.60021700	-3.23225200
C	-1.29267900	3.23579400	-1.87596600
C	-2.22888300	3.69348100	-0.89596100
C	-3.31770800	4.49471200	-1.31175400
C	-3.47825000	4.83211700	-2.64292800
H	0.62157300	2.27099000	-2.16709800
H	-2.68702500	4.65622700	-4.65264100
H	-0.76009500	3.25710000	-3.97236500
C	-0.17218500	2.45632100	-1.45033900
C	-2.02854700	3.32240500	0.47496200
H	-4.02922000	4.84366700	-0.56737600
H	-4.31921300	5.44818400	-2.94844100
C	-0.96883000	2.55241400	0.86347200
C	0.02790700	2.12887400	-0.09067300
H	-2.74820600	3.66770100	1.21353200

H	-0.84875100	2.27690500	1.90504700	C	0.11659300	-3.20760900	-0.96652200
C	1.16620100	1.28747100	0.22412600	C	0.54149000	-3.49113400	0.36745000
H	2.00774900	1.44032900	-0.45461800	C	1.43815500	-4.56025000	0.59475900
C	1.58649000	1.05419100	1.66359400	C	1.90315100	-5.33104100	-0.45574500
H	0.72473700	0.74553900	2.26449500	H	-1.22394700	-2.01697500	-2.18485000
H	2.29434000	0.21736300	1.71599600	H	1.84423600	-5.66652700	-2.59468400
C	4.49740600	3.56305600	3.85675900	H	0.27310500	-3.80945200	-3.03803300
C	4.27584200	3.85590400	2.36582200	C	-0.79024100	-2.12053300	-1.19076500
C	3.59092800	2.67927600	1.65084900	C	0.02503100	-2.68314000	1.43379600
C	2.26561200	2.28097800	2.33013000	H	1.75492600	-4.77203000	1.61354900
C	2.49932200	1.99756900	3.82773500	H	2.59104300	-6.15073700	-0.26837800
C	3.18054400	3.17380000	4.54434700	C	-0.84899300	-1.66051200	1.20679600
H	3.41943700	2.94230800	0.59902400	C	-1.31810800	-1.35537000	-0.12723500
H	3.64987900	4.75533600	2.26346700	H	0.34445900	-2.90695300	2.44942500
H	5.23086100	4.08415800	1.87570500	H	-1.22100300	-1.07249000	2.03902800
H	5.21703000	2.73780000	3.96012400	C	-2.09430500	-0.17779100	-0.46197400
H	4.94483600	4.43343700	4.35377300	H	-2.66729000	-0.27985500	-1.38830000
H	1.57707900	3.13831100	2.25286800	C	-2.79251000	0.65825600	0.59076200
H	1.54406300	1.75973300	4.31526100	H	-2.10376700	0.88343300	1.41536700
H	3.12816800	1.09995500	3.92414600	H	-3.04562400	1.62991700	0.15070100
H	2.50245400	4.04060600	4.54520600	C	-6.98280000	0.08337700	1.90138900
H	3.35935400	2.91748700	5.59642900	C	-6.47761700	-0.73114800	0.70098000
H	4.26485100	1.80960300	1.64923300	C	-5.19016400	-0.13245800	0.11270700
Zn	1.92064900	-1.44023500	-0.43294600	C	-4.07915600	0.02024700	1.17005200
C	1.29031200	-0.80602100	-2.35734700	C	-4.60266100	0.83390700	2.37055600
C	2.05734400	0.12725700	-3.08869400	C	-5.88694700	0.23667900	2.96648900
C	0.83327500	-1.93576700	-3.07618300	H	-4.84038400	-0.75590500	-0.71967500
C	2.30272400	-0.01801100	-4.45603500	H	-6.28059900	-1.76465300	1.02327800
H	2.49153800	0.98927700	-2.58301300	H	-7.25340600	-0.78982100	-0.07358000
C	1.08333700	-2.10266600	-4.44091000	H	-7.29243400	1.08115200	1.55609000
H	0.26198500	-2.70532200	-2.55755100	H	-7.87419200	-0.38789000	2.33559200
C	1.80965200	-1.13435500	-5.13736600	H	-3.82753200	-0.98885300	1.53617700
H	2.89031700	0.72758400	-4.98682300	H	-3.82406700	0.90128100	3.14294900
H	0.71698200	-2.98629500	-4.95823500	H	-4.80077700	1.86563800	2.04115100
H	2.00521000	-1.25618200	-6.19965100	H	-5.66123600	-0.75050200	3.39713200
I	4.36025600	-1.99826500	0.31680700	H	-6.24490100	0.86235500	3.79454600
C	-6.98762500	-0.67878200	3.01755900	H	-5.41182100	0.85929700	-0.31186000
C	-6.07235100	0.00137800	2.24560900	C	-0.64529800	2.03176300	-1.24338200
C	-5.27026900	-0.68669500	1.29479500	C	-1.34296600	2.67046800	-2.28502900
C	-5.42869800	-2.10322000	1.14784100	C	-0.17762900	2.83945600	-0.19196700
C	-6.38054500	-2.77442300	1.95725100	C	-1.55163300	4.05363700	-2.28632000
C	-7.14252100	-2.07933700	2.87199900	H	-1.73534900	2.08506100	-3.11580100
H	-4.20720300	1.05701400	0.59207300	C	-0.38115800	4.22468700	-0.18872300
H	-7.59446400	-0.14371800	3.74271200	H	0.35656300	2.39165100	0.64376700
H	-5.94948500	1.07645200	2.35461900	C	-1.06905900	4.83893200	-1.23654800
C	-4.32139000	-0.01917300	0.48254900	H	-2.09504300	4.51699900	-3.10781300
C	-4.62385400	-2.78221300	0.19000800	H	-0.00256600	4.82252200	0.63835700
H	-6.49811400	-3.84958500	1.84628700	H	-1.23087100	5.91413100	-1.23400800
H	-7.86677400	-2.60551600	3.48774300	C	5.89002000	0.22421400	2.87280600
C	-3.70961500	-2.10820400	-0.57808800	C	4.99396400	-0.38963100	2.02612900
C	-3.53956700	-0.69660400	-0.44326200	C	4.30935500	0.35523400	1.02689500
H	-4.74187900	-3.85697900	0.07734100	C	4.56786400	1.76020000	0.91248700
H	-3.10814900	-2.65399200	-1.29644700	C	5.49696000	2.36256500	1.79987600
C	-2.63634900	0.08044200	-1.29298600	C	6.14397000	1.61345800	2.75899800
H	-2.73882800	1.15597600	-1.18268800	H	3.19507100	-1.31300900	0.22416000
C	-1.79536500	-0.37936200	-2.26748500	H	6.40703200	-0.35573400	3.63252900
H	-1.72078300	-1.43336300	-2.50511900	H	4.79731700	-1.45600300	2.10989800
H	-1.39030700	0.30759000	-3.00331000	C	3.38441000	-0.24491100	0.13676700
				C	3.88079100	2.49572600	-0.09318800
				H	5.69081200	3.42892300	1.71031300
				H	6.85335900	2.08663400	3.43254500
				C	2.98822800	1.88663700	-0.93946200
				C	2.72092600	0.48747500	-0.83856900
				H	4.07365700	3.56203000	-0.18433700
CP11							
Ni	-0.30845000	0.15879600	-1.25904700				
C	1.48090400	-5.05559200	-1.77283100				
C	0.60360500	-4.01529500	-2.02230100				

H	2.47507200	2.47653300	-1.69030700
C	1.80872800	-0.21831900	-1.75028200
H	1.83853500	-1.30105600	-1.65890000
C	1.09519200	0.31681000	-2.80322500
H	1.17573100	1.35802100	-3.09260200
H	0.65396600	-0.34738800	-3.54386600

ZnI₂

I	0.00000000	0.00000000	-2.52895000
Zn	0.00000000	0.00000000	-0.00000800
I	0.00000000	0.00000000	2.52895400

TS9

Ni	-0.24177900	0.84283200	-1.16622600
C	2.32823200	-3.76923400	-2.13398200
C	1.27314000	-2.89060800	-2.30210400
C	0.66829500	-2.26117800	-1.18812600
C	1.15745100	-2.55728200	0.11966400
C	2.23786600	-3.45878400	0.26412200
C	2.81659300	-4.05522600	-0.84107400
H	-0.89958800	-1.28138800	-2.31423500
H	2.78020100	-4.24606400	-2.99965800
H	0.89324200	-2.67473700	-3.29842600
C	-0.42376900	-1.34087200	-1.33621800
C	0.52151800	-1.93956900	1.24453900
H	2.60965900	-3.67537600	1.26273800
H	3.64378500	-4.74864600	-0.71626400
C	-0.53310800	-1.08422300	1.09446600
C	-1.07029700	-0.77472700	-0.20920300
H	0.89808800	-2.16683400	2.23912000
H	-0.98821100	-0.63581700	1.97190800
C	-2.12910500	0.23457800	-0.42041900
H	-2.59228300	0.13197300	-1.40411200
C	-3.19671800	0.38593400	0.66763200
H	-2.72890000	0.66953100	1.61736700
H	-3.85595200	1.21960100	0.39997800
C	-6.67945500	-2.30024100	1.11806900
C	-5.76087200	-2.50906300	-0.09456300
C	-4.87267100	-1.28101400	-0.35365200
C	-4.05047300	-0.88390600	0.88866200
C	-4.98424900	-0.68561500	2.10020700
C	-5.86951900	-1.91341200	2.36422800
H	-4.20849800	-1.48397200	-1.20315500
H	-5.11985500	-3.38501700	0.08454000
H	-6.35517400	-2.73666200	-0.98891700
H	-7.40075400	-1.50047300	0.89266400
H	-7.26785800	-3.20645300	1.31122900
H	-3.37341900	-1.71986600	1.12300000
H	-4.38912900	-0.45088400	2.99326300
H	-5.62533800	0.19044400	1.91638100
H	-5.23358300	-2.76122700	2.65944500
H	-6.54043500	-1.71782500	3.21069900
H	-5.50637700	-0.42924300	-0.64731000
C	-1.55433200	2.14850900	-0.47881100
C	-2.37116300	2.90664600	-1.34015400
C	-1.17125500	2.73261800	0.74587700
C	-2.74932700	4.20966500	-1.01413500
H	-2.70512900	2.47681700	-2.28258600
C	-1.54005700	4.04091600	1.06605000
H	-0.56729300	2.16460200	1.45052000
C	-2.33123400	4.78732700	0.18850000
H	-3.37171500	4.77730900	-1.70249700
H	-1.21341200	4.47627400	2.00800200

H	-2.62701100	5.80153500	0.44282700
C	6.33235300	-0.96540200	1.50574200
C	5.40690800	-0.97108600	0.48523300
C	4.47033700	0.08980300	0.34466500
C	4.50392200	1.16749100	1.28825000
C	5.47008600	1.14467600	2.32727700
C	6.36616300	0.10282700	2.43576200
H	3.49185300	-0.70814700	-1.40724700
H	7.04279100	-1.78250800	1.60101900
H	5.37468200	-1.79162800	-0.22739600
C	3.50794400	0.11493300	-0.69655400
C	3.55995100	2.22156200	1.13990500
H	5.49223700	1.96648600	3.03971200
H	7.10223500	0.09723600	3.23528900
C	2.63793700	2.21598200	0.12258700
C	2.59324600	1.15030800	-0.83006100
H	3.58025600	3.04468000	1.85101700
H	1.92813500	3.03301600	0.04173300
C	1.61877200	1.12485600	-1.93816000
H	1.77573100	0.31959600	-2.65423600
C	0.75618800	2.16762800	-2.29465500
H	0.78958600	3.13629900	-1.80585300
H	0.30145400	2.16917800	-3.28363200

3

C	4.78758300	-1.69478200	-1.00989900
C	3.50653800	-1.34342000	-1.37526800
C	2.66747800	-0.62082200	-0.48496100
C	3.17681000	-0.26120300	0.80407400
C	4.50161900	-0.63730700	1.15087900
C	5.29067400	-1.33846300	0.26551700
H	0.96388600	-0.52280400	-1.81196900
H	5.41841900	-2.24769000	-1.70084200
H	3.11903500	-1.61621400	-2.35434200
C	1.34046500	-0.24306800	-0.82951600
C	2.33057100	0.46531900	1.68600200
H	4.88440300	-0.36120300	2.13084600
H	6.30283000	-1.62094100	0.54234500
C	1.05359100	0.81492700	1.31701100
C	0.53055000	0.45827000	0.04102800
H	2.71405100	0.74903500	2.66360200
H	0.43355800	1.38800500	2.00123100
C	-0.89855400	0.84067300	-0.34242500
H	-1.02588900	0.56178300	-1.39579000
C	-1.94416600	0.04794100	0.47995900
H	-1.77098500	0.23127800	1.54912700
H	-2.94256100	0.44968100	0.25589300
C	-3.35442200	-4.07100900	-0.29211200
C	-2.48908200	-3.38896100	-1.36163400
C	-2.43923900	-1.86504700	-1.16348800
C	-1.95658000	-1.47547300	0.24868200
C	-2.83087100	-2.17263700	1.31115900
C	-2.88326100	-3.69635700	1.12066600
H	-1.79348300	-1.41833900	-1.93006900
H	-1.46698000	-3.79268700	-1.31054500
H	-2.86685700	-3.62438200	-2.36509500
H	-4.40135100	-3.75720900	-0.41983000
H	-3.33640100	-5.16051300	-0.42452600
H	-0.92849800	-1.84967000	0.36842800
H	-2.45478500	-1.93221500	2.31482600
H	-3.85285900	-1.76551800	1.25669100
H	-1.88034600	-4.11558400	1.28992800
H	-3.54081700	-4.14777600	1.87489500

H	-3.44506900	-1.44535100	-1.32271500
C	-1.09189600	2.35936500	-0.27728100
C	-0.51612000	3.15549900	-1.28028800
C	-1.80317100	3.00162300	0.74441100
C	-0.64597500	4.54261500	-1.26690300
H	0.04587800	2.67590300	-2.07886700
C	-1.93428400	4.39381100	0.76362000
H	-2.26958700	2.41980200	1.53336800
C	-1.35778900	5.16983700	-0.24057700
H	-0.19335600	5.13480900	-2.05818000
H	-2.49270400	4.86836700	1.56662900
H	-1.46234700	6.25144500	-0.22697000

TS10

Ni	-0.95017200	-0.67207400	-0.27131000
I	-2.56230900	0.90577100	-1.50533900
C	-4.99933600	-2.63412800	2.14257700
C	-5.19659500	-1.11338000	2.09258000
C	-3.96012300	-0.40230100	1.46463500
C	-3.72486000	-1.02083800	0.11571600
C	-3.43324800	-2.49814200	0.12400400
C	-4.67892700	-3.19868700	0.75251400
H	-4.14525000	0.67205300	1.38666700
H	-6.09156300	-0.87361600	1.50267300
H	-5.35930500	-0.70432700	3.09738000
H	-4.17650700	-2.87287200	2.83173400
H	-5.89715600	-3.11785700	2.54714100
H	-4.50641700	-0.77445400	-0.59632000
H	-3.27405000	-2.88687700	-0.88412400
H	-2.55067900	-2.73275600	0.72596500
H	-5.54361600	-3.06390900	0.08852600
H	-4.47980500	-4.27660200	0.80018300
H	-3.10295100	-0.55487500	2.12673400
C	5.82567300	-3.57757600	1.24730000
C	4.45347600	-3.67701400	1.17463700
C	3.71593400	-2.90894400	0.23280300
C	4.42763000	-2.02760000	-0.64413800
C	5.84075600	-1.94778600	-0.54489000
C	6.52743000	-2.70484500	0.38002800
H	1.77415700	-3.67337400	0.78893100
H	6.37618300	-4.17073400	1.97269800
H	3.91423100	-4.34755800	1.84002700
C	2.30273800	-2.98832800	0.12789000
C	3.67878800	-1.26642100	-1.58486900
H	6.37541700	-1.27719400	-1.21394700
H	7.60977800	-2.63552300	0.44672900
C	2.31139200	-1.36486400	-1.65810000
C	1.58392300	-2.24106500	-0.79443800
H	4.21065300	-0.59515200	-2.25547000
H	1.77370400	-0.76292400	-2.38361100
C	0.11803000	-2.39667900	-0.87729600
H	-0.27288500	-3.20471100	-0.26042100
C	-0.70203500	-1.88727300	-1.88397700
H	-0.29387000	-1.29570600	-2.69905000
H	-1.65265600	-2.36124800	-2.10608400
C	1.30870500	6.34528800	0.55201500
C	0.42320700	5.32761400	0.82914800
C	0.84665100	3.96988800	0.82078900
C	2.21634800	3.67716800	0.51697800
C	3.10400500	4.74841400	0.23634900
C	2.66285700	6.05393700	0.25303200
H	-1.07631300	3.13202900	1.32958200
H	0.97105700	7.37829500	0.56095000

H	-0.61696800	5.54896500	1.05715400
C	-0.03765000	2.89959600	1.10395500
C	2.62852800	2.31634000	0.51254600
H	4.14267800	4.52078200	0.00696100
H	3.35229600	6.86559200	0.03639000
C	1.74627700	1.30155600	0.79175900
C	0.37850600	1.57609600	1.09684300
H	3.66608600	2.08347200	0.28386200
H	2.09774600	0.27587800	0.77775300
C	-0.59030800	0.51168500	1.42361700
H	-1.55978000	0.88456800	1.74292000
C	-0.28030700	-0.82667500	1.65645100
H	0.74501600	-1.18326200	1.66792100
H	-0.98681900	-1.45413400	2.19705800

TS11

Ni	-0.09674900	-0.66232600	1.24343800
I	-0.41825400	-0.07233400	3.69418100
C	6.57099100	-2.52825500	-0.90865100
C	5.66386900	-1.83705900	-0.13663300
C	4.49520600	-1.27321600	-0.71878700
C	4.27613600	-1.43703000	-2.12606900
C	5.23020700	-2.15323400	-2.89350800
C	6.35315700	-2.68807700	-2.29943400
H	3.71306400	-0.43668600	1.11400100
H	7.45994300	-2.95482000	-0.45231500
H	5.82888000	-1.71328200	0.93091700
C	3.54230800	-0.55536000	0.04586500
C	3.10735200	-0.86294500	-2.69963200
H	5.06098700	-2.27410300	-3.96093700
H	7.07689600	-3.23555100	-2.89684800
C	2.20101200	-0.17408800	-1.93158600
C	2.39813600	-0.01043000	-0.52494900
H	2.94444400	-0.96991800	-3.76963000
H	1.33156800	0.27255800	-2.40496600
C	1.45211400	0.71956700	0.32604500
H	1.83131500	0.99189200	1.30977100
C	0.25233700	1.28027600	-0.06646500
H	-0.21674000	1.04975400	-1.01627500
H	-0.34708200	1.83026000	0.65081900
C	0.02609100	6.33092500	-0.70787000
C	1.40859000	5.79235600	-0.30614000
C	1.33058000	4.29199200	0.08647800
C	0.67677200	3.51295100	-1.01662400
C	-0.68011500	3.99451400	-1.44158400
C	-0.60811500	5.49662300	-1.83231100
H	2.32925000	3.90326100	0.31500400
H	2.10596200	5.90954900	-1.14749400
H	1.81968400	6.37211700	0.53017300
H	-0.63648300	6.31798100	0.17012700
H	0.10784000	7.37971200	-1.02071300
H	1.32928900	3.11577300	-1.79367500
H	-1.07678700	3.40455700	-2.27659400
H	-1.39295500	3.89468600	-0.60823400
H	-0.00911000	5.60067800	-2.74775700
H	-1.61478800	5.86582900	-2.06700200
H	0.73368000	4.21303200	1.00804900
C	-5.81995400	-0.71597200	-3.40181500
C	-4.46111500	-0.83933200	-3.21437700
C	-3.93673200	-1.29857200	-1.97525800
C	-4.84744400	-1.63521600	-0.92125600
C	-6.24154500	-1.49570600	-1.14565200
C	-6.71898400	-1.04625500	-2.35791000

H	-1.85874600	-1.18388100	-2.55314700
H	-6.20850800	-0.36397500	-4.35359300
H	-3.76927500	-0.58680200	-4.01475800
C	-2.54472800	-1.43464200	-1.74571700
C	-4.31368400	-2.09753500	0.31389500
H	-6.92913100	-1.75012700	-0.34257400
H	-7.78877100	-0.94399100	-2.51799900
C	-2.96037800	-2.22582100	0.50405800
C	-2.03908200	-1.89252700	-0.53695700
H	-4.99995100	-2.34861500	1.11891900
H	-2.58724200	-2.56965000	1.46360300
C	-0.58136200	-2.01166700	-0.36889800
H	0.00988300	-1.69050000	-1.22431000
C	0.08711500	-2.65281000	0.65776800
H	-0.43555700	-3.19598800	1.44055000
H	1.15246700	-2.84566600	0.57289300

TS2-*t*Bu

C	-4.59446400	0.95772000	0.56827300
C	-3.36452400	1.48191700	0.23551100
C	-2.27602400	0.63113400	-0.10238000
C	-2.48295400	-0.78716700	-0.09035900
C	-3.76010000	-1.29547800	0.25586300
C	-4.79606800	-0.44398300	0.57902800
H	-0.85221900	2.21454500	-0.45430700
H	-5.41686300	1.62050800	0.82426800
H	-3.20889100	2.55835500	0.22667200
C	-0.99835700	1.13586600	-0.44798700
C	-1.38682700	-1.63019600	-0.43198500
H	-3.91084000	-2.37275400	0.26254600
H	-5.77061900	-0.84575500	0.84283800
C	-0.16200500	-1.11027600	-0.76235800
C	0.06863500	0.30370200	-0.77689700
H	-1.53799100	-2.70752300	-0.42949100
H	0.64875800	-1.78374600	-1.02247700
C	1.35322100	0.88799000	-1.13566400
H	1.37396800	1.97752600	-1.14019100
C	2.51745800	0.23059600	-1.41477100
H	2.54886600	-0.84541900	-1.55602200
H	3.35868800	0.78100000	-1.82263900
C	3.85829000	-0.05505500	0.56387200
C	2.97810800	-0.93715500	1.40365500
H	2.82458400	-1.92062700	0.94349200
H	3.42909200	-1.11548500	2.39666400
H	1.99590800	-0.48207000	1.57414600
C	5.07463200	-0.69346000	-0.04802900
H	5.55037500	-0.04101500	-0.79059400
H	5.83916000	-0.91025800	0.71987000
H	4.83575900	-1.64823400	-0.53265600
C	3.99892000	1.37007700	1.02085600
H	4.58362600	1.43075500	1.95619900
H	4.51911400	1.98865200	0.27930400
H	3.02187300	1.82416100	1.22260700

TS7-*t*Bu-1

Ni	0.22305400	1.98553100	0.55651200
C	0.93359500	3.13361300	-1.10885300
C	-5.63638100	-2.54904700	0.95636500
C	-4.96912800	-1.39118600	1.28832200
C	-4.00766700	-0.83295000	0.40218200
C	-3.74380600	-1.49227000	-0.84395500
C	-4.44846500	-2.68215800	-1.15602800
C	-5.37430200	-3.19933700	-0.27484000

H	-3.51941800	0.85871700	1.64935800
H	-6.37039500	-2.96838300	1.63793300
H	-5.17169600	-0.88869800	2.23071200
C	-3.30315400	0.35731900	0.70772000
C	-2.78419600	-0.91909800	-1.72540500
H	-4.25084900	-3.17946900	-2.10206400
H	-5.91062400	-4.11032100	-0.52341600
C	-2.11808800	0.23755000	-1.40240100
C	-2.36930400	0.90634500	-0.16459000
H	-2.58903500	-1.41117700	-2.67496400
H	-1.39870800	0.64863500	-2.10363700
C	-1.67986100	2.14640900	0.22546600
H	-2.06852400	2.59677500	1.13993800
C	-1.07237300	3.08140600	-0.70743300
H	-1.26741100	2.90192600	-1.76031700
H	-1.16948700	4.12561400	-0.42502400
C	3.89529900	-3.86362500	-1.38631800
C	2.73158100	-3.23838700	-0.99773900
C	2.76441200	-2.17495500	-0.05459700
C	4.02687800	-1.76236500	0.48866900
C	5.20562100	-2.42741400	0.06866900
C	5.14085600	-3.45486000	-0.84924900
H	0.63157100	-1.82825300	-0.03640300
H	3.86293100	-4.67699200	-2.10497200
H	1.77351100	-3.55312800	-1.40349900
C	1.58943100	-1.51056100	0.37116500
C	4.04710900	-0.70577700	1.44419000
H	6.16170500	-2.11888300	0.48305300
H	6.04979500	-3.95942200	-1.16319200
C	2.89227200	-0.07875900	1.83961400
C	1.62848700	-0.47156900	1.29684800
H	5.00038000	-0.41158400	1.87560800
H	2.93897900	0.69608400	2.59936500
C	0.36560700	0.16203500	1.68675200
H	-0.53101800	-0.37269700	1.38057600
C	0.19858700	1.27013700	2.50042100
H	1.03644800	1.74555700	3.00595800
H	-0.78243800	1.49774000	2.90554300
C	1.22498200	1.98957900	-2.08482800
H	1.27955700	1.00851800	-1.60026900
H	0.47666300	1.94111600	-2.88128400
H	2.19802900	2.16814100	-2.56240700
C	0.84233000	4.47887400	-1.83132200
H	0.09004000	4.47426000	-2.62513900
H	0.62526700	5.30447500	-1.14697900
H	1.81333500	4.68446000	-2.29969600
C	1.99796400	3.23862400	-0.00184100
H	1.89278600	4.14159900	0.60462000
H	2.09888500	2.35663000	0.68000600
H	2.98451100	3.24847400	-0.48364500

TS7-*t*Bu-2

Ni	-0.89332700	1.57474000	-0.24785800
C	-1.20550800	3.69174500	-0.13678000
C	6.18381800	-1.30030000	-0.72598700
C	4.95512700	-1.00553200	-1.27477100
C	4.11207900	-0.02830900	-0.67846300
C	4.56152300	0.64888900	0.50160100
C	5.83144800	0.32245500	1.04233400
C	6.62538000	-0.63153500	0.44226000
H	2.51153600	-0.21858600	-2.11309900
H	6.82301200	-2.04560100	-1.19042100
H	4.61613000	-1.51272600	-2.17457200

C	2.84066900	0.29722400	-1.21466200	Zn	3.03040800	0.82879200	0.43519900
C	3.71234700	1.63193000	1.08256600	C	1.42294100	0.38879400	1.67842500
H	6.17132300	0.83833400	1.93675600	C	1.66480100	-0.06818400	2.99400200
H	7.59737700	-0.87259100	0.86256400	C	0.09817100	0.79054700	1.38849100
C	2.48994500	1.93169300	0.53345800	C	0.66446500	-0.08154900	3.96981100
C	2.02348700	1.26043300	-0.63812400	H	2.66960000	-0.38105100	3.27420200
H	4.05030700	2.15235000	1.97528000	C	-0.92191300	0.76816300	2.35961600
H	1.87177300	2.69090200	1.00036200	H	-0.11857700	1.25717300	0.43143400
C	0.73682400	1.58524200	-1.28582600	C	-0.63459200	0.34052500	3.65559800
H	0.52299900	0.96273900	-2.15566100	H	0.89798400	-0.40041600	4.98352500
C	0.22081400	2.95031500	-1.36703800	H	-1.91784600	1.12149800	2.10391000
H	0.89960400	3.72694600	-1.02636100	H	-1.40546200	0.35484000	4.42288300
H	-0.26525300	3.19166600	-2.30859700	I	5.50457300	0.23772300	1.21963200
C	-0.49678800	4.06948900	1.16625300	C	-7.11372100	-3.17280800	-1.20469200
H	-0.27868500	3.20114600	1.79831200	C	-5.77347600	-3.48660700	-1.18255100
H	0.44185400	4.59866400	0.97768500	C	-4.92056300	-2.95386800	-0.17667800
H	-1.13994200	4.74357400	1.74736600	C	-5.47872000	-2.08459200	0.81818400
C	-2.53583700	2.97160700	0.13442200	C	-6.86461900	-1.78323800	0.76822800
H	-3.18562900	2.92338200	-0.74179700	C	-7.66421600	-2.31409200	-0.22082100
H	-2.47808500	1.92907600	0.57116800	H	-3.12186900	-3.92284800	-0.87371900
H	-3.05931900	3.49450300	0.94441100	H	-7.75643200	-3.58428200	-1.97765100
C	-1.47402500	4.92069100	-1.00797900	H	-5.34888700	-4.14658900	-1.93508900
H	-0.55622800	5.46932400	-1.23922600	C	-3.53731400	-3.25399900	-0.12207700
H	-1.97156800	4.66052700	-1.94728600	C	-4.61715400	-1.56460600	1.82461300
H	-2.13649400	5.60227800	-0.45931400	H	-7.28716400	-1.12836700	1.52640300
P	-1.28499300	-0.60395800	0.05916800	H	-8.72395800	-2.07697000	-0.24908500
C	-3.02180400	-0.86765000	-0.49757600	C	-3.27855700	-1.87048900	1.84908200
C	-3.94327800	-1.63815300	0.22704400	C	-2.70631200	-2.72643700	0.85949800
C	-3.43574600	-0.25535200	-1.69495700	H	-5.03997400	-0.91932700	2.59097000
C	-5.24850900	-1.79838800	-0.24297100	H	-2.64935700	-1.46226100	2.63139100
H	-3.64942100	-2.11063100	1.15832400	C	-1.28451300	-3.10362700	0.85534800
C	-4.73729800	-0.42688500	-2.16663000	H	-1.05911700	-3.94200300	0.19978900
H	-2.73520100	0.35070100	-2.26593000	C	-0.30242700	-2.71904800	1.77736300
C	-5.64686800	-1.19787300	-1.43844100	H	-0.52534300	-2.05206500	2.60561700
H	-5.95368400	-2.39538900	0.32794200	H	0.59389200	-3.31943700	1.89706800
H	-5.04129900	0.04269500	-3.09778600	C	3.22753800	-3.49675100	-2.65545800
H	-6.66258300	-1.32682300	-1.80053900	C	3.56831300	-3.13951400	-1.20478100
C	-1.22170400	-1.10465800	1.82312600	C	2.50269100	-2.18806500	-0.58879700
C	-1.19881600	-2.45858300	2.20216800	C	1.12186100	-2.80959000	-0.71953200
C	-1.23063400	-0.11885600	2.82208300	C	0.76031400	-3.10938100	-2.16923200
C	-1.19363900	-2.81069100	3.55189800	C	1.81250600	-4.07808500	-2.77151500
H	-1.17586700	-3.23677500	1.44559000	H	2.76391200	-1.99520800	0.45637800
C	-1.22484700	-0.47369200	4.17159600	H	3.62141900	-4.05377500	-0.59712700
H	-1.23540500	0.93271600	2.54735900	H	4.54570600	-2.64937000	-1.13366400
C	-1.20734000	-1.82050200	4.53753400	H	3.30382700	-2.59568000	-3.27972300
H	-1.17528300	-3.85952400	3.83319500	H	3.96089700	-4.21303700	-3.04701000
H	-1.22790400	0.29963600	4.93416900	H	1.07058200	-3.73399600	-0.13395700
H	-1.19909600	-2.09862400	5.58730400	H	-0.23844100	-3.55792300	-2.25194500
C	-0.28428900	-1.86690200	-0.82377100	H	0.76511400	-2.19068800	-2.76699400
C	-0.73390300	-2.45517200	-2.01647400	H	1.76159900	-5.04196900	-2.24508800
C	0.97074500	-2.23346000	-0.30781900	H	1.55536200	-4.27467500	-3.81997700
C	0.05644300	-3.39764600	-2.67667800	H	2.54201100	-1.23871200	-1.14125900
H	-1.70583700	-2.19752900	-2.42402400	C	-5.67138800	4.93167800	0.53983600
C	1.75087600	-3.18426400	-0.96674800	C	-5.36132200	3.60980500	0.31165000
H	1.33577300	-1.79262900	0.61434300	C	-4.10252500	3.24486500	-0.24019300
C	1.29689700	-3.76609100	-2.15253400	C	-3.15728200	4.27486700	-0.55968600
H	-0.30599600	-3.85238800	-3.59402200	C	-3.50805400	5.62676600	-0.31236900
H	2.71504500	-3.46420100	-0.55285300	C	-4.73591400	5.94845700	0.22563700
H	1.90456800	-4.50782400	-2.66282400	H	-4.46727800	1.11512400	-0.24562600
				H	-6.63568200	5.20109700	0.96153300
				H	-6.07636800	2.82563000	0.54922600
				C	-3.74910400	1.89642200	-0.48705900
				C	-1.90218300	3.90147400	-1.11933100
				H	-2.79065800	6.40684600	-0.55408300
TS12							
Ni	-0.05766800	-1.53120600	0.18334600				
I	2.49837100	1.89674200	-2.00426700				

H	-4.99205300	6.98786200	0.41111000
C	-1.58601700	2.58698900	-1.35151100
C	-2.51443000	1.54870900	-1.02660400
H	-1.18573600	4.67995300	-1.36829000
H	-0.62232900	2.33957200	-1.78606900
C	-2.23289600	0.13799400	-1.25966000
H	-3.07423700	-0.52649600	-1.06673500
C	-1.07947900	-0.43647000	-1.69664500
H	-0.21137200	0.14475300	-2.00431600
H	-1.12679600	-1.47416700	-2.00915500

CP12

Ni	-0.24483300	-1.25488200	0.29355500
C	1.24752900	-2.06016200	-0.55317400
C	1.28275500	-2.54350900	-1.87320000
C	2.45319700	-2.08697300	0.17121600
C	2.46591400	-3.02058300	-2.44907100
H	0.37574400	-2.55236000	-2.47574600
C	3.64054500	-2.56008700	-0.39776900
H	2.47625400	-1.73846600	1.20247100
C	3.65262300	-3.03065100	-1.71238100
H	2.45779700	-3.38800600	-3.47366800
H	4.55628000	-2.56252500	0.19014400
H	4.57254300	-3.40433500	-2.15547600
C	-6.28287000	2.93722800	-1.66527900
C	-5.62540300	1.81736900	-1.20737600
C	-4.53125900	1.93464900	-0.30663900
C	-4.12349600	3.24108600	0.11961200
C	-4.82347900	4.37479200	-0.36875400
C	-5.87874700	4.22794400	-1.24262900
H	-4.15118700	-0.18526400	-0.13906900
H	-7.11681100	2.83491200	-2.35416700
H	-5.93423800	0.82590900	-1.53002400
C	-3.83180800	0.80391000	0.18424800
C	-3.03741000	3.34648200	1.03175300
H	-4.51211200	5.36408100	-0.04185800
H	-6.40619800	5.10320400	-1.61160500
C	-2.37868200	2.23043800	1.48708100
C	-2.75627400	0.92178300	1.05506100
H	-2.74181200	4.33330700	1.38020400
H	-1.57935800	2.33908100	2.21442600
C	-2.09062600	-0.29297700	1.54824900
H	-2.70076900	-1.19074400	1.48345600
C	-0.88294300	-0.38095100	2.19041800
H	-0.26978600	0.49886500	2.36902600
H	-0.61959200	-1.26069200	2.76675500
C	-1.61592200	-5.93280100	0.51985400
C	-0.71626600	-5.42946400	1.65905500
C	0.07155900	-4.17237900	1.23332400
C	-0.87632600	-3.06322300	0.76534800
C	-1.76807000	-3.55696800	-0.38380900
C	-2.55461700	-4.82636000	0.01606600
H	0.69349400	-3.82281400	2.06837700
H	-1.33908300	-5.19497700	2.53606800
H	-0.02132500	-6.22078000	1.97181700
H	-0.98252900	-6.27341200	-0.31283800
H	-2.19819500	-6.80506000	0.84609400
H	-1.53328800	-2.83456400	1.62092700
H	-2.47816000	-2.77814100	-0.70041500
H	-1.14575000	-3.78905200	-1.25798500
H	-3.27160700	-4.57099700	0.81114800
H	-3.14751200	-5.18582400	-0.83649200
H	0.76289800	-4.44557000	0.42840200

C	5.44205000	4.18184000	1.44138000
C	4.11541300	3.81221800	1.42624300
C	3.63765200	2.85479100	0.49014200
C	4.55955800	2.27831100	-0.44311300
C	5.91970500	2.68019800	-0.40136700
C	6.35302700	3.61020100	0.51920200
H	1.58194700	2.90366900	1.14635900
H	5.79556900	4.91432500	2.16198600
H	3.41347500	4.24927900	2.13291900
C	2.27995900	2.45197800	0.44335300
C	4.07084500	1.32158300	-1.37633200
H	6.61744800	2.24015500	-1.11000000
H	7.39752600	3.90911800	0.54099400
C	2.74993000	0.95156000	-1.39684100
C	1.81688200	1.52037900	-0.47672200
H	4.76892000	0.87334700	-2.07902600
H	2.41452700	0.20545500	-2.10821000
C	0.38797300	1.19956600	-0.48597700
H	-0.19915400	1.75646400	0.23984000
C	-0.28929200	0.37893200	-1.33488200
H	0.19345600	-0.11604000	-2.16876200
H	-1.37585900	0.38425200	-1.33334900

TS13

C	-7.34871400	-1.66030600	1.25742000
C	-6.40074200	-0.66215100	1.21202200
C	-5.45421600	-0.60595600	0.15279200
C	-5.50235000	-1.60694100	-0.87118500
C	-6.49076700	-2.62163800	-0.79595200
C	-7.39458700	-2.64949700	0.24450500
H	-4.43676600	1.16337100	0.85563300
H	-8.06643300	-1.69282100	2.07259400
H	-6.36329300	0.09822200	1.98865900
C	-4.46473500	0.40564300	0.07461600
C	-4.55193700	-1.53913700	-1.92848100
H	-6.52370800	-3.38004500	-1.57468400
H	-8.14693500	-3.43204200	0.29165600
C	-3.60827000	-0.54425200	-1.97641200
C	-3.54311600	0.45947300	-0.96184700
H	-4.58519900	-2.29550500	-2.70922900
H	-2.90013200	-0.52079000	-2.79788900
C	-2.56282600	1.54880800	-0.98569900
H	-2.62738400	2.23458700	-0.14359300
C	-1.64640200	1.81745500	-1.94862900
H	-1.60327800	1.26253300	-2.87845100
H	-1.07054200	2.73608200	-1.91850100
C	7.30945900	-1.56068800	-0.25306100
C	6.26236100	-0.87193700	-0.82475100
C	4.92598000	-1.34186300	-0.70076600
C	4.68670800	-2.55129200	0.02975400
C	5.78666800	-3.23822000	0.60546200
C	7.07070800	-2.75554400	0.46963000
H	4.02144400	0.24333500	-1.85351200
H	8.32558300	-1.18894900	-0.35545900
H	6.44492000	0.04485200	-1.38104000
C	3.82477900	-0.66137200	-1.28043200
C	3.34622800	-3.01453300	0.14274800
H	5.59897700	-4.15603600	1.15833100
H	7.90489700	-3.29037700	0.91566100
C	2.30190200	-2.32630300	-0.42267600
C	2.51966700	-1.11994600	-1.15695800
H	3.15623500	-3.93385300	0.69232600
H	1.29130600	-2.70490400	-0.31124800

C	1.42540200	-0.38874700	-1.81718400
H	1.77781400	0.35620500	-2.53359500
C	0.08993600	-0.80434100	-1.95176000
H	-0.26605200	-1.71382200	-1.47138100
H	-0.45864900	-0.52625800	-2.84733600
Ni	0.11188400	0.70551900	-0.61987500
C	0.34800600	0.54152300	1.24225600
C	1.44861800	-0.12539600	1.82502800
C	-0.89158400	0.46868700	1.91095700
C	1.28849200	-0.90989300	2.96352400
H	2.43262900	-0.03188400	1.37644700
C	-1.04963600	-0.33580200	3.04555800
H	-1.74848100	1.01849600	1.53820900
C	0.03572400	-1.02960800	3.57778600
H	2.14985300	-1.42980900	3.37652500
H	-2.02634700	-0.40139200	3.51985000
H	-0.08335800	-1.63728200	4.47077400
C	1.39611600	5.24978200	0.01768600
C	0.49328300	4.79500700	1.17301900
C	-0.17910500	3.44180900	0.86087800
C	0.86978800	2.37255100	0.53169800
C	1.77960500	2.80976700	-0.64379200
C	2.43578500	4.17570400	-0.32825900
H	-0.78593300	3.12835400	1.71773200
H	1.09412200	4.69693900	2.08883300
H	-0.27422500	5.55240900	1.38085700
H	0.77543900	5.45350600	-0.86835200
H	1.89552500	6.19396900	0.27068700
H	1.54168700	2.32485600	1.39071800
H	2.56508900	2.06705700	-0.81460100
H	1.21699600	2.90509400	-1.58316500
H	3.12362000	4.05047800	0.52057300
H	3.04686500	4.49359200	-1.18370300
H	-0.86640600	3.59221600	0.01919200

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C	-0.92064000	-0.19367400	0.00087000
C	-1.82089100	-1.26771900	0.00527600
C	-1.44870700	1.10711900	-0.00453700
C	-3.20137700	-1.05642600	0.00434100
H	-1.43361500	-2.28457900	0.00949500
C	-2.82672600	1.32475100	-0.00549100
H	-0.77687000	1.96204600	-0.00805700
C	-3.71019900	0.24272400	-0.00105300
H	-3.87754400	-1.90770000	0.00782800
H	-3.21150600	2.34156100	-0.00971700
H	-4.78376000	0.41182000	-0.00180000
C	3.45726500	0.36665000	-0.00162700
C	2.78012600	-0.17010800	1.26846700
C	1.27002800	0.11503400	1.26837400
C	0.57908400	-0.44236300	0.00193600
C	1.26997300	0.10407900	-1.26930300
C	2.78006800	-0.18105600	-1.26700600
H	0.79944700	-0.31282500	2.16252700
H	2.94287300	-1.25638200	1.33321800
H	3.24371300	0.26714900	2.16218400
H	3.39725600	1.46536300	-0.00636900
H	4.52500700	0.11246300	-0.00055400
H	0.72869600	-1.53283900	0.00663800
H	0.79934600	-0.33148000	-2.15970600
H	1.10622400	1.18963400	-1.33136500
H	2.94281100	-1.26785000	-1.32238200
H	3.24361400	0.24846700	-2.16448700

H	1.10628900	1.20108400	1.32107500
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CP1'

Ni	0.00000100	-0.00008100	-0.00055500
C	2.71043600	-0.68529900	-0.22799700
C	1.37146500	-2.45213300	-0.94630500
C	2.46710900	-3.27227800	-1.13207300
C	3.77070900	-2.79977000	-0.84001900
C	3.85216500	-1.48886400	-0.38147700
C	2.71024600	0.68556400	0.22768200
C	1.37070000	2.45219100	0.94545400
C	2.46613900	3.27250600	1.13167600
C	3.76993000	2.80020400	0.84012900
C	3.85178400	1.48931800	0.38160500
H	0.37159800	-2.80656300	-1.17699500
H	2.30239500	-4.27077600	-1.51906200
H	4.81687500	-1.06724500	-0.11813500
H	0.37066800	2.80647400	1.17566600
H	2.30111700	4.27097400	1.51860600
H	4.81666400	1.06787100	0.11861100
N	1.44964800	1.17538100	0.50106100
N	1.45001900	-1.17530900	-0.50187800
C	5.03534300	-3.65891800	-0.99891900
C	5.03435200	3.65959200	0.99943900
C	4.71622600	-5.06486900	-1.54265700
H	5.64287700	-5.64117100	-1.64393400
H	4.05340800	-5.62132200	-0.87012100
H	4.24394500	-5.02207500	-2.53081200
C	5.72722400	-3.81775000	0.37639800
H	6.63553400	-4.42567700	0.27981500
H	6.01658600	-2.84988300	0.79949400
H	5.06250500	-4.31062500	1.09502200
C	6.00959200	-2.97002000	-1.98442100
H	6.92043800	-3.56984800	-2.10379600
H	5.54899900	-2.84999300	-2.97161700
H	6.30895300	-1.97689500	-1.63293200
C	6.00855300	2.97078300	1.98504400
H	6.30820900	1.97776600	1.63350300
H	6.91924500	3.57079500	2.10466400
H	5.54779800	2.85054100	2.97213900
C	5.72647200	3.81874700	-0.37572300
H	6.63463200	4.42686100	-0.27889600
H	6.01611800	2.85098700	-0.79887200
H	5.06178300	4.31156000	-1.09441800
C	4.71482500	5.06540100	1.54330500
H	4.05211100	5.62184900	0.87066600
H	4.24225900	5.02236100	2.53131500
H	5.64134500	5.64184900	1.64494500
C	-2.71026800	-0.68566600	0.22761100
C	-1.37083600	-2.45242600	0.94524200
C	-2.46634300	-3.27264500	1.13153700
C	-3.77010700	-2.80020500	0.84013300
C	-3.85187400	-1.48930500	0.38162700
C	-2.71037700	0.68523000	-0.22800500
C	-1.37128700	2.45202200	-0.94621000
C	-2.46688800	3.27222200	-1.13202200
C	-3.77051600	2.79976200	-0.84004100
C	-3.85206000	1.48885100	-0.38152000
H	-0.37083000	-2.80680900	1.17539900
H	-2.30137700	-4.27113600	1.51843200
H	-4.81674100	-1.06775700	0.11875500
H	-0.37137900	2.80643100	-1.17676900
H	-2.30211200	4.27072200	-1.51897600

H	-4.81680700	1.06728200	-0.11823900
N	-1.44992900	1.17520200	-0.50181100
N	-1.44970300	-1.17561100	0.50087600
C	-5.03461600	-3.65944200	0.99961100
C	-5.03510600	3.65898000	-0.99895900
C	-4.71510800	-5.06550900	1.54281700
H	-5.64169300	-5.64181100	1.64469800
H	-4.05282800	-5.62184300	0.86965400
H	-4.24205700	-5.02292500	2.53061400
C	-5.72732400	-3.81797400	-0.37532100
H	-6.63558100	-4.42591300	-0.27832200
H	-6.01692900	-2.85001300	-0.79803600
H	-5.06304200	-4.31070100	-1.09445100
C	-6.00828800	-2.97081900	1.98587200
H	-6.91900900	-3.57074800	2.10571300
H	-5.54707400	-2.85095200	2.97279700
H	-6.30796300	-1.97765200	1.63477600
C	-6.00935700	2.97016100	-1.98451100
H	-6.30877800	1.97703900	-1.63306400
H	-6.92017200	3.57003600	-2.10389600
H	-5.54874200	2.85014200	-2.97169800
C	-5.72701700	3.81781000	0.37634200
H	-6.63528800	4.42579400	0.27975300
H	-6.01645000	2.84994900	0.79940200
H	-5.06228900	4.31062300	1.09500000
C	-4.71589800	5.06493100	-1.54264500
H	-4.05305500	5.62132000	-0.87008200
H	-4.24361000	5.02214400	-2.53079700
H	-5.64251400	5.64128900	-1.64391300

bipyridyl

C	0.73710500	1.23698300	-0.12418900
C	2.58531200	2.37364400	-0.83090100
C	3.42785500	1.28225100	-0.59969800
C	2.89000900	0.09538200	-0.09161500
C	1.50686600	0.09837300	0.14377100
C	-0.73710100	1.23698500	0.12417500
C	-2.58530500	2.37364900	0.83088400
C	-3.42786200	1.28227800	0.59961800
C	-2.89002000	0.09541200	0.09152700
C	-1.50687400	0.09839800	-0.14384900
H	2.99989000	3.30119500	-1.22504100
H	4.48576900	1.37969700	-0.81473100
H	1.02184600	-0.77782100	0.56217900
H	-2.99989000	3.30121400	1.22498400
H	-4.48579700	1.37976600	0.81452800
H	-1.02185300	-0.77779700	-0.56225600
N	-1.27254200	2.37364600	0.60499500
N	1.27255200	2.37365000	-0.60499000
C	3.73136600	-1.15394700	0.21584700
C	-3.73137100	-1.15393700	-0.21586500
C	5.21967300	-0.95060200	-0.12526100
H	5.77881700	-1.86442300	0.10489100
H	5.36808300	-0.73126200	-1.18879000
H	5.66405700	-0.13617200	0.45800400
C	3.20057700	-2.34607700	-0.61557300
H	3.78804200	-3.24744500	-0.40320400
H	2.15342200	-2.56949200	-0.38573300
H	3.27172200	-2.13926400	-1.68952900
C	3.61787300	-1.48711900	1.72269300
H	4.20849500	-2.38068600	1.95840400
H	3.99188400	-0.66028000	2.33698000
H	2.58246800	-1.68296600	2.02036600

C	-3.61777000	-1.48750700	-1.72260500
H	-2.58237700	-1.68354400	-2.02018700
H	-4.20844200	-2.38108800	-1.95813400
H	-3.99166900	-0.66081000	-2.33715200
C	-3.20063600	-2.34585100	0.61592100
H	-3.78804700	-3.24729500	0.40372000
H	-2.15344200	-2.56923100	0.38622400
H	-3.27189500	-2.13875100	1.68981300
C	-5.21970800	-0.95050300	0.12504500
H	-5.36828800	-0.73133100	1.18858200
H	-5.66389400	-0.13591800	-0.45816200
H	-5.77890400	-1.86423400	-0.10533900

TS1'

Ni	-0.07318900	-0.09988900	-1.41747900
I	-0.39362000	2.61025000	-0.51003300
C	-3.09355400	5.97590400	2.49849200
C	-1.56111100	6.03404800	2.59646400
C	-0.90667400	4.80573600	1.91601400
C	-1.39864200	4.68394800	0.49229600
C	-2.90190100	4.60010300	0.36310000
C	-3.55927800	5.82767700	1.04161200
H	0.18536000	4.88752400	1.94892900
H	-1.19946200	6.95225700	2.11159000
H	-1.24440400	6.08721600	3.64693700
H	-3.45995100	5.11887800	3.08318100
H	-3.53679500	6.87374100	2.94878100
H	-0.94040800	5.39992100	-0.19198200
H	-3.20306600	4.53862700	-0.68863300
H	-3.26471200	3.68724400	0.85634300
H	-3.29572300	6.73577800	0.48049500
H	-4.65279600	5.73500400	0.99460600
H	-1.17848400	3.90217300	2.47952300
C	-5.17220900	-5.29622600	-0.51377000
C	-4.02182900	-4.85063800	-1.12630800
C	-3.80011300	-3.46168600	-1.34254800
C	-4.80237000	-2.53169400	-0.90936000
C	-5.97551100	-3.02266500	-0.28136600
C	-6.16014900	-4.37505900	-0.08595800
H	-1.87524800	-3.68459200	-2.29337100
H	-5.32698300	-6.36055700	-0.35668500
H	-3.26378200	-5.55792000	-1.45537600
C	-2.62905000	-2.96946200	-1.96857400
C	-4.57235200	-1.14511300	-1.13166100
H	-6.73147200	-2.31112800	0.04376100
H	-7.06392200	-4.73920600	0.39509400
C	-3.42832300	-0.69844200	-1.74623600
C	-2.41652800	-1.61195900	-2.18522900
H	-5.32709000	-0.43187900	-0.80736900
H	-3.28673400	0.36745100	-1.89684000
C	-1.17728500	-1.15808000	-2.83454500
H	-0.52438400	-1.96164700	-3.17301500
C	-0.89762800	0.14989900	-3.26863800
H	-1.64942800	0.93340100	-3.23873800
H	-0.10678900	0.30396900	-3.99869100
C	1.59853800	-1.14041100	0.63703100
C	-0.63541700	-1.38142100	1.23827500
C	-0.30134000	-1.95056400	2.45742800
C	1.05424800	-2.12915600	2.80109700
C	1.99190800	-1.70780300	1.85674300
C	2.52352100	-0.66280200	-0.39309400
C	2.71138500	0.37185400	-2.46697100
C	4.09490100	0.31656200	-2.43088800

C	4.74641200	-0.25365100	-1.31618200
C	3.92050100	-0.74023400	-0.30259600
H	-1.67461500	-1.24052900	0.95572000
H	-1.09988500	-2.25207300	3.12372100
H	3.04980100	-1.81511500	2.06803800
H	2.19405900	0.82155900	-3.30905600
H	4.65191500	0.72361800	-3.26559300
H	4.36332900	-1.19129200	0.57820500
N	1.92278300	-0.09867200	-1.48546400
N	0.27533500	-0.97899900	0.33582100
C	1.51094400	-2.74752700	4.13218700
C	6.27542800	-0.34870800	-1.19189500
C	0.32019800	-3.14175900	5.02680300
H	0.69054500	-3.57618000	5.96200400
H	-0.29835600	-2.27555900	5.28764900
H	-0.32111300	-3.88968200	4.54681700
C	2.37868300	-1.72344500	4.90262000
H	2.71383400	-2.15157800	5.85511900
H	3.27000700	-1.43438400	4.33569200
H	1.81071200	-0.81192100	5.11998000
C	2.34620900	-4.01902200	3.84796500
H	2.68219900	-4.47011800	4.78945900
H	1.75434900	-4.76512500	3.30569600
H	3.23608500	-3.79794500	3.24895400
C	6.73743500	0.42565400	0.06597900
H	6.29354100	0.01982000	0.98122800
H	7.82768300	0.36526200	0.16912800
H	6.45943300	1.48351500	0.00030500
C	6.68900900	-1.83442500	-1.06180800
H	7.77852500	-1.91792400	-0.96793700
H	6.24215400	-2.30729600	-0.18073900
H	6.37885000	-2.40764300	-1.94290000
C	6.99450900	0.24733700	-2.41721700
H	6.72943600	-0.27822200	-3.34174100
H	6.76394200	1.31065800	-2.54819100
H	8.07876300	0.15862100	-2.28696200

CP2'

Ni	0.08248200	-1.69214000	-0.02671100
I	-0.09511800	-3.06005100	2.20845900
C	-0.99022600	0.98781300	0.35300700
C	1.12046500	0.84513500	1.28450900
C	1.07318300	2.16784400	1.71783200
C	-0.06147900	2.94689600	1.46169300
C	-1.10162300	2.31740200	0.76209300
C	-2.05455400	0.25449500	-0.37782400
C	-2.66480800	-1.75566200	-1.34362200
C	-3.92386200	-1.27105000	-1.68670200
C	-4.27433200	0.04553000	-1.36208600
C	-3.30012100	0.80046000	-0.69337500
H	1.98755400	0.22193000	1.47912800
H	1.92620100	2.56724400	2.25211600
H	-2.00550500	2.87081900	0.53660100
H	-2.37907000	-2.77779200	-1.57284600
H	-4.61359300	-1.93242300	-2.19614200
H	-3.51949300	1.82203200	-0.40710700
N	-1.74456600	-1.02078300	-0.71165100
N	0.12107300	0.26216600	0.61508800
C	-0.19958300	4.41081400	1.90700100
C	-5.64181600	0.66150600	-1.69481200
C	1.04999900	4.90784400	2.65823200
H	0.90782200	5.95265300	2.95489200
H	1.23536400	4.32895000	3.56994600

H	1.94836200	4.86232000	2.03228700
C	-1.42055100	4.54351500	2.84891300
H	-1.53197100	5.58429000	3.17485000
H	-2.35315000	4.24824400	2.35629000
H	-1.30010500	3.91855500	3.74068000
C	-0.40789100	5.30498100	0.66095100
H	-0.51163000	6.35340700	0.96401900
H	0.44464600	5.23200200	-0.02365300
H	-1.31026200	5.02982100	0.10436500
C	-6.33730600	1.09521500	-0.38177400
H	-5.75223400	1.84163000	0.16584600
H	-7.31544500	1.53733900	-0.60416500
H	-6.49415900	0.23860700	0.28299000
C	-5.43614500	1.89701900	-2.60410300
H	-6.40456100	2.34965300	-2.84679300
H	-4.82281700	2.66499500	-2.12084600
H	-4.94674900	1.61835400	-3.54421000
C	-6.56251600	-0.33314200	-2.42689700
H	-6.13437300	-0.66087600	-3.38109400
H	-6.77062300	-1.22080000	-1.81901200
H	-7.52190800	0.14812200	-2.64504600
C	5.84809100	2.24488100	-2.45840600
C	4.62230000	1.66702000	-2.70487500
C	4.20338800	0.51076700	-1.99016300
C	5.08437800	-0.04545600	-1.00556500
C	6.34025200	0.57386500	-0.77463800
C	6.71667000	1.69433100	-1.48360600
H	2.28828600	0.32015200	-2.96972900
H	6.15513300	3.12721800	-3.01388900
H	3.95581900	2.08802300	-3.45448000
C	2.94888500	-0.10868300	-2.21794000
C	4.65724100	-1.20268700	-0.29718200
H	7.00444200	0.14626800	-0.02683900
H	7.68181200	2.15837700	-1.29920400
C	3.43692700	-1.78348900	-0.54469600
C	2.54606600	-1.24172000	-1.52446900
H	5.31851700	-1.63101400	0.45273400
H	3.14032200	-2.66174200	0.02054900
C	1.22710800	-1.83930900	-1.79843600
H	0.65049600	-1.33133100	-2.57019000
C	0.79479200	-3.09627100	-1.37183000
H	1.44343800	-3.77879900	-0.83253500
H	-0.06192800	-3.56246200	-1.85139800

TS3'

C	2.21148600	5.51526300	-1.80289900
C	1.62942600	4.26638900	-1.85190300
C	2.23139800	3.15177300	-1.20130800
C	3.46375000	3.35514700	-0.49317600
C	4.03416500	4.64871900	-0.46083600
C	3.42441600	5.71158000	-1.10078200
H	0.73283000	1.71256300	-1.77855900
H	1.74087700	6.35522100	-2.30762000
H	0.69895900	4.11295200	-2.39462200
C	1.66142700	1.85977700	-1.23038200
C	4.06270200	2.23211000	0.15665000
H	4.96669000	4.79579500	0.07946900
H	3.87517500	6.69967400	-1.06791500
C	3.49408300	0.98945400	0.11214200
C	2.25831300	0.75354700	-0.59325600
H	4.99006600	2.38434600	0.70422800
H	3.96329900	0.16616200	0.63944800
C	1.65168500	-0.53339300	-0.66525300

H	0.73243100	-0.58722800	-1.24569400
C	2.35924200	-1.83291800	-0.39838100
H	2.93263400	-1.77621100	0.53336000
H	1.61260900	-2.62320400	-0.24172400
C	4.29664300	-4.25678900	-3.56210200
C	3.52472000	-2.99771800	-3.98433800
C	2.57673800	-2.51536800	-2.87435000
C	3.31266300	-2.28281400	-1.54160700
C	4.08781500	-3.54935500	-1.13135000
C	5.04015200	-4.03253800	-2.23670300
H	2.06947600	-1.59506900	-3.19039200
H	4.24148600	-2.19658600	-4.21828300
H	2.95968900	-3.18783700	-4.90646000
H	3.58920000	-5.09132800	-3.44265100
H	5.00091300	-4.55477800	-4.34974900
H	4.04424200	-1.47466700	-1.69916100
H	4.64636400	-3.36051200	-0.20519000
H	3.36643800	-4.34868900	-0.89990800
H	5.82905600	-3.28085400	-2.38822200
H	5.54576700	-4.95469000	-1.92185200
H	1.78899300	-3.26999900	-2.71751100
Ni	0.05821700	-0.44634300	1.56942400
I	1.63563900	-1.01569400	3.47033900
C	-2.43269900	-0.77452900	0.21527200
C	-1.55630000	-2.84588300	0.76585700
C	-2.65114800	-3.50892400	0.21912500
C	-3.69645700	-2.77623400	-0.35948500
C	-3.55751400	-1.38028000	-0.34479400
C	-2.21617100	0.69072100	0.28082600
C	-0.78926900	2.36558100	1.00248900
C	-1.63444200	3.36020700	0.51790300
C	-2.83249200	3.01292200	-0.11952300
C	-3.10279600	1.63986600	-0.22681600
H	-0.74186600	-3.39180000	1.23264100
H	-2.67298100	-4.59097000	0.25888100
H	-4.33702500	-0.75978800	-0.77141600
H	0.14411500	2.61499600	1.49600500
H	-1.33762500	4.39383300	0.64389200
H	-4.01463100	1.30922900	-0.71053600
N	-1.06204400	1.05805900	0.89413800
N	-1.43504300	-1.51146600	0.76649100
C	-4.94231000	-3.42699700	-0.97950300
C	-3.81956800	4.04615000	-0.68343100
C	-4.89570000	-4.96439500	-0.89483500
H	-5.79972900	-5.38419600	-1.34893300
H	-4.03488900	-5.37753700	-1.43276200
H	-4.85500100	-5.31563400	0.14237500
C	-5.04021900	-3.02308700	-2.47050100
H	-5.92810900	-3.47751600	-2.92533700
H	-5.12093000	-1.93820300	-2.59750500
H	-4.16099700	-3.36231600	-3.02970700
C	-6.20228800	-2.93457500	-0.22724600
H	-7.10045000	-3.38964300	-0.66082300
H	-6.16054100	-3.20812900	0.83292400
H	-6.31833100	-1.84723900	-0.28886900
C	-3.98632000	3.81490900	-2.20476800
H	-4.37203700	2.81445500	-2.42840000
H	-4.69188000	4.54349700	-2.62083600
H	-3.03058700	3.93114500	-2.72826300
C	-5.18949500	3.87843500	0.01720400
H	-5.90545600	4.60888200	-0.37735600
H	-5.61216600	2.88046400	-0.14115200
H	-5.10163100	4.03808700	1.09763800
C	-3.33399700	5.49119900	-0.46208300

H	-3.22371400	5.72640800	0.60246100
H	-2.37492600	5.68065600	-0.95723500
H	-4.06498000	6.19177400	-0.88004300

CP6'

Ni	-0.34560700	-1.02549300	-0.40712400
I	-1.30414600	-3.42849200	-0.66141400
C	-0.06932800	2.40113900	5.29079900
C	-0.37024700	1.37831800	4.41967800
C	-0.96793400	1.64563700	3.15529400
C	-1.25591600	3.00714300	2.80837300
C	-0.93582900	4.03887100	3.72993300
C	-0.35410500	3.74631500	4.94402300
H	-1.08014100	-0.41283700	2.52206800
H	0.38592200	2.18017100	6.25282800
H	-0.15653600	0.34579300	4.68721700
C	-1.29063900	0.61697300	2.23748700
C	-1.86803600	3.25814500	1.55238300
H	-1.16126600	5.06885000	3.46112500
H	-0.11464100	4.54429700	5.64189300
C	-2.16094100	2.23267700	0.68227100
C	-1.86524500	0.86789200	0.99286600
H	-2.11857700	4.28399200	1.28871400
H	-2.65716000	2.46813100	-0.25452500
C	-2.12812600	-0.27161600	0.06092900
H	-2.43703300	-1.12747500	0.66432800
C	-3.13816500	-0.07519400	-1.07197900
H	-2.84322500	0.75298200	-1.73533400
H	-3.11816300	-0.97356700	-1.70019500
C	-7.54168000	-0.40964100	-0.74801800
C	-6.69310200	-0.78730300	0.47494400
C	-5.22333600	-1.02923800	0.09427300
C	-4.60578600	0.17846000	-0.63755600
C	-5.47132500	0.55395100	-1.85716400
C	-6.94212000	0.79777200	-1.48406800
H	-4.64344700	-1.26576000	0.99398500
H	-6.74697400	0.02514200	1.21544100
H	-7.10560400	-1.68006800	0.96286700
H	-7.58471200	-1.26690700	-1.43639500
H	-8.57618600	-0.19765700	-0.44690900
H	-4.62298000	1.03248300	0.05795200
H	-5.05648600	1.44563500	-2.34911500
H	-5.41530300	-0.26057500	-2.59599100
H	-7.00822400	1.68429200	-0.83529500
H	-7.52787800	1.02646300	-2.38448300
H	-5.15448900	-1.91314000	-0.55733300
C	2.49488300	-0.62019400	-0.34783900
C	2.03841300	-2.76469700	0.37300500
C	3.36583100	-2.96653300	0.74657200
C	4.31002400	-1.94824300	0.57702100
C	3.83442600	-0.75524000	0.01195200
C	1.92074100	0.59163900	-0.96431400
C	-0.01452900	1.63970200	-1.65349200
C	0.69976200	2.69359100	-2.21614900
C	2.09578000	2.71754300	-2.14117200
C	2.69082800	1.62186800	-1.49973100
H	1.29077900	-3.54215000	0.48892900
H	3.63765800	-3.92557700	1.16998400
H	4.50943300	0.07989900	-0.13383300
H	-1.09249800	1.61769700	-1.70687100
H	0.14421500	3.48411800	-2.70515700
H	3.77037800	1.55562500	-1.43634900
N	0.56208400	0.60703800	-1.02420500

N	1.59826400	-1.61831100	-0.16157300	H	-8.67743900	0.98999700	1.09553300
C	5.78617100	-2.08556800	0.97726400	H	-4.69266900	-0.18260400	1.47568100
C	2.95892100	3.84418000	-2.72567900	H	-4.73778100	2.06746800	2.52083600
C	6.09862600	-3.47254800	1.56998000	H	-5.30204200	2.77821800	1.01100200
H	7.15922900	-3.52574800	1.83827000	H	-6.82083100	0.73144400	2.71973800
H	5.51892400	-3.66847200	2.47898400	H	-7.21723800	2.43883000	2.55180600
H	5.89908600	-4.27759100	0.85381500	H	-5.55194500	1.21949000	-1.10090900
C	6.12677500	-1.01137900	2.03843100	C	2.21580700	0.21732000	0.30173400
H	7.17947200	-1.09562700	2.33235300	C	1.96042200	-2.01412600	-0.23842500
H	5.96752300	0.00436200	1.66099800	C	3.30460600	-2.27555500	0.00491000
H	5.51215000	-1.13572300	2.93693600	C	4.15593500	-1.24938400	0.43153200
C	6.67405300	-1.87693800	-0.27331800	C	3.57050100	0.01538700	0.56875000
H	7.73190000	-1.97062200	-0.00179800	C	1.55552300	1.53413700	0.33862500
H	6.45347200	-2.62470200	-1.04328300	C	-0.40447100	2.68826000	-0.04976800
H	6.53216000	-0.88559000	-0.71687900	C	0.21707000	3.91417500	0.16112100
C	3.79504800	4.48258600	-1.59022800	C	1.57669300	3.96663900	0.49022900
H	4.45930000	3.75527300	-1.11131400	C	2.23429400	2.73266600	0.56234700
H	4.41972700	5.28843600	-1.99262000	H	1.29931800	-2.80177500	-0.57297200
H	3.14833700	4.90815400	-0.81489500	H	3.66371000	-3.28587700	-0.14614000
C	3.90699300	3.25609500	-3.79869400	H	4.17799200	0.85611400	0.88131300
H	4.53133700	4.05103300	-4.22276000	H	-1.44770000	2.64392900	-0.32518200
H	4.57603900	2.49480000	-3.38353300	H	-0.37679100	4.81381000	0.05666200
H	3.34085400	2.79611300	-4.61629400	H	3.29599600	2.70363600	0.77535300
C	2.10476300	4.94591300	-3.38082600	N	0.22537500	1.51016500	0.05785000
H	1.50995800	4.55972500	-4.21630500	N	1.40794600	-0.80419700	-0.08040100
H	1.42508600	5.41729400	-2.66194900	C	5.64868800	-1.45460200	0.72814300
H	2.75901100	5.72938800	-3.77792400	C	2.34023700	5.27524600	0.73926300

CP7'

Ni	-0.48554500	-0.29795600	-0.37603600
I	-0.25250900	-0.18063200	-3.18781600
C	-0.05361200	-5.73029200	0.16208200
C	-0.54963000	-4.59168800	-0.45081400
C	-1.01596700	-3.49958200	0.31881100
C	-0.99118300	-3.59644000	1.74303300
C	-0.47722900	-4.76804400	2.34279700
C	-0.01274100	-5.81736300	1.56824900
H	-1.71253900	-2.32232900	-1.36902700
H	0.29907100	-6.56185800	-0.44200800
H	-0.58800200	-4.52143600	-1.53543000
C	-1.54031300	-2.31155300	-0.29728200
C	-1.51807100	-2.50750100	2.51707100
H	-0.45777600	-4.83770700	3.42818100
H	0.37659500	-6.71358500	2.04373200
C	-2.04277800	-1.39565100	1.92538000
C	-2.10882400	-1.27584900	0.48481200
H	-1.49850600	-2.58965000	3.60160900
H	-2.44214800	-0.59305900	2.53732800
C	-2.49551000	-0.08924700	-0.23331200
H	-2.79601700	-0.26437100	-1.26413600
C	-3.24280700	1.04111000	0.44068200
H	-2.71653900	1.37842100	1.34465400
H	-3.27791100	1.90297100	-0.23996800
C	-7.65322900	1.23827900	0.78843200
C	-7.03902400	0.08068800	-0.01229200
C	-5.57998800	0.36929400	-0.40131600
C	-4.70855600	0.70534500	0.82401600
C	-5.33803400	1.86324500	1.62305400
C	-6.79588000	1.57762100	2.01691700
H	-5.16222600	-0.48924500	-0.93995400
H	-7.07626000	-0.83706600	0.59349300
H	-7.63394000	-0.11767300	-0.91297100
H	-7.72648900	2.12613100	0.14262600

H	-8.67743900	0.98999700	1.09553300
H	-4.69266900	-0.18260400	1.47568100
H	-4.73778100	2.06746800	2.52083600
H	-5.30204200	2.77821800	1.01100200
H	-6.82083100	0.73144400	2.71973800
H	-7.21723800	2.43883000	2.55180600
H	-5.55194500	1.21949000	-1.10090900
C	2.21580700	0.21732000	0.30173400
C	1.96042200	-2.01412600	-0.23842500
C	3.30460600	-2.27555500	0.00491000
C	4.15593500	-1.24938400	0.43153200
C	3.57050100	0.01538700	0.56875000
C	1.55552300	1.53413700	0.33862500
C	-0.40447100	2.68826000	-0.04976800
C	0.21707000	3.91417500	0.16112100
C	1.57669300	3.96663900	0.49022900
C	2.23429400	2.73266600	0.56234700
H	1.29931800	-2.80177500	-0.57297200
H	3.66371000	-3.28587700	-0.14614000
H	4.17799200	0.85611400	0.88131300
H	-1.44770000	2.64392900	-0.32518200
H	-0.37679100	4.81381000	0.05666200
H	3.29599600	2.70363600	0.77535300
N	0.22537500	1.51016500	0.05785000
N	1.40794600	-0.80419700	-0.08040100
C	5.64868800	-1.45460200	0.72814300
C	2.34023700	5.27524600	0.73926300
C	6.08427100	-2.91698000	0.51700500
H	7.15136800	-3.01812200	0.74280800
H	5.54103400	-3.60415000	1.17565600
H	5.93461500	-3.24182900	-0.51871500
C	5.93400000	-1.06691000	2.19901100
H	6.99826200	-1.20319100	2.42410200
H	5.68283700	-0.02059900	2.40353400
H	5.35772800	-1.69192700	2.89055800
C	6.48340700	-0.55512200	-0.21525200
H	7.55276800	-0.69225200	-0.01609800
H	6.29722600	-0.80570500	-1.26536600
H	6.25349700	0.50695200	-0.07875500
C	2.94036100	5.25129300	2.16563700
H	3.63415100	4.41520800	2.30452200
H	3.49447300	6.17785800	2.35600000
H	2.15361600	5.16434200	2.92361900
C	3.48049900	5.40522100	-0.29945000
H	4.03374900	6.33730000	-0.13467900
H	4.19491200	4.57803400	-0.23007800
H	3.08369800	5.41993000	-1.32043900
C	1.42699000	6.50958800	0.61610800
H	0.99724500	6.60095600	-0.38769300
H	0.60601300	6.48444200	1.34183600
H	2.00916100	7.41729200	0.80840200

TS4'-t

C	-1.27449300	5.52483200	-1.95055100
C	-1.02259700	4.17069000	-2.02270900
C	0.09515900	3.59538100	-1.35259100
C	0.96332000	4.46123300	-0.60497200
C	0.67617200	5.84485200	-0.54883600
C	-0.42056300	6.37231100	-1.20482200
H	-0.28602400	1.56547800	-1.97067000
H	-2.12770200	5.94815900	-2.47479800
H	-1.67166100	3.52024600	-2.60559900
C	0.37720700	2.21293100	-1.39963400

C	2.08777200	3.87928000	0.05810800
H	1.33777300	6.49336700	0.02134500
H	-0.62684400	7.43788800	-1.15435700
C	2.34680300	2.53817200	-0.00981200
C	1.48990100	1.64176500	-0.74817700
H	2.74467200	4.52959600	0.63161600
H	3.19982600	2.13052800	0.52203600
C	1.73583900	0.24550100	-0.83275600
H	1.01325700	-0.32932300	-1.40920800
C	3.02970000	-0.43501000	-0.49035900
H	3.43445000	-0.04990000	0.45216300
H	2.83922900	-1.50247600	-0.31539200
C	6.11815500	-1.45327500	-3.50081200
C	4.80111200	-0.83516800	-3.99336400
C	3.69655900	-0.93287500	-2.92868100
C	4.12436200	-0.30788100	-1.58768800
C	5.44866600	-0.93030100	-1.10651400
C	6.55735500	-0.83151900	-2.16639900
H	2.78116700	-0.45018600	-3.29380400
H	4.96968800	0.22352700	-4.24064100
H	4.47451500	-1.32257700	-4.92157200
H	5.98075800	-2.53689000	-3.36646300
H	6.90420700	-1.32961300	-4.25717900
H	4.29758800	0.76642500	-1.75927700
H	5.77046000	-0.44737300	-0.17454600
H	5.27515200	-1.98968000	-0.86114300
H	6.81029200	0.22701200	-2.32771000
H	7.47165500	-1.31744300	-1.80162100
H	3.44720800	-1.99333600	-2.76189900
Ni	0.33211400	-0.66542300	1.74042500
I	2.13146800	-0.48729600	3.49552000
C	-1.79133600	-1.78604300	0.21248000
C	-0.14746100	-3.37828700	0.56411400
C	-0.87864200	-4.35303200	-0.10913900
C	-2.13284400	-4.03898800	-0.64885600
C	-2.57361400	-2.71915400	-0.46690100
C	-2.18454100	-0.37489400	0.44630400
C	-1.54940100	1.62831400	1.41641600
C	-2.70835700	2.26313000	0.97749500
C	-3.65779400	1.55189400	0.23429000
C	-3.36422100	0.20270100	-0.02091800
H	0.82130100	-3.60264800	1.00040400
H	-0.45716200	-5.34670900	-0.19724900
H	-3.53919400	-2.41787300	-0.85609700
H	-0.79710000	2.16309900	1.98720400
H	-2.84317600	3.31063900	1.21448300
H	-4.06100200	-0.39917200	-0.59283100
N	-1.28371500	0.34099200	1.16383800
N	-0.57976400	-2.12060200	0.72530000
C	-3.00818900	-5.05435200	-1.39882500
C	-4.95773300	2.17927000	-0.29134300
C	-2.33939200	-6.43893500	-1.49151700
H	-2.99617400	-7.12761700	-2.03373400
H	-1.38724900	-6.39770700	-2.03259200
H	-2.15503200	-6.87117300	-0.50154200
C	-3.26820200	-4.54067400	-2.83560300
H	-3.89556100	-5.25469500	-3.38169900
H	-3.78479900	-3.57493200	-2.83926300
H	-2.32940900	-4.42174900	-3.38813900
C	-4.35625900	-5.21180400	-0.65452500
H	-4.99350200	-5.93221200	-1.18048300
H	-4.20230000	-5.57669900	0.36709000
H	-4.90475700	-4.26575500	-0.59389700
C	-5.01312200	2.03108900	-1.83089500

H	-4.99290500	0.98228800	-2.14592300
H	-5.93790400	2.47495300	-2.21743400
H	-4.16749200	2.54192000	-2.30489900
C	-6.16567600	1.44714900	0.34139900
H	-7.10320300	1.88029800	-0.02646200
H	-6.17261800	0.37983600	0.09455200
H	-6.15437200	1.53903000	1.43320800
C	-5.05537200	3.67765900	0.05323000
H	-5.06511200	3.84804600	1.13569200
H	-4.22568900	4.24878400	-0.37840300
H	-5.98752200	4.08667700	-0.35150600

CP8'-t

Ni	0.25747200	0.30542100	1.27106000
I	0.82675000	0.65158400	3.79586300
C	6.56777000	-1.73781300	0.83079200
C	5.55954700	-0.84287700	1.11258900
C	4.49859300	-0.62122700	0.18858300
C	4.50298100	-1.35467500	-1.04487200
C	5.55768400	-2.26639700	-1.30630400
C	6.57072200	-2.45710600	-0.39059000
H	3.46722600	0.84741900	1.38581100
H	7.36922600	-1.89556900	1.54791800
H	5.55694100	-0.29163700	2.04984200
C	3.45258800	0.29730600	0.44733700
C	3.43597000	-1.12624300	-1.95709700
H	5.55515600	-2.81416000	-2.24674900
H	7.37410100	-3.15793200	-0.60163900
C	2.42555700	-0.23979600	-1.67096700
C	2.39957900	0.51329700	-0.44852900
H	3.43245500	-1.66741700	-2.90179700
H	1.63027100	-0.09598800	-2.39617800
C	1.29222500	1.42644600	-0.10644200
H	1.62894800	2.19812700	0.59512000
C	0.44153300	2.01344600	-1.22786700
H	-0.03436200	1.20753300	-1.80746600
H	-0.38960500	2.57735400	-0.77957500
C	1.46003700	5.54120500	-3.70605200
C	2.38697100	5.18014100	-2.53580500
C	1.70100800	4.23088300	-1.53997800
C	1.16760300	2.95630400	-2.22104600
C	0.24590800	3.33241100	-3.39760200
C	0.92658000	4.27859300	-4.39944500
H	2.39953400	3.96567800	-0.73768400
H	3.29291700	4.69579600	-2.92951300
H	2.72077100	6.08998100	-2.02000300
H	0.61146000	6.13060800	-3.32672400
H	1.98559100	6.17974900	-4.42817200
H	2.03231600	2.41369600	-2.63382000
H	-0.09370500	2.42161200	-3.91111100
H	-0.65926300	3.81874900	-2.99952500
H	1.76354700	3.75154200	-4.88134100
H	0.22661000	4.54972400	-5.20115300
H	0.85902400	4.75629300	-1.06067500
C	-2.39776100	-0.29557300	0.27932600
C	-2.40845100	1.74039800	1.38492800
C	-3.76162200	1.93285200	1.12069800
C	-4.47604400	0.96865100	0.39755500
C	-3.75462900	-0.16074200	-0.01734800
C	-1.57378400	-1.47052300	-0.10331000
C	0.52958800	-2.43875400	0.00077300
C	0.09248700	-3.57439800	-0.67656500
C	-1.23936700	-3.66871500	-1.09737300

C	-2.06806400	-2.57761900	-0.79234600
H	-1.83411400	2.46292500	1.95670400
H	-4.23817800	2.83247900	1.48936100
H	-4.25805400	-0.94225600	-0.57372200
H	1.55921800	-2.34174100	0.32777000
H	0.80486800	-4.36745500	-0.86557600
H	-3.10948500	-2.59708500	-1.09035000
N	-0.27693700	-1.40981600	0.28462100
N	-1.73708000	0.66122800	0.97123800
C	-5.96968600	1.10057400	0.06357700
C	-1.80225200	-4.88322400	-1.85075300
C	-6.57114500	2.41087400	0.60606300
H	-7.63309100	2.46239800	0.34316100
H	-6.49944400	2.47280500	1.69776000
H	-6.08295300	3.29338400	0.17733500
C	-6.73797900	-0.08700400	0.69253100
H	-7.80638100	-0.00623500	0.46130700
H	-6.38789500	-1.05182200	0.31024200
H	-6.62589000	-0.09675000	1.78238700
C	-6.15110800	1.07896400	-1.47346900
H	-7.21377700	1.16965100	-1.72639500
H	-5.61743100	1.91125100	-1.94584500
H	-5.78277900	0.14819000	-1.91800600
C	-2.95415600	-5.50515500	-1.02459400
H	-3.77302000	-4.79619300	-0.86199700
H	-3.36646800	-6.37333400	-1.55160700
H	-2.59994900	-5.84007100	-0.04335500
C	-2.34199200	-4.42322200	-3.22660800
H	-2.74981500	-5.28049500	-3.77455700
H	-3.14221400	-3.68195500	-3.12759600
H	-1.54578700	-3.97931300	-3.83462300
C	-0.73215500	-5.96616200	-2.08526400
H	0.10232000	-5.59259500	-2.68939400
H	-0.32919700	-6.35380900	-1.14288400
H	-1.17692600	-6.80949200	-2.62425800

CP4'

Ni	1.92853800	-0.00041400	0.00002600
I	4.42742100	-0.00024800	-0.00001200
C	-0.81246200	0.74119000	0.00005300
C	0.52481900	2.63116100	-0.00016700
C	-0.58364100	3.47341600	-0.00017000
C	-1.87581400	2.93182800	-0.00001000
C	-1.96104800	1.53097400	0.00009200
C	-0.81263200	-0.74110400	0.00009000
C	0.52424900	-2.63137200	0.00010200
C	-0.58439100	-3.47337500	0.00005100
C	-1.87645700	-2.93151100	0.00003300
C	-1.96138900	-1.53064300	0.00003900
H	1.53513600	3.02886800	-0.00025500
H	-0.41889200	4.54376300	-0.00032800
H	-2.93369800	1.05276200	0.00021500
H	1.53448100	-3.02928800	0.00007500
H	-0.41987800	-4.54375700	-0.00003700
H	-2.93393500	-1.05222000	-0.00001700
N	0.42673000	-1.29498100	0.00012900
N	0.42701900	1.29481200	-0.00004600
C	-3.15107200	3.78819700	0.00001700
C	-3.15190300	-3.78760600	-0.00005200
C	-2.83617700	5.29610500	-0.00043600
H	-3.77161500	5.86585900	-0.00039900
H	-2.26854500	5.59550300	0.88786500
H	-2.26889500	5.59503700	-0.88911700

C	-3.98300500	3.46355700	1.26431000
H	-4.89851500	4.06637000	1.27622100
H	-4.27918600	2.40975200	1.30163400
H	-3.41781600	3.68611100	2.17626600
C	-3.98354100	3.46292200	-1.26375500
H	-4.89906400	4.06571700	-1.27556800
H	-3.41875000	3.68503600	-2.17606400
H	-4.27972800	2.40909600	-1.30043900
C	-3.98403600	-3.46252900	1.26399700
H	-4.27993600	-2.40863500	1.30106900
H	-4.89971300	-4.06509100	1.27580700
H	-3.41911300	-3.68507700	2.17611800
C	-3.98403600	-3.46240100	-1.26406200
H	-4.89966800	-4.06502800	-1.27596900
H	-4.28002200	-2.40852800	-1.30100000
H	-3.41908400	-3.68478200	-2.17620700
C	-2.83735600	-5.29558700	-0.00014000
H	-2.26981000	-5.59479200	-0.88856200
H	-2.27012700	-5.59497500	0.88842000
H	-3.77292500	-5.86512600	-0.00035600

TS5'

Ni	-1.20968100	0.00007800	-1.06542200
I	-3.57267400	0.00023600	-1.91382700
C	-4.52300400	-0.00022700	3.54199400
C	-3.66064700	-1.27252900	3.53495600
C	-2.68759000	-1.27917600	2.32625700
C	-1.91030600	-0.00023800	2.26057700
C	-2.68745500	1.27877000	2.32651100
C	-3.66051200	1.27198500	3.53520900
H	-2.02165900	-2.14957600	2.37807900
H	-3.08036900	-1.32333600	4.46779300
H	-4.29796200	-2.16638000	3.50633300
H	-5.17230600	-0.00010400	2.65445100
H	-5.18651100	-0.00027900	4.41708600
H	-0.84450100	-0.00031500	2.47511900
H	-2.02143200	2.14908900	2.37850500
H	-3.28882000	1.39107800	1.40956000
H	-3.08022800	1.32254400	4.46805600
H	-4.29773300	2.16590900	3.50676400
H	-3.28896700	-1.39123800	1.40928400
C	1.43742400	-0.74111900	-0.34871500
C	0.15010900	-2.63278100	-0.70006000
C	1.22111300	-3.47378500	-0.41090300
C	2.46782000	-2.93057100	-0.07318800
C	2.54761100	-1.52977200	-0.04989000
C	1.43744900	0.74113200	-0.34865800
C	0.15020200	2.63286400	-0.69986600
C	1.22123600	3.47380900	-0.41064600
C	2.46792300	2.93052600	-0.07296900
C	2.54766400	1.52972300	-0.04977300
H	-0.82365200	-3.03226600	-0.96669500
H	1.06391100	-4.54436900	-0.45559600
H	3.48609700	-1.05036700	0.20341000
H	-0.82354500	3.03240300	-0.96647500
H	1.06407100	4.54440300	-0.45526100
H	3.48613400	1.05026700	0.20349000
N	0.24181500	1.29623600	-0.67295800
N	0.24177000	-1.29615700	-0.67305700
C	3.70068300	-3.78517500	0.25770600
C	3.70081500	3.78506300	0.25798800
C	3.39899400	-5.29352600	0.17548600
H	4.30311200	-5.86202400	0.41857000

H	2.62042600	-5.59396600	0.88578300
H	3.08246600	-5.59293000	-0.83003800
C	4.17586700	-3.46010900	1.69450700
H	5.05786700	-4.06158900	1.94358200
H	4.45062300	-2.40588800	1.80742500
H	3.39376200	-3.68385800	2.42863600
C	4.83202700	-3.45814200	-0.74677600
H	5.72053800	-4.05911200	-0.52062500
H	4.52358300	-3.68099400	-1.77431200
H	5.12533700	-2.40368800	-0.70561300
C	4.17599000	3.45987300	1.69476400
H	4.45071000	2.40563500	1.80760300
H	5.05801000	4.06130500	1.94388300
H	3.39389400	3.68359400	2.42891100
C	4.83214700	3.45806400	-0.74651900
H	5.72068000	4.05898600	-0.52032400
H	5.12542000	2.40359700	-0.70543500
H	4.52371100	3.68100300	-1.77403900
C	3.39918000	5.29343100	0.17588000
H	3.08266200	5.59292100	-0.82962100
H	2.62062300	5.59384500	0.88620000
H	4.30331800	5.86187900	0.41900600

TS6'-t

Ni	1.20847700	0.00044700	-1.09741000
I	3.58313300	0.00075300	-1.90243500
C	4.54297700	-0.00000700	3.44642600
C	3.68202600	1.27019100	3.53101600
C	2.59853100	1.28557600	2.42487600
C	1.83228000	-0.00077400	2.39515000
C	2.59946500	-1.28657900	2.42435400
C	3.68295500	-1.27086900	3.53049200
H	1.92695600	2.14305000	2.56043400
H	3.19435600	1.31149600	4.51583700
H	4.31249200	2.16529900	3.44866900
H	5.09574300	0.00039200	2.49576100
H	5.29390900	0.00010300	4.24767500
H	0.74660200	-0.00120000	2.40759800
H	1.92851000	-2.14459400	2.55956300
H	3.10905900	-1.43635300	1.45597500
H	3.19532200	-1.31294200	4.51529900
H	4.31407400	-2.16548200	3.44776700
H	3.10802100	1.43611700	1.45656100
C	-1.43376000	0.74119100	-0.36468700
C	-0.14739400	2.63279400	-0.72011500
C	-1.21680500	3.47380500	-0.42481600
C	-2.46186900	2.93061100	-0.08147500
C	-2.54218200	1.52971300	-0.05961000
C	-1.43353900	-0.74124600	-0.36484200
C	-0.14661400	-2.63238800	-0.72070500
C	-1.21576300	-3.47378300	-0.42554800
C	-2.46097700	-2.93103500	-0.08204600
C	-2.54171300	-1.53016600	-0.05988900
H	0.82537600	3.03222900	-0.99035900
H	-1.05940400	4.54437400	-0.46872900
H	-3.47955300	1.05035000	0.19778700
H	0.82626900	-3.03147000	-0.99106400
H	-1.05804200	-4.54429500	-0.46969100
H	-3.47921700	-1.05113900	0.19764800
N	-0.23907800	-1.29593300	-0.69392700
N	-0.23945400	1.29630400	-0.69362100
C	-3.69254300	3.78521800	0.25728400
C	-3.69137900	-3.78608300	0.25658900

C	-3.39080100	5.29355400	0.17507400
H	-4.29338900	5.86201000	0.42381300
H	-2.60827500	5.59297200	0.88142800
H	-3.07979600	5.59403000	-0.83185800
C	-4.15952700	3.45853200	1.69643100
H	-5.03977900	4.06014200	1.95124100
H	-4.43417800	2.40431700	1.80964800
H	-3.37313500	3.68099700	2.42633400
C	-4.82964600	3.45959700	-0.74114300
H	-5.71660300	4.06061800	-0.50918900
H	-4.52707200	3.68355200	-1.77018700
H	-5.12316500	2.40521900	-0.69946400
C	-4.15840000	-3.45983300	1.69582200
H	-4.43336500	-2.40572400	1.80926700
H	-5.03845900	-4.06176100	1.95054700
H	-3.37191000	-3.68221000	2.42564600
C	-4.82862200	-3.46060200	-0.74172400
H	-5.71538800	-4.06193700	-0.50985400
H	-5.12245800	-2.40632000	-0.69981800
H	-4.52602500	-3.68425700	-1.77082600
C	-3.38918500	-5.29431100	0.17405800
H	-3.07813100	-5.59448800	-0.83294900
H	-2.60653800	-5.59363700	0.88031700
H	-4.29159000	-5.86309100	0.42271900

CP9'-t

Ni	-1.52431000	-0.00187000	0.29636300
I	-3.26320600	0.00390900	2.22847900
C	-4.00224400	-0.00989200	-3.86657200
C	-3.21128700	1.25996400	-3.51853600
C	-2.77235700	1.25735700	-2.03635200
C	-1.98522500	-0.00552600	-1.66564900
C	-2.77189200	-1.27005800	-2.03176300
C	-3.21083800	-1.27820200	-3.51393000
H	-2.17733200	2.16046700	-1.83548200
H	-2.31699000	1.31553100	-4.15777800
H	-3.81185100	2.15441600	-3.73712500
H	-4.94844500	-0.00904200	-3.30484900
H	-4.27201800	-0.01187800	-4.93161900
H	-1.02530900	-0.00634200	-2.20987400
H	-2.17657400	-2.17225300	-1.82764700
H	-3.67209200	-1.34194300	-1.40219000
H	-2.31653400	-1.33578000	-4.15298300
H	-3.81109200	-2.17365600	-3.72924800
H	-3.67256600	1.33120200	-1.40702700
C	1.27050200	-0.74131200	0.15019900
C	-0.03555000	-2.64599400	0.33488100
C	1.07355300	-3.47864100	0.21952300
C	2.34975100	-2.92335600	0.05479200
C	2.42000000	-1.52297200	0.02405000
C	1.26919100	0.74233300	0.14868000
C	-0.04034200	2.64503500	0.32915900
C	1.06730800	3.47943000	0.21238700
C	2.34454800	2.92610300	0.04917300
C	2.41733700	1.52578000	0.02133200
H	-1.03362300	-3.05219500	0.46764100
H	0.92342800	-4.55008900	0.26309500
H	3.38168700	-1.03849200	-0.09588800
H	-1.03919200	3.04965300	0.46091000
H	0.91525100	4.55069400	0.25373000
H	3.37994000	1.04278600	-0.09723300
N	0.04837300	1.31095500	0.29436200
N	0.05072800	-1.31181100	0.29739700

C	3.62563700	-3.76790000	-0.08277800	N	-0.00295700	-1.25726900	0.03480400
C	3.61895300	3.77265500	-0.08976000	N	0.46306300	1.30391800	-0.08513200
C	3.32961200	-5.27848800	-0.02353100	C	4.38559900	3.10429600	0.57481500
H	4.26478900	-5.83909700	-0.12695400	C	3.15045600	-4.26172900	-0.39218100
H	2.87587000	-5.56933100	0.93061300	C	4.34939300	4.64425300	0.57740600
H	2.66389600	-5.59697900	-0.83367400	H	5.35826100	5.03420900	0.75024800
C	4.59656000	-3.41484000	1.06992400	H	4.00021900	5.04643900	-0.38023900
H	5.51314600	-4.00972200	0.98323900	H	3.70419700	5.03653800	1.37147600
H	4.88441000	-2.35818300	1.05576200	C	5.34675900	2.63990800	-0.54600900
H	4.14486100	-3.62690300	2.04538500	H	6.34369700	3.06667300	-0.38600900
C	4.29899300	-3.45476800	-1.44085900	H	5.45266600	1.54998000	-0.57065200
H	5.21369200	-4.04860200	-1.55144400	H	4.99177600	2.96558200	-1.53016100
H	3.63333100	-3.69736600	-2.27671400	C	4.92042000	2.62501200	1.94595000
H	4.57648900	-2.39885500	-1.52817100	H	5.91381400	3.05021700	2.13056100
C	4.59010900	3.42383700	1.06404000	H	4.25876200	2.94183000	2.75985700
H	4.87989100	2.36767800	1.05224400	H	5.01208000	1.53456100	1.99285800
H	5.50563900	4.02020400	0.97640600	C	3.96922700	-3.94719400	-1.66765600
H	4.13767400	3.63716200	2.03888400	H	4.42426500	-2.95175500	-1.62868600
C	4.29335700	3.45782700	-1.44692700	H	4.77804500	-4.67797900	-1.78308500
H	5.20701500	4.05308300	-1.55847000	H	3.33892500	-3.99363200	-2.56266300
H	4.57280100	2.40223400	-1.53187100	C	4.07471900	-4.18591800	0.84711600
H	3.62755400	3.69741600	-2.28353700	H	4.88573600	-4.91752400	0.75511000
C	3.32016700	5.28282800	-0.03387300	H	4.53138500	-3.19663700	0.95852700
H	2.65417900	5.59836200	-0.84495000	H	3.52119600	-4.40636200	1.76675000
H	2.86553400	5.57489900	0.91947000	C	2.60356900	-5.69729300	-0.50529900
H	4.25436600	5.84490900	-0.13815600	H	2.02888800	-5.98676900	0.38181200
				H	1.96450600	-5.82314400	-1.38655900
				H	3.43757600	-6.40070000	-0.60120800

CP10'

Ni	-1.29057800	0.22135200	-0.01785600
I	-2.76671900	2.07798300	-1.02021900
C	-5.54390700	-1.69842800	1.34668000
C	-4.74713300	-2.41401500	0.24502900
C	-3.71136600	-1.47037800	-0.40547800
C	-2.78568000	-0.84024300	0.64334200
C	-3.59902700	-0.10642500	1.72372500
C	-4.61296300	-1.06241800	2.39034000
H	-3.13726900	-2.02402300	-1.16371700
H	-4.22792600	-3.28093100	0.68427000
H	-5.42805400	-2.81305800	-0.51976500
H	-6.15932900	-0.91020100	0.88870100
H	-6.23991200	-2.39832900	1.82935000
H	-2.25587700	-1.64993500	1.17351300
H	-2.93324700	0.31574200	2.48952800
H	-4.14141600	0.73660900	1.28270600
H	-4.07276400	-1.85752600	2.92740300
H	-5.20097900	-0.51986400	3.14365300
H	-4.23601700	-0.67548200	-0.94880000
C	1.57023700	0.54192500	0.07854000
C	0.60882100	2.63449000	-0.04932400
C	1.83887700	3.25843300	0.15137000
C	2.99676300	2.49471400	0.33385600
C	2.82880800	1.10244300	0.29152400
C	1.31322300	-0.90981200	0.00790400
C	-0.29590900	-2.56051500	-0.10120800
C	0.66661200	-3.55579700	-0.23944300
C	2.02618100	-3.22709200	-0.24577400
C	2.32200200	-1.86240000	-0.12382600
H	-0.30129400	3.20608300	-0.19880600
H	1.86738500	4.34104100	0.16391000
H	3.68226900	0.45147100	0.44105000
H	-1.34702700	-2.81557100	-0.09750100
H	0.33018100	-4.57994300	-0.34352600
H	3.35274300	-1.53002800	-0.15443600

TS7'

Ni	-0.14507900	-1.58047800	-0.05916600
C	0.83607800	-4.49024500	3.26692800
C	-0.67169600	-4.44404600	2.98217700
C	-1.01091100	-3.44958600	1.84473100
C	-0.18073000	-3.77519400	0.59687000
C	1.32920000	-3.78410700	0.87190700
C	1.64063400	-4.80085900	1.99663400
H	-2.08349400	-3.49663700	1.62249100
H	-1.02085400	-5.44343700	2.68817700
H	-1.22849100	-4.16877700	3.88599700
H	1.16114800	-3.52175900	3.67557600
H	1.04737600	-5.23904600	4.03918300
H	-0.44918300	-4.77902600	0.26209600
H	1.88455800	-4.04890900	-0.03617700
H	1.69186100	-2.79840600	1.19481100
H	1.39856900	-5.81290700	1.64368900
H	2.71663900	-4.78932900	2.20916500
H	-0.80235600	-2.43070100	2.21104600
C	-5.37400800	2.65394900	-2.67297700
C	-4.21343600	1.93412100	-2.85002100
C	-3.96980700	0.75100200	-2.09738400
C	-4.95905100	0.32121000	-1.15089100
C	-6.14271800	1.08448800	-0.99226300
C	-6.34801000	2.22737200	-1.73647300
H	-2.05039600	0.31799500	-2.98111700
H	-5.55001300	3.55316500	-3.25650100
H	-3.46877900	2.25868200	-3.57286300
C	-2.79017000	-0.01319200	-2.25450800
C	-4.71025400	-0.86930000	-0.41152800
H	-6.89124000	0.75158600	-0.27730200
H	-7.26047000	2.80287500	-1.61079000
C	-3.55686900	-1.59346400	-0.58652500
C	-2.55242600	-1.17978700	-1.52352800

H	-5.46282700	-1.21102300	0.29538700	C	-0.21859600	-0.21952800	4.38953900
H	-3.41887900	-2.50802400	-0.01699900	H	0.28579900	-2.31653600	4.35279400
C	-1.30836200	-1.91287400	-1.72201800	H	-0.54840900	1.89794500	4.13414200
H	-0.68444400	-1.56283500	-2.54214700	H	-0.64694000	-0.25273500	5.38822900
C	-1.03572600	-3.24217500	-1.20324800	I	4.91502100	1.06309400	1.18799400
H	-1.91285000	-3.81189800	-0.90577500	C	2.57401100	-4.56149800	-1.84827000
H	-0.34329700	-3.83359800	-1.79912100	C	2.95972000	-3.96525000	-0.48806500
C	0.95270700	0.94818900	0.66952400	C	2.54033700	-2.47999800	-0.38756800
C	-1.09930400	0.63981400	1.70843800	C	1.03259000	-2.30007000	-0.63555300
C	-1.03296600	1.88668100	2.32025200	C	0.67870400	-2.87501700	-2.01841200
C	0.07905800	2.71240000	2.10868800	C	1.08033600	-4.36235300	-2.14074600
C	1.07434100	2.20562900	1.25615500	H	2.83579100	-2.12500200	0.61286800
C	1.94897300	0.36930600	-0.26829400	H	2.46679100	-4.53403900	0.31452500
C	2.46714700	-1.42796800	-1.63373800	H	4.04070000	-4.05523400	-0.32085500
C	3.64888400	-0.83095400	-2.06037800	H	3.16270700	-4.07018900	-2.63631400
C	4.01196700	0.42952700	-1.56736800	H	2.83297000	-5.62805200	-1.88219000
C	3.12088500	1.01759800	-0.65462900	H	0.52236400	-2.87836500	0.14861700
H	-1.96224800	-0.00382500	1.84888600	H	-0.38957500	-2.76402100	-2.24197100
H	-1.85542600	2.19724300	2.95190300	H	1.20745600	-2.30195700	-2.78906800
H	1.95046900	2.80657900	1.04711600	H	0.48960500	-4.96397400	-1.43152100
H	2.17446700	-2.40497800	-2.00638000	H	0.83518600	-4.73356300	-3.14506200
H	4.27049500	-1.36000800	-2.77159200	H	3.12167800	-1.91354900	-1.12623100
H	3.34782000	1.99405600	-0.24526300	C	-2.73652800	-0.46646500	-0.13383400
N	1.63229800	-0.85635500	-0.75672500	C	-2.05902400	-2.66520100	-0.11740400
N	-0.13141800	0.16624900	0.90961700	C	-3.34744700	-3.11822900	0.14564800
C	0.23298800	4.09973500	2.74552600	C	-4.39600800	-2.20417600	0.29115000
C	5.29784100	1.15838000	-1.97966300	C	-4.04835900	-0.85589000	0.14432600
C	-0.96675400	4.46077400	3.64156600	C	-2.33915500	0.94632800	-0.30008600
H	-0.81146900	5.45378500	4.07481800	C	-0.59413300	2.42681700	-0.55641600
H	-1.90560700	4.49405800	3.07729000	C	-1.45414200	3.51965300	-0.58379600
H	-1.08487300	3.75668200	4.47307200	C	-2.83607800	3.32642100	-0.48211100
C	0.34661400	5.16066900	1.62283500	C	-3.25735800	1.99854400	-0.34034000
H	0.45657000	6.15648700	2.06549800	H	-1.25133600	-3.37763900	-0.22046600
H	1.21501200	4.98911600	0.97763000	H	-3.50679200	-4.18562600	0.23689000
H	-0.54863400	5.16796300	0.99137300	H	-4.80972000	-0.09479900	0.25979500
C	1.51774700	4.11846000	3.61011600	H	0.47291900	2.57078300	-0.67131600
H	1.64066700	5.10585800	4.06790800	H	-1.02389100	4.50694400	-0.69665100
H	1.46590800	3.37690700	4.41499200	H	-4.31568700	1.78060900	-0.27130000
H	2.41728800	3.91476500	3.01920100	N	-1.00771600	1.15876400	-0.41914500
C	4.92377900	2.51045900	-2.63586300	N	-1.73254300	-1.37265600	-0.25813300
H	4.37033700	3.16310200	-1.95209200	C	-5.84394000	-2.61171300	0.59695200
H	5.83447700	3.04123100	-2.93345300	C	-3.85837200	4.47109700	-0.52606700
H	4.31140600	2.36127000	-3.53203000	C	-6.00148900	-4.13973700	0.71166900
C	6.15958600	1.41397900	-0.71848900	H	-7.04661800	-4.38523400	0.92821100
H	7.08031700	1.93622200	-0.99978300	H	-5.72996200	-4.64983300	-0.21952800
H	5.64007100	2.03561800	0.01871000	H	-5.39165300	-4.55383900	1.52257000
H	6.43990600	0.47344900	-0.23142400	C	-6.76545000	-2.10843600	-0.54034400
C	6.12996200	0.33934900	-2.98438400	H	-7.80414100	-2.39096100	-0.33373700
H	6.44881700	-0.62229100	-2.56641400	H	-6.73258500	-1.01854600	-0.64358300
H	5.58187500	0.15033100	-3.91440000	H	-6.47965600	-2.54616400	-1.50336500
H	7.03466800	0.89644900	-3.24705900	C	-6.27962500	-1.97191400	1.93738900
				H	-7.31376300	-2.25291700	2.16777900
				H	-5.64320900	-2.31146100	2.76212900
				H	-6.23217000	-0.87818700	1.90517600
				C	-4.80784600	4.25732500	-1.72973800
				H	-5.35720900	3.31251000	-1.65717500
				H	-5.54476400	5.06757100	-1.77360100
				H	-4.25247200	4.25162700	-2.67416400
				C	-4.67851200	4.47207300	0.78659000
				H	-5.41463800	5.28393800	0.76754000
				H	-5.22387200	3.53326900	0.93130100
				H	-4.03028900	4.62211200	1.65721900
				C	-3.17999500	5.84572500	-0.67798300
				H	-2.50917300	6.06560400	0.16021400
TS12'							
Ni	0.16141800	-0.54749100	-0.41296600				
I	1.91311300	0.66070100	-2.30597600				
Zn	2.52788500	0.27742900	0.45796000				
C	0.90675100	-0.13485100	1.76968600				
C	0.86272700	-1.32504300	2.52727800				
C	0.38442400	1.01817800	2.40081500				
C	0.30386600	-1.37568900	3.80709500				
H	1.27428200	-2.24417600	2.11944700				
C	-0.16770500	0.98409500	3.68325600				
H	0.41108300	1.97782300	1.88927700				

H	-2.60483200	5.91738600	-1.60786800
H	-3.94376900	6.63029600	-0.70245100

CP12'

Ni	1.45021400	0.23072400	-0.02893400
C	2.58073300	1.72183100	-0.32029300
C	3.12152800	2.51629900	0.71099900
C	2.83699000	2.14693600	-1.63982900
C	3.85700600	3.67658600	0.44587100
H	2.97234900	2.22159600	1.74940600
C	3.58043200	3.30109300	-1.91599900
H	2.44879800	1.56918000	-2.47820900
C	4.09150800	4.07594600	-0.87266600
H	4.25409800	4.26648600	1.27062100
H	3.76090100	3.59403200	-2.94919000
H	4.66859600	4.97352000	-1.08310700
C	4.76801700	-3.21532700	0.80143200
C	4.93885300	-2.35605800	-0.46034800
C	3.63722100	-1.60657400	-0.81769900
C	3.09176000	-0.78804800	0.36830300
C	2.96716100	-1.63163900	1.65675600
C	4.28216400	-2.37049500	1.98882400
H	3.82316000	-0.93636100	-1.66709500
H	5.73578600	-1.61880000	-0.28357800
H	5.26927100	-2.97880400	-1.30437400
H	4.03466200	-4.01355300	0.60073100
H	5.71093800	-3.72089900	1.05166700
H	3.86968500	-0.04833900	0.59083000
H	2.69450600	-0.98137300	2.49972400
H	2.16666600	-2.38234300	1.59084700
H	5.05601300	-1.62969200	2.23872300
H	4.15302900	-3.00235000	2.87972400
H	2.90750400	-2.34901200	-1.17882700
C	-1.40458400	0.63744800	0.03044600
C	-0.32060800	2.67159100	-0.07098000
C	-1.51791900	3.36735700	0.07906900
C	-2.72376600	2.67357700	0.22947800
C	-2.63357300	1.27454000	0.20122900
C	-1.23837000	-0.82857000	-0.04355300
C	0.25709200	-2.57193600	-0.18003400
C	-0.76671800	-3.50931000	-0.29257000
C	-2.10247600	-3.09620600	-0.27147500
C	-2.30983500	-1.71548100	-0.14988600
H	0.62342700	3.19298200	-0.17364900
H	-1.48351400	4.44998500	0.08190700
H	-3.52875600	0.67618500	0.32357000
H	1.28947400	-2.88939800	-0.19873900
H	-0.49648200	-4.55306600	-0.39597400
H	-3.31936300	-1.32220600	-0.15717100
N	0.05316100	-1.25382100	-0.04472200
N	-0.24700400	1.33264000	-0.09275000
C	-4.08251300	3.36397600	0.41926900
C	-3.29260800	-4.05937700	-0.38635700
C	-3.95714600	4.89925500	0.41444200
H	-4.94676200	5.34871100	0.55077700
H	-3.31672500	5.25919600	1.22748800
H	-3.55292200	5.27299600	-0.53306700
C	-4.69116100	2.92763500	1.77377900
H	-5.66398000	3.41099600	1.92192600
H	-4.84721400	1.84468000	1.82382800
H	-4.03994400	3.21169400	2.60796700
C	-5.03119700	2.94817300	-0.73080800
H	-6.00713100	3.43203200	-0.60699800

H	-4.62519600	3.24636400	-1.70396400
H	-5.19791500	1.86587600	-0.75393000
C	-4.18088700	-3.92280700	0.87373800
H	-4.57151600	-2.90639800	0.99172000
H	-5.03820300	-4.60252100	0.80463100
H	-3.62002000	-4.17440500	1.78084100
C	-4.12086400	-3.69949200	-1.64341500
H	-4.97646300	-4.37856100	-1.73636900
H	-4.51147700	-2.67725700	-1.59882300
H	-3.51605100	-3.78847800	-2.55278300
C	-2.83932000	-5.52668800	-0.50568600
H	-2.22903700	-5.69423700	-1.40032000
H	-2.26340900	-5.84859900	0.36932200
H	-3.71740700	-6.17728300	-0.57989400

TS13'

Ni	1.40676600	-0.10223100	-0.01139500
C	2.90846400	-1.21552600	-0.03787900
C	3.22613900	-1.98364600	-1.20854200
C	3.03437900	-1.91181500	1.20923400
C	3.57626600	-3.32480600	-1.13330600
H	3.18267800	-1.50418700	-2.18429400
C	3.36353800	-3.26520800	1.26570100
H	2.85207500	-1.37900100	2.13897500
C	3.64466000	-3.99020100	0.10307800
H	3.79382200	-3.86964400	-2.05091300
H	3.41414500	-3.75826100	2.23533300
H	3.92363900	-5.03892000	0.15405900
C	4.57270800	3.23693000	0.00592100
C	4.73163800	2.32251000	1.23075500
C	3.61770000	1.25774200	1.29311200
C	3.56588400	0.44488300	-0.01851700
C	3.38754600	1.36300600	-1.25274700
C	4.50472300	2.42666100	-1.29799400
H	3.79944400	0.58844000	2.14165700
H	5.70751200	1.81710800	1.17892800
H	4.73630600	2.91882100	2.15331100
H	3.64856200	3.82688500	0.11278200
H	5.39636400	3.96150400	-0.03904400
H	4.57931400	0.04179800	-0.12928700
H	3.41035600	0.76832200	-2.17334100
H	2.41459400	1.87232500	-1.23991100
H	5.46950200	1.92316000	-1.45977800
H	4.35219400	3.09626000	-2.15526800
H	2.65851200	1.75449900	1.49071100
C	-1.37671200	-0.62826200	-0.07032900
C	-0.17004700	-2.57417500	-0.41072500
C	-1.31831800	-3.35310600	-0.32241500
C	-2.56273200	-2.75489200	-0.06544500
C	-2.55857000	-1.36003100	0.06406500
C	-1.29706600	0.83999400	0.03270100
C	0.09153700	2.66275400	0.30175000
C	-0.97376500	3.55402200	0.23814100
C	-2.27820500	3.07311300	0.04728800
C	-2.40727300	1.68290800	-0.06038800
H	0.80414600	-3.01985900	-0.58754800
H	-1.22350600	-4.42468100	-0.45147400
H	-3.48044300	-0.83507900	0.29062900
H	1.10314300	3.03205600	0.44480000
H	-0.76913300	4.61296100	0.34111700
H	-3.38250100	1.24352800	-0.23873000
N	-0.03639500	1.32945400	0.20648900
N	-0.17927300	-1.23539300	-0.29191300

C	-3.86968800	-3.54864900	0.08529700
C	-3.51086000	3.98378900	-0.05617100
C	-3.65491100	-5.06159000	-0.10991400
H	-4.61006900	-5.58658700	0.00244900
H	-3.26617700	-5.29297900	-1.10811500
H	-2.96210800	-5.47420300	0.63206600
C	-4.89093900	-3.06289900	-0.97125600
H	-5.83128500	-3.61860800	-0.87321700
H	-5.12111500	-1.99806200	-0.85782200
H	-4.50929900	-3.21693300	-1.98696100
C	-4.44774500	-3.31838600	1.50242800
H	-5.38438500	-3.87574900	1.62491700
H	-3.74619100	-3.65821400	2.27257400
H	-4.66266400	-2.26074600	1.68900400
C	-4.17398800	3.79093800	-1.44134100
H	-4.49562500	2.75621200	-1.60018400
H	-5.05901000	4.43248900	-1.52912600
H	-3.48161800	4.05417400	-2.24892000
C	-4.52082300	3.60738800	1.05446900
H	-5.40958700	4.24638100	0.98976200
H	-4.85251300	2.56711300	0.96972100
H	-4.07945100	3.73862500	2.04892200
C	-3.14681400	5.47201900	0.10429900
H	-2.69062900	5.67769000	1.07939000
H	-2.45597300	5.80977000	-0.67655200
H	-4.05315200	6.08284500	0.02879500

CP1-2

Ni	0.22185000	-2.07448600	-0.40562500
C	3.90756200	0.13098700	2.08566000
C	4.98728200	-0.89376500	1.67451000
C	2.58717900	-0.51222100	1.62503600
H	3.93411500	0.34590600	3.15665200
H	4.06549800	1.07151100	1.54915900
H	5.24879900	-1.57839200	2.49552700
H	5.91391700	-0.42173600	1.32811300
H	1.85326700	0.20049000	1.24319900
H	2.09924200	-1.09580300	2.41657600
N	4.35524400	-1.63330000	0.58398800
C	5.08399300	-2.58492000	-0.22935500
H	5.50308500	-3.38853800	0.39034500
H	4.39159000	-3.01575200	-0.95410400
H	5.90558800	-2.08755300	-0.75832200
C	3.00895000	-1.47932400	0.53415700
O	2.27436000	-2.06954200	-0.27198900
C	-6.72601900	0.56097800	-0.63082500
C	-5.80735600	-0.44756400	-0.82302600
C	-4.61901700	-0.51297700	-0.04410100
C	-4.39677400	0.49479800	0.95036900
C	-5.36184200	1.52012700	1.12475600
C	-6.50307400	1.55624400	0.35240600
H	-3.84249100	-2.30421800	-0.96572600
H	-7.62881900	0.59620800	-1.23522100
H	-5.97949500	-1.21182600	-1.57776900
C	-3.65410900	-1.53893400	-0.21422200
C	-3.20680500	0.41654500	1.72600800
H	-5.18593600	2.28061400	1.88286600
H	-7.23544400	2.34632800	0.49540700
C	-2.29193800	-0.59003600	1.53203000
C	-2.49346000	-1.60674000	0.54581200
H	-3.03087700	1.17215300	2.48940500
H	-1.39475300	-0.61775500	2.14290700
C	-1.51219200	-2.68547800	0.31283400

H	-1.88371800	-3.47152800	-0.34878500
C	-0.42910200	-3.02129100	1.18023800
H	-0.29602500	-2.50606100	2.13216100
H	-0.07138200	-4.05144100	1.18793900
C	1.17545900	4.91332500	0.64135400
C	0.39636300	3.82046200	0.33122600
C	0.91516300	2.75283300	-0.45301900
C	2.26898900	2.83625800	-0.91821700
C	3.04481600	3.97683300	-0.58355900
C	2.51280900	4.99380200	0.18020500
H	-0.88408300	1.55432900	-0.42336600
H	0.76479500	5.72172900	1.24046800
H	-0.63129900	3.75820100	0.68144100
C	0.13990700	1.61277200	-0.78638700
C	2.77478400	1.76578300	-1.70825700
H	4.06910400	4.03813000	-0.94539300
H	3.11623500	5.86283700	0.42843600
C	1.99898400	0.67354600	-2.01093900
C	0.65213800	0.56637000	-1.54441500
H	3.79342300	1.83175600	-2.08548200
H	2.40930400	-0.12033800	-2.62627900
C	-0.19880200	-0.60009400	-1.83675300
H	-1.26467500	-0.42381700	-1.70691100
C	0.19733800	-1.78601600	-2.43870000
H	1.21305600	-1.94376800	-2.79298400
H	-0.55277400	-2.46042400	-2.84370100

CP1-3

Ni	1.26749500	0.05694300	0.54423000
C	5.83772100	1.91098500	0.18021900
C	6.40090100	0.69977400	-0.59508800
C	4.46825100	1.42603500	0.68960900
H	6.50855200	2.23278400	0.98063700
H	5.70553700	2.75535000	-0.50427500
H	7.05502800	0.07256700	0.03019600
H	6.97215800	0.98992000	-1.48452500
H	3.68305400	2.18379900	0.69454200
H	4.51460000	1.01477500	1.70608800
N	5.20293800	-0.04137300	-0.97819200
C	5.24438300	-1.16961700	-1.88547800
H	5.88272000	-1.97043500	-1.48818600
H	4.22730600	-1.54641000	-2.00469000
H	5.63812100	-0.86135400	-2.86117900
C	4.10352600	0.29472100	-0.25357600
O	3.01038700	-0.27677100	-0.36594200
C	-2.83635100	-2.86241700	-0.90866900
C	-2.24058200	-3.49939100	0.36509500
C	-1.61501200	-2.26147000	-1.62563800
H	-3.38116400	-3.59119100	-1.51439100
H	-3.53079700	-2.06436400	-0.63028700
H	-2.01725600	-4.56979600	0.23437500
H	-2.89900500	-3.40220700	1.23599000
H	-1.81522200	-1.31209600	-2.12788700
H	-1.18296200	-2.94569600	-2.36784800
N	-1.00546900	-2.74915400	0.57922700
C	-0.22284700	-2.90200100	1.78824400
H	0.16426500	-3.92687900	1.87547300
H	0.60982200	-2.19469800	1.75518600
H	-0.83992200	-2.68413100	2.66740100
C	-0.59660000	-2.05778300	-0.51370800
O	0.44391800	-1.39557100	-0.61814100
C	-6.07972500	0.70268300	-0.08418600
C	-4.97218500	0.39153700	0.67612600

C	-3.70373200	0.97869600	0.40369800
C	-3.60631300	1.91195400	-0.68148300
C	-4.76390800	2.21216800	-1.44296100
C	-5.97776800	1.62184300	-1.15657900
H	-2.63871800	-0.02229900	1.99109100
H	-7.03978400	0.24476800	0.14175700
H	-5.05573900	-0.30671200	1.50708000
C	-2.54414700	0.67728900	1.16123100
C	-2.33542600	2.49808200	-0.94227100
H	-4.67870900	2.92232000	-2.26333000
H	-6.85724800	1.86197600	-1.74825800
C	-1.23126700	2.17586000	-0.19324500
C	-1.29950100	1.23957200	0.89045600
H	-2.24919000	3.21248500	-1.75908300
H	-0.27340200	2.62867800	-0.43041900
C	-0.11020400	0.83990600	1.65881100
H	-0.35467400	0.22344200	2.52926400
C	1.14907700	1.55822900	1.70196600
H	1.22303500	2.54312500	1.22869000
H	1.71326400	1.51037100	2.63810900

CP1-4

Ni	0.04116600	0.44739100	0.17075800
C	-2.03433100	-1.56262400	-1.10109700
C	-2.25968300	-0.10187400	-1.53431000
C	-2.22923500	-1.53102200	0.42352000
H	-2.73513300	-2.23422800	-1.60574800
H	-1.01742500	-1.88368700	-1.33677800
H	-3.32954400	0.10382500	-1.69631800
H	-1.71569100	0.17410900	-2.44144300
H	-1.56993000	-2.22215500	0.95373400
H	-3.26302000	-1.76061800	0.71839200
N	-1.79926600	0.70896000	-0.38317300
C	-2.27625400	2.09769600	-0.32829700
H	-3.36513300	2.13287300	-0.47763700
H	-2.04238900	2.50229500	0.65717300
H	-1.78620200	2.69176100	-1.10340600
C	-1.95563900	-0.08747100	0.83914100
O	-2.11784900	0.41811300	1.94730700
C	2.73823100	1.13945400	-1.13111200
C	2.85995900	0.95480600	0.39187000
C	2.31044200	-0.25000300	-1.62612400
H	1.96508000	1.88263000	-1.35447300
H	3.67924800	1.48425200	-1.57027500
H	2.72066100	1.87945300	0.95860300
H	3.84095200	0.53051500	0.65749300
H	3.18173500	-0.88606200	-1.84126000
H	1.69092500	-0.23065800	-2.52626400
N	1.81050400	-0.03174300	0.72744000
C	1.92550600	-0.69929300	2.03010900
H	1.67115500	-0.00253800	2.83222100
H	1.23724300	-1.54467800	2.03997500
H	2.94926700	-1.07214700	2.17736300
C	1.56674300	-0.88947300	-0.44792500
O	1.21565700	-2.07231100	-0.36319200

CP1-5

Ni	0.19555900	-0.54282000	-0.12734100
C	3.01474500	-3.18643500	-1.34966500
C	3.44525400	-2.48714700	-0.04578400
C	1.51340400	-2.83435000	-1.47719800
H	3.61088500	-2.85723400	-2.20706800
H	3.15073100	-4.26830800	-1.24643000

H	3.77395200	-1.44601800	-0.24847100
H	4.27027700	-2.99960000	0.46495400
H	0.89450900	-3.72103700	-1.66407200
H	1.32280200	-2.12822500	-2.29064500
N	2.23862700	-2.52103300	0.75986800
C	2.29714800	-1.85336100	2.03723900
H	2.56181600	-0.78019700	1.94468300
H	1.31881300	-1.92575200	2.51875200
H	3.04337500	-2.33739800	2.67985300
C	1.12714900	-2.21683800	-0.11485100
O	-0.11037600	-2.28846600	0.35714100
C	-4.47607600	-1.68959500	0.19853200
C	-5.07244600	-0.28587000	-0.04394500
C	-3.03288200	-1.41299300	0.65473900
H	-5.05915200	-2.26193400	0.92449600
H	-4.46899500	-2.25191800	-0.74115300
H	-5.61179000	0.09682700	0.83680200
H	-5.76380500	-0.25472600	-0.89431200
H	-2.28084200	-2.13004700	0.31547200
H	-2.94321500	-1.35904100	1.74813500
N	-3.89583900	0.53525200	-0.31533000
C	-3.99308200	1.89322900	-0.80307400
H	-4.52813200	2.53467100	-0.08888800
H	-2.98007500	2.27526500	-0.94063400
H	-4.52647500	1.92088900	-1.76088400
C	-2.73063400	-0.03367000	0.09954200
O	-1.62697000	0.52884400	0.03561100
C	2.47248200	4.30672900	-0.51268900
C	1.69329900	4.07900000	0.79851900
C	1.91095200	3.22986900	-1.45499700
H	2.35369100	5.32476200	-0.89229800
H	3.54008800	4.13522900	-0.34024100
H	0.79144900	4.70785000	0.86058000
H	2.29539600	4.27543200	1.69297700
H	2.64198300	2.80911100	-2.14988400
H	1.06762200	3.59960400	-2.05306400
N	1.32225000	2.66659100	0.73963300
C	0.75583300	1.99930700	1.89657300
H	-0.20534000	2.45201400	2.17395500
H	0.59393600	0.94288300	1.65241000
H	1.44585300	2.07813200	2.74474700
C	1.38629000	2.15260100	-0.51598600
O	1.07373500	1.01452200	-0.88839500

TS14

Ni	0.49015500	-1.38909700	-0.09637400
I	4.12004300	1.10961500	-0.47162300
C	4.96922800	-2.92836900	0.95522600
C	4.62363700	-2.61021600	-0.50511500
C	3.12096600	-2.28930900	-0.68191600
C	2.56698100	-1.32770900	0.34233500
C	3.05696300	-1.45414400	1.76203200
C	4.56122300	-1.78058900	1.88787200
H	2.91618900	-1.93618500	-1.69630500
H	5.20486000	-1.74647200	-0.84411600
H	4.87774500	-3.45700600	-1.15457900
H	4.46174100	-3.85584700	1.26346000
H	6.04557600	-3.11886200	1.04767400
H	2.02823500	-0.39738300	0.05053700
H	2.79882500	-0.55675500	2.33155200
H	2.50710400	-2.28900200	2.21987100
H	5.13692100	-0.88194100	1.64328300
H	4.77788700	-2.03872700	2.93181300

H	2.56991600	-3.23669000	-0.55516700
C	-6.83102500	-1.85457800	-1.13010500
C	-5.55988200	-2.37531800	-1.23082700
C	-4.55085300	-2.01685000	-0.29520700
C	-4.87983300	-1.10460800	0.76024700
C	-6.19856000	-0.58675700	0.83686300
C	-7.15414000	-0.95176800	-0.08733000
H	-2.99480200	-3.23711900	-1.16355700
H	-7.59291200	-2.13584900	-1.85188400
H	-5.31075700	-3.06968600	-2.02993500
C	-3.23183800	-2.53238900	-0.36816700
C	-3.86354900	-0.75617900	1.69345900
H	-6.44444600	0.10378200	1.64022600
H	-8.16083900	-0.54895900	-0.01836200
C	-2.59496400	-1.26905400	1.59222100
C	-2.24822000	-2.17926500	0.54688900
H	-4.10717000	-0.06554000	2.49721700
H	-1.84289300	-0.97570400	2.31751400
C	-0.90453300	-2.77267200	0.42809700
H	-0.83376200	-3.56519000	-0.31714900
C	0.13164800	-2.67645600	1.37065100
H	-0.00857600	-2.15554200	2.31612800
H	0.88657800	-3.45851800	1.38839700
C	-0.69345000	5.65812300	0.94392600
C	0.03552800	4.60779000	0.43133800
C	-0.61788400	3.44925600	-0.07121800
C	-2.04902600	3.38899100	-0.03719400
C	-2.77048200	4.48841800	0.49526100
C	-2.10854800	5.59821700	0.97575400
H	1.19127000	2.40737000	-0.63742400
H	-0.18454500	6.53882300	1.32594500
H	1.12153300	4.64754700	0.40402300
C	0.10503500	2.35420400	-0.60799800
C	-2.69018200	2.22441300	-0.54559300
H	-3.85689300	4.44195500	0.51767600
H	-2.67197400	6.43429800	1.38137200
C	-1.96531500	1.17573800	-1.05364900
C	-0.53841700	1.22236100	-1.09319000
H	-3.77621600	2.17363900	-0.52767500
H	-2.48672700	0.30467900	-1.43640200
C	0.27914700	0.13271600	-1.65607100
H	1.31668700	0.40740700	-1.85431900
C	-0.15797700	-1.09445100	-2.10455500
H	-1.20984000	-1.36221900	-2.12473500
H	0.50460500	-1.72245800	-2.69478900

CP13

Ni	0.39244700	1.15487300	0.08000300
C	2.55257800	5.37662700	-0.45436500
C	1.11841800	5.40528200	0.08993800
C	0.37226500	4.07740200	-0.21363700
C	1.17784100	2.91531800	0.34417400
C	2.59083600	2.83781700	-0.22449200
C	3.33433800	4.16952100	0.07961300
H	-0.63132800	4.11366700	0.22672700
H	1.13643400	5.56807300	1.17615300
H	0.55244900	6.23764000	-0.34470500
H	2.52662500	5.33820400	-1.55283600
H	3.07224000	6.30460600	-0.18801600
H	1.21308100	2.98683400	1.43761000
H	3.15649800	1.99963500	0.20045500
H	2.56702500	2.69353700	-1.31155600
H	3.47155400	4.26593500	1.16520900

H	4.33579600	4.12388000	-0.36439100
H	0.25700900	3.98938400	-1.30187200
C	4.99911400	-3.96830000	-0.50274100
C	4.62865600	-2.76420700	0.05176100
C	3.26600800	-2.50394900	0.36561900
C	2.28149900	-3.51398600	0.09778900
C	2.69730400	-4.74317000	-0.47270600
C	4.02615400	-4.96448700	-0.76666500
H	3.59847700	-0.52444200	1.15641200
H	6.04119300	-4.16178300	-0.73840400
H	5.37270200	-1.99955000	0.25938800
C	2.84795800	-1.28221800	0.94052100
C	0.92278600	-3.24737200	0.42821300
H	1.95418400	-5.51069500	-0.67190000
H	4.33474200	-5.91023900	-1.20211000
C	0.54160900	-2.05222000	0.98643200
C	1.51168300	-1.03399400	1.25245100
H	0.18136200	-4.02114300	0.24651800
H	-0.49845100	-1.89433600	1.25144200
C	1.15938700	0.26361100	1.83771000
H	2.00469300	0.86838400	2.16195800
C	-0.11133400	0.74696200	2.08962000
H	-1.00089200	0.13347300	1.96735100
H	-0.24521900	1.66381300	2.65433500
C	-6.51628800	-0.51866300	0.84126700
C	-5.53096200	0.38114100	0.50373800
C	-4.33465800	-0.06242900	-0.12582200
C	-4.16779800	-1.46101600	-0.40574600
C	-5.20236000	-2.35977800	-0.04679700
C	-6.35022000	-1.89837200	0.56353100
H	-3.43853200	1.89262500	-0.29381400
H	-7.42807600	-0.17451100	1.31980400
H	-5.65588500	1.44087300	0.71045300
C	-3.30423500	0.83136100	-0.49350600
C	-2.97057400	-1.89169900	-1.04708500
H	-5.08108600	-3.41798500	-0.26220400
H	-7.13784700	-2.59570500	0.83312200
C	-1.98290600	-1.00337800	-1.39055700
C	-2.13397100	0.39259000	-1.11311500
H	-2.85604300	-2.94731000	-1.27951600
H	-1.09416600	-1.36179800	-1.89942100
C	-1.12740500	1.38743800	-1.47647800
H	-1.45492800	2.42124400	-1.39275500
C	0.13578600	1.15331200	-1.99136800
H	0.46393000	0.15367400	-2.27180300
H	0.70488300	1.97270600	-2.41550800

TS15

Ni	-0.36494700	-1.57173200	-1.43960900
C	6.90348300	-0.29944800	1.51291000
C	5.82273400	-1.07590600	1.15767300
C	4.99132300	-0.70761500	0.06460400
C	5.29589300	0.48718000	-0.66566000
C	6.41787800	1.26428600	-0.27590400
C	7.20419500	0.88122400	0.79009500
H	3.66326000	-2.40747300	0.20757100
H	7.53169900	-0.59121300	2.34990900
H	5.59106200	-1.98416200	1.70876200
C	3.87612500	-1.48814300	-0.33441500
C	4.45507300	0.84843200	-1.75636400
H	6.64870100	2.16825700	-0.83459400
H	8.06111500	1.48370100	1.07861100
C	3.38152500	0.07300300	-2.11499100

C	3.07355500	-1.12981700	-1.40902200
H	4.67726200	1.75899100	-2.30719700
H	2.76428700	0.37469200	-2.95555600
C	2.01118700	-2.05233700	-1.82706000
H	1.95302700	-2.97903800	-1.25970700
C	1.22573600	-1.96269900	-2.94542300
H	1.30849500	-1.13176900	-3.64193800
H	0.70690500	-2.84663400	-3.29817500
C	3.58652700	4.93680500	0.73012700
C	3.34735600	3.58054200	0.77348200
C	2.03101400	3.06819300	0.60412000
C	0.95502500	3.99078800	0.39269500
C	1.23491600	5.38052500	0.35083300
C	2.52220900	5.84636000	0.51521700
H	2.57166600	0.98973300	0.81904500
H	4.59669300	5.31509000	0.86339400
H	4.16375600	2.88251500	0.93869700
C	1.74948100	1.67920600	0.64757800
C	-0.35947200	3.46818500	0.23898800
H	0.41381200	6.07554200	0.18982000
H	2.72427300	6.91365900	0.48358300
C	-0.60234900	2.11925500	0.29455400
C	0.45864100	1.18133700	0.50264000
H	-1.18418300	4.15894900	0.07939700
H	-1.61895200	1.76197200	0.17738300
C	0.21593300	-0.25861400	0.64495200
H	1.10421100	-0.86188200	0.82127400
C	-1.01344100	-0.84105300	0.88915400
H	-1.93823200	-0.30134300	0.72273000
H	-1.09313400	-1.91356100	1.02077000
C	-6.11100100	3.30673600	0.43881600
C	-5.59408300	2.04519800	0.24225200
C	-4.58121100	1.81823400	-0.72914900
C	-4.10769100	2.92548000	-1.50609500
C	-4.66108600	4.21249700	-1.27992800
C	-5.64046400	4.40071400	-0.32825600
H	-4.40088700	-0.30673200	-0.37612500
H	-6.88484000	3.46740200	1.18434300
H	-5.95578100	1.20368200	0.82842100
C	-4.02473000	0.53306700	-0.95734000
C	-3.09704700	2.68559700	-2.47926600
H	-4.30114300	5.04972100	-1.87342000
H	-6.05753400	5.39044200	-0.16416400
C	-2.57849900	1.43023600	-2.67442400
C	-3.03709700	0.31534700	-1.90832700
H	-2.73527900	3.52151900	-3.07321200
H	-1.80830000	1.28525100	-3.42565600
C	-2.55028000	-1.05508800	-2.12934500
H	-3.02094100	-1.82419000	-1.52016600
C	-1.73254300	-1.47634800	-3.14879300
H	-1.35448900	-0.78987800	-3.90196100
H	-1.66571100	-2.53453900	-3.37486400
I	-0.85653200	-4.21068600	-0.80367600
C	-2.13212500	-2.19021800	5.58291600
C	-0.73644000	-1.57385000	5.39621900
C	-0.39242800	-1.41949300	3.89093000
C	-1.48194900	-0.65760100	3.19212700
C	-2.86569400	-1.22421600	3.34178400
C	-3.21387900	-1.38393400	4.84663700
H	0.57880300	-0.92612000	3.76935600
H	-0.70504300	-0.58605600	5.87741900
H	0.02575900	-2.19133000	5.88917200
H	-2.12599000	-3.22095400	5.19917600
H	-2.37525700	-2.25580700	6.65127900

H	-1.39440200	0.42878900	3.19370300
H	-3.61387000	-0.59314500	2.84620200
H	-2.91652700	-2.21830200	2.87179400
H	-3.30176600	-0.38795100	5.30320900
H	-4.19341800	-1.86877200	4.95037000
H	-0.30217900	-2.42651800	3.45593600

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I	1.02560300	0.00000500	0.00000100
C	-1.25185800	0.00003100	0.00004000
C	-1.69160900	0.57256000	-1.34424700
H	-1.33732300	1.59759400	-1.48456700
H	-1.33708900	-0.03643200	-2.18050500
H	-2.79124800	0.58532800	-1.37447800
C	-1.69162100	0.87784400	1.16792700
H	-1.33663400	0.48748600	2.12579600
H	-1.33794800	1.90683800	1.05837100
H	-2.79126100	0.89695400	1.19464700
C	-1.69156300	-1.45047000	0.17626000
H	-1.33718100	-2.08441400	-0.64128800
H	-1.33715800	-1.87029300	1.12181300
H	-2.79121000	-1.48311800	0.18027500

TS1''

Ni	1.22215700	0.06518900	0.66782300
C	-4.74768100	-5.13985700	-0.07272600
C	-3.41374300	-4.79508900	-0.09890600
C	-2.94331900	-3.65576700	0.60908500
C	-3.88098500	-2.86782800	1.35134500
C	-5.24759300	-3.24774400	1.35679200
C	-5.67354200	-4.35946200	0.66197700
H	-0.86665600	-3.88960900	0.05867000
H	-5.09411200	-6.01556400	-0.61509300
H	-2.70016300	-5.39528400	-0.65893000
C	-1.57644800	-3.27604000	0.61046800
C	-3.39891800	-1.72922100	2.05618100
H	-5.95667100	-2.64424200	1.91841600
H	-6.72284800	-4.64146200	0.67532800
C	-2.06811900	-1.39499700	2.04495300
C	-1.11864600	-2.17688600	1.32051300
H	-4.10916200	-1.11974800	2.60981100
H	-1.73260600	-0.51830100	2.59110900
C	0.33016000	-1.92900500	1.37336000
H	0.93259500	-2.57362500	0.73756200
C	0.99290600	-1.22221400	2.35556400
H	0.44592900	-0.73956200	3.16191900
H	2.04083300	-1.42856700	2.53872900
C	-6.06700800	-1.00157200	-2.08252900
C	-4.72795300	-1.32387600	-2.09402000
C	-3.75614400	-0.41263100	-1.59861800
C	-4.19371800	0.84996900	-1.08224800
C	-5.58040400	1.15205400	-1.08359700
C	-6.49810400	0.24851600	-1.57440200
H	-2.04750200	-1.66919200	-2.00257500
H	-6.79955100	-1.70859700	-2.46226500
H	-4.39674400	-2.28704600	-2.47380800
C	-2.36920900	-0.71155500	-1.60131100
C	-3.21289400	1.75299900	-0.58756400
H	-5.90753700	2.11278800	-0.69220100
H	-7.55727700	0.49198300	-1.57294900
C	-1.87726700	1.43622200	-0.60986300
C	-1.42456000	0.18508700	-1.12908300
H	-3.53622200	2.71190500	-0.18866000

H	-1.15638800	2.14950500	-0.22401600
C	0.01087200	-0.13859500	-1.24674400
H	0.24656600	-1.16409900	-1.52193100
C	1.00464200	0.81044200	-1.34119200
H	0.76181600	1.86779300	-1.33594500
H	1.98401800	0.53469200	-1.71531900
C	0.15068000	7.42794800	-1.27795100
C	0.94749300	6.30752700	-1.19351100
C	0.73126900	5.33696600	-0.17785700
C	-0.33148600	5.54414600	0.76014700
C	-1.13454300	6.70836000	0.64667200
C	-0.90005700	7.63106500	-0.34991900
H	2.34449700	4.02815000	-0.77179300
H	0.32605200	8.16233600	-2.05929600
H	1.75461700	6.15020400	-1.90501700
C	1.53252200	4.17155900	-0.06145100
C	-0.53700600	4.56647200	1.77353200
H	-1.93972600	6.86176600	1.36149000
H	-1.52087300	8.51939300	-0.42724400
C	0.25857100	3.45043800	1.86013300
C	1.32430100	3.22869200	0.93454000
H	-1.34175100	4.71740900	2.48946400
H	0.07216200	2.72458800	2.64589400
C	2.22222000	2.06237600	1.02488000
H	2.99992600	2.01194100	0.26679700
C	2.33320000	1.21764300	2.10795900
H	1.74508600	1.37040100	3.00810000
H	3.21030700	0.58849100	2.20480400
I	3.64834500	-1.36607500	-0.17476900
C	6.04173400	-2.81448200	-1.03668200
C	5.42058800	-3.87028300	-1.90545000
H	4.87477800	-3.43452000	-2.74860300
H	6.20549100	-4.52639300	-2.32731600
H	4.73316100	-4.50898100	-1.34131200
C	6.57992700	-3.25987000	0.29266200
H	7.51336500	-3.83708700	0.15116100
H	6.81940000	-2.41021200	0.94028800
H	5.87432400	-3.90927600	0.82097800
C	6.78637700	-1.71314200	-1.73520200
H	7.02312500	-0.88741000	-1.05635400
H	7.74566400	-2.09532700	-2.13296700
H	6.22071800	-1.31275200	-2.58281200

CP5''

C	4.66388200	-1.02584500	0.30444200
C	3.39251600	-1.51203600	0.08578800
C	2.29212200	-0.62649400	-0.09375100
C	2.53511300	0.78756200	-0.04221400
C	3.84945100	1.25414500	0.18376600
C	4.89784900	0.36850600	0.35449600
H	0.80481300	-2.16422700	-0.35798200
H	5.49322300	-1.71510700	0.43952400
H	3.21197000	-2.58383700	0.04712600
C	0.97884900	-1.09067100	-0.31947100
C	1.42474000	1.67020500	-0.22361300
H	4.02598200	2.32686400	0.22167500
H	5.90374800	0.74101000	0.52743500
C	0.16088600	1.19995600	-0.44119300
C	-0.11861500	-0.21682000	-0.49884600
H	1.60546600	2.74232900	-0.18417600
H	-0.65316800	1.90562100	-0.57017100
C	-1.40783000	-0.74422800	-0.72529900
H	-1.48398400	-1.83033700	-0.74107000

C	-2.67784100	0.01318800	-0.95761400
H	-2.46923900	1.06262900	-1.19754200
H	-3.17561700	-0.40870500	-1.84522000
C	-3.72219400	-0.01602500	0.20998500
C	-3.13491000	0.65622100	1.46383300
H	-2.23202700	0.13984700	1.80775500
H	-2.86780900	1.70190700	1.26579300
H	-3.86215300	0.64938400	2.28515400
C	-4.12099800	-1.46674000	0.53861200
H	-4.89950900	-1.48777100	1.31101600
H	-4.51664700	-1.98131100	-0.34648000
H	-3.26839600	-2.04437700	0.91279100
C	-4.97000600	0.76020500	-0.25100900
H	-5.41954700	0.30045400	-1.14008300
H	-5.73277300	0.77912300	0.53712600
H	-4.72242200	1.79973300	-0.50014200

TS3''

Ni	-0.50114300	-1.36330000	0.70383600
C	6.28948600	0.57739800	-1.08512700
C	5.02781100	0.89694700	-0.63481000
C	4.27459900	-0.03502600	0.13006900
C	4.84649900	-1.31488000	0.42644800
C	6.14823400	-1.61265800	-0.05194000
C	6.85470300	-0.68797300	-0.79101400
H	2.54489800	1.23433900	0.37679200
H	6.85754500	1.29562300	-1.66997400
H	4.58649700	1.86523000	-0.85874700
C	2.97463000	0.26231600	0.60791600
C	4.08177400	-2.23926200	1.19269900
H	6.58038100	-2.58483600	0.17263600
H	7.85072300	-0.92776200	-1.15297200
C	2.82505900	-1.92286100	1.64392500
C	2.24367900	-0.65041900	1.35563600
H	4.51160000	-3.21198500	1.41891500
H	2.26789800	-2.65100700	2.22565200
C	0.90298200	-0.26412700	1.82198700
H	0.62784500	0.76796300	1.60604500
C	0.05413200	-0.98952700	2.64809500
H	0.34079600	-1.93926100	3.09244800
H	-0.80174300	-0.49490300	3.10104200
I	-1.32259000	-2.92647500	-1.04678800
C	1.81307100	4.93426800	0.28872400
C	0.75327200	4.32612000	0.92719100
C	-0.02142200	3.32837200	0.26863000
C	0.32232700	2.97118800	-1.07981400
C	1.41477300	3.61341800	-1.70636600
C	2.14999500	4.57679300	-1.03860600
H	-1.36213200	2.95594700	1.91694600
H	2.39412300	5.69383300	0.80457100
H	0.49366300	4.60144200	1.94674700
C	-1.10512900	2.67594500	0.89688900
C	-0.46065600	1.97012300	-1.73563900
H	1.66786900	3.33943900	-2.72791400
H	2.98386400	5.06653300	-1.53378000
C	-1.50944400	1.35263600	-1.11301500
C	-1.87352200	1.67894100	0.24860900
H	-0.20311900	1.69674000	-2.75612300
H	-2.07074200	0.59259400	-1.64421600
C	-2.93221500	1.04384000	0.94023700
H	-3.07868500	1.36298300	1.97191600
C	-3.94807800	0.08975800	0.39339600
H	-3.59653300	-0.37459100	-0.53338900

H	-4.07683600	-0.73354300	1.11157900
C	-5.37160800	0.69547100	0.13023100
C	-5.29477600	1.79024000	-0.94905000
H	-4.64916300	2.61903800	-0.63749000
H	-4.89882400	1.39177700	-1.89126000
H	-6.29125300	2.20026200	-1.15460200
C	-5.95928000	1.28424300	1.42638700
H	-6.98338600	1.63899300	1.25824000
H	-5.99558700	0.53199300	2.22478700
H	-5.37220200	2.13577500	1.78928600
C	-6.27798600	-0.44765700	-0.36384600
H	-6.36356400	-1.24149800	0.38827800
H	-7.28845000	-0.07817000	-0.57799000
H	-5.88368800	-0.89912900	-1.28211100

CP6''

Ni	-0.90721600	-1.19882800	-0.19827400
I	-1.28989700	-2.36910000	2.01834000
C	1.55738800	3.66528400	3.12119500
C	0.62450000	2.69168500	2.83871300
C	0.16620300	2.49291900	1.50777200
C	0.69017200	3.31995700	0.46188800
C	1.64618000	4.31433500	0.78498600
C	2.07119900	4.48407700	2.08654700
H	-1.19906800	0.89063400	1.98957300
H	1.90329300	3.80816100	4.14101300
H	0.22792200	2.05854300	3.62816500
C	-0.80001400	1.50706000	1.18868400
C	0.21957000	3.10872900	-0.86641600
H	2.04097600	4.94308300	-0.00967300
H	2.80543200	5.24939500	2.32272600
C	-0.70430100	2.13604200	-1.15051400
C	-1.25185000	1.30387200	-0.11817200
H	0.60334200	3.74380800	-1.66191500
H	-1.04851300	2.01398200	-2.17229500
C	-2.22753200	0.22790500	-0.37930900
H	-2.78231000	-0.04093600	0.52082100
C	-3.12154700	0.21776900	-1.60614000
H	-2.56628100	0.51563400	-2.50495900
H	-3.44600200	-0.81632600	-1.77300600
C	-4.43400600	1.07133200	-1.52935000
C	5.94190900	0.74097400	-1.17480800
C	4.62320300	0.83111800	-1.55934800
C	3.73656400	-0.26632600	-1.37887500
C	4.23894300	-1.47184600	-0.78755300
C	5.60330600	-1.53235800	-0.40190900
C	6.43701400	-0.45169700	-0.59074100
H	1.99809700	0.71275200	-2.20344400
H	6.60986400	1.58610500	-1.31702700
H	4.23968800	1.74544500	-2.00578700
C	2.37585700	-0.20764000	-1.76446300
C	3.34581100	-2.56419200	-0.61310200
H	5.98044700	-2.44780700	0.04754000
H	7.47973500	-0.50960000	-0.29085500
C	2.03153600	-2.48081600	-1.00140500
C	1.51528400	-1.28529500	-1.59256900
H	3.72066300	-3.48028100	-0.16350400
H	1.38018100	-3.33566800	-0.85275600
C	0.11057300	-1.15654900	-2.01332000
H	-0.12690700	-0.24185300	-2.54916800
C	-0.85016000	-2.16679500	-1.97423500
H	-0.60224600	-3.18802300	-1.69560600
H	-1.78089700	-2.04921700	-2.51739800

C	-5.33089900	0.57733400	-0.37754800
H	-5.53525400	-0.49722300	-0.46251200
H	-4.87760700	0.75544500	0.60384100
H	-6.29384200	1.10226400	-0.39188100
C	-5.17994000	0.86815200	-2.86388700
H	-5.42420500	-0.18877200	-3.02806900
H	-6.11997700	1.43310300	-2.87327500
H	-4.57728900	1.21051700	-3.71480500
C	-4.13946800	2.57102700	-1.34417800
H	-3.62651400	2.77385800	-0.39837600
H	-3.51380800	2.96251100	-2.15567700
H	-5.07531700	3.14360000	-1.34368300

CP7''

Ni	0.82406700	-0.07060600	-0.90882700
I	0.56244200	-2.44610200	-1.81768400
C	1.60090000	5.21094700	-1.42389600
C	1.99145300	3.88414100	-1.48549600
C	1.71193500	2.99950900	-0.41949000
C	1.02955600	3.49497700	0.73131900
C	0.64170700	4.85261400	0.76984600
C	0.92037700	5.69800000	-0.29039500
H	2.80976000	1.31455300	-1.22950300
H	1.82236200	5.88043300	-2.25019300
H	2.52485500	3.50921500	-2.35599900
C	2.11064900	1.61794000	-0.45036900
C	0.77077700	2.59163300	1.81987400
H	0.12223500	5.22740100	1.64855700
H	0.61750200	6.74036100	-0.24862600
C	1.16673100	1.28778300	1.78957800
C	1.91158100	0.75883600	0.66563300
H	0.24641700	2.97705600	2.69153300
H	0.95705300	0.63758000	2.63104800
C	2.23715600	-0.62190400	0.45835100
H	3.06180700	-0.79810900	-0.23244800
C	2.03166800	-1.71281800	1.48404000
H	1.17246700	-1.47789200	2.12505400
H	1.76233300	-2.62832900	0.94747800
C	3.26044500	-2.04404600	2.39207100
C	-5.67532900	0.25568700	2.58840200
C	-4.52577700	0.82773900	2.09036500
C	-3.93726400	0.34850200	0.88830600
C	-4.55970900	-0.74172200	0.19758100
C	-5.74295400	-1.30904000	0.73662200
C	-6.28913700	-0.82292700	1.90529900
H	-2.28635500	1.74149100	0.87316200
H	-6.11640100	0.62976600	3.50827400
H	-4.05168000	1.65640200	2.61147100
C	-2.75618500	0.91325700	0.34667700
C	-3.96460400	-1.21106300	-1.00726700
H	-6.21285100	-2.13733100	0.21178700
H	-7.19537800	-1.26696000	2.30813100
C	-2.82051700	-0.64337500	-1.50747200
C	-2.18797200	0.44219200	-0.82914000
H	-4.43285100	-2.03975500	-1.53257200
H	-2.38280800	-1.03261500	-2.41914900
C	-0.98739800	1.11670800	-1.34362100
H	-0.72148200	2.02212400	-0.80266500
C	-0.29394500	0.83853200	-2.49972100
H	-0.59582600	0.05688800	-3.18606100
H	0.42864300	1.55719400	-2.87608900
C	3.67561200	-0.83365900	3.24844500
H	3.97363700	0.02017800	2.62918900

H	2.85726900	-0.50690500	3.90265300
H	4.52719500	-1.08933200	3.89111100
C	4.45733300	-2.50248600	1.53595600
H	5.28389400	-2.83336500	2.17675600
H	4.18117200	-3.33983900	0.88396800
H	4.84049600	-1.69492800	0.90147800
C	2.84210600	-3.19924400	3.32319300
H	2.55510300	-4.08767600	2.74807900
H	3.66594100	-3.48190800	3.99017800
H	1.98702200	-2.91561100	3.94964100

TS4-t''

Ni	0.82565300	-0.61401100	-0.41111300
C	-4.42455900	4.96076400	0.21992100
C	-3.11192700	4.54495200	0.18145700
C	-2.73956100	3.37712400	-0.53940000
C	-3.75397800	2.63727900	-1.23053900
C	-5.09730300	3.09194100	-1.17105400
C	-5.42712400	4.22772500	-0.46189600
H	-0.62920100	3.49448600	-0.08759600
H	-4.69623700	5.85521800	0.77377500
H	-2.34038500	5.10711200	0.70256200
C	-1.39825000	2.91897600	-0.60027100
C	-3.37283900	1.46565800	-1.94351000
H	-5.86397500	2.52791800	-1.69682000
H	-6.45867600	4.56724300	-0.42606200
C	-2.06640400	1.04757500	-1.98574300
C	-1.04281100	1.78326800	-1.31401500
H	-4.14196500	0.89091000	-2.45331100
H	-1.81115900	0.13458900	-2.51396500
C	0.37874100	1.40955700	-1.39419300
H	1.05258700	2.02651000	-0.79813600
C	0.94248700	0.53700600	-2.29066300
H	0.35228900	-0.00424600	-3.02058900
H	2.01462700	0.52301200	-2.44379300
C	-7.01687200	-0.61755700	1.24957900
C	-5.78366600	-0.00471400	1.27966400
C	-4.59260800	-0.77729600	1.36191200
C	-4.69150500	-2.20609800	1.41063800
C	-5.97674100	-2.80536900	1.37740300
C	-7.11408500	-2.02998700	1.29946800
H	-3.23762400	0.90335400	1.36131400
H	-7.92171000	-0.01907000	1.18681500
H	-5.70329700	1.07860000	1.23473500
C	-3.30845500	-0.18107700	1.39857100
C	-3.49251200	-2.96991200	1.48823000
H	-6.05048600	-3.88965000	1.41252000
H	-8.09274300	-2.50171700	1.27427200
C	-2.26257400	-2.36500000	1.52250600
C	-2.14914200	-0.94140200	1.48299600
H	-3.56479300	-4.05434000	1.51145300
H	-1.36694900	-2.97414100	1.56004000
C	-0.86905700	-0.24585900	1.58514000
H	-0.94289700	0.84021400	1.55677600
C	0.36880500	-0.78657700	1.78425600
H	0.51775200	-1.85069900	1.93990100
H	1.18979900	-0.13133000	2.06120300
I	-0.01221100	-2.81629900	-1.59976900
C	4.97135400	4.95994000	-0.46977900
C	4.60246700	3.71771400	-0.93839400
C	4.27586500	2.66588000	-0.03612400
C	4.34535500	2.92382100	1.37357100
C	4.72786400	4.20964200	1.82286000

C	5.03453500	5.21089100	0.92204800
H	3.87667700	1.19488300	-1.55459600
H	5.21723800	5.75345100	-1.17013700
H	4.55539500	3.52405700	-2.00746400
C	3.89188800	1.38091100	-0.48315600
C	4.03429400	1.85576500	2.26684400
H	4.77910600	4.39810500	2.89277400
H	5.32790000	6.19411300	1.27904600
C	3.66509500	0.61984500	1.80745000
C	3.56357700	0.33327800	0.39773100
H	4.10603400	2.03648600	3.33712300
H	3.45887700	-0.16840700	2.52353200
C	3.14816400	-0.95297800	-0.10900800
H	3.23461800	-1.06536600	-1.18847900
C	3.27349000	-2.24651000	0.66099000
H	3.10478800	-2.08371500	1.73260500
H	2.48841700	-2.93121100	0.32082400
C	4.63719900	-3.00958400	0.50347500
C	4.88915000	-3.36529800	-0.97420500
H	5.78391400	-3.99278300	-1.06940200
H	4.04275200	-3.91640900	-1.40070300
H	5.05149700	-2.47082500	-1.58643100
C	4.52086100	-4.31238400	1.31929100
H	3.70031400	-4.93959200	0.95075600
H	5.44668700	-4.89701000	1.25258900
H	4.33498000	-4.10301100	2.38050600
C	5.81313400	-2.17754100	1.04503900
H	5.93959700	-1.24184400	0.49002700
H	5.67048100	-1.92308200	2.10283000
H	6.75059100	-2.74187600	0.96386900

CP8-t''

Ni	0.02959000	-0.88849300	0.58985100
C	-1.92802500	6.58611900	-1.79034100
C	-2.31110200	5.31688100	-1.41649700
C	-1.63157000	4.63134400	-0.37341000
C	-0.53903100	5.28237900	0.28633600
C	-0.16950100	6.58977800	-0.12114300
C	-0.84784600	7.22843900	-1.13722200
H	-2.83236900	2.83509400	-0.46339900
H	-2.45488500	7.10073700	-2.58908000
H	-3.14081700	4.82156800	-1.91504500
C	-1.99888900	3.32435000	0.03710100
C	0.13146100	4.58890300	1.33394500
H	0.65923400	7.08185200	0.38233100
H	-0.55578900	8.22983300	-1.44108500
C	-0.24823700	3.32438300	1.70946400
C	-1.33190600	2.65853400	1.05597000
H	0.95296400	5.08501600	1.84550900
H	0.27162800	2.82875700	2.52376400
C	-1.77337700	1.31045300	1.42897500
H	-2.66661400	0.96043500	0.91465500
C	-1.20628700	0.48161600	2.33505100
H	-0.33820700	0.74927800	2.92931300
H	-1.68868600	-0.45626900	2.59355600
C	7.49867000	1.42145200	0.01492900
C	6.16655900	1.70795000	0.21548300
C	5.15578800	0.95416900	-0.44021600
C	5.54213700	-0.11225300	-1.31559600
C	6.92157800	-0.38192300	-1.50118300
C	7.87924900	0.36755600	-0.85116500
H	3.48702000	2.02780800	0.41250800
H	8.26361300	2.00215800	0.52284300

H	5.86950800	2.51389400	0.88219000
C	3.77704700	1.22040800	-0.25642600
C	4.52142800	-0.86305900	-1.96601400
H	7.21323200	-1.19312300	-2.16383500
H	8.93329100	0.14990800	-1.00015700
C	3.19494300	-0.57891000	-1.77054500
C	2.79515400	0.48251900	-0.90220300
H	4.81286100	-1.67692300	-2.62535300
H	2.44079400	-1.17480800	-2.27459200
C	1.39651600	0.85159500	-0.69554300
H	1.23845000	1.68895200	-0.01680100
C	0.29342200	0.31671000	-1.30058800
H	0.37759900	-0.43810400	-2.07517600
H	-0.66691700	0.81494900	-1.21340700
I	1.80017200	-1.93206600	2.16021700
C	-6.94821900	-0.45734700	1.22173300
C	-5.73492500	-1.07863000	1.41977000
C	-4.74400800	-1.08888700	0.39770300
C	-5.03798100	-0.43986700	-0.84737800
C	-6.29632600	0.19014100	-1.01998000
C	-7.23402900	0.18428000	-0.00864300
H	-3.28589100	-2.22293300	1.51111400
H	-7.69410900	-0.45849500	2.01206500
H	-5.51724800	-1.57269400	2.36391700
C	-3.48629400	-1.71870800	0.56690100
C	-4.04311300	-0.46743200	-1.86568200
H	-6.51250000	0.67747800	-1.96830200
H	-8.19562200	0.66922200	-0.15246600
C	-2.83357700	-1.08642000	-1.66916400
C	-2.50694100	-1.73386700	-0.43048400
H	-4.26125100	0.00772300	-2.82008300
H	-2.10788100	-1.09246400	-2.47629800
C	-1.19332300	-2.35087000	-0.17966200
H	-1.21197100	-2.93668800	0.74600900
C	-0.45076500	-3.09441600	-1.28902500
H	-0.52359400	-2.53935600	-2.23440100
H	0.61784700	-3.12361700	-1.03483300
C	-0.87678000	-4.57253800	-1.57909100
C	-2.34490500	-4.65984400	-2.03419800
H	-3.03341500	-4.32288200	-1.25279600
H	-2.52566700	-4.04543200	-2.92513000
H	-2.60651200	-5.69548800	-2.28599300
C	-0.66959600	-5.45135800	-0.33067100
H	-0.87877500	-6.50316200	-0.56242200
H	0.36154900	-5.38511100	0.03676100
H	-1.33506100	-5.15844400	0.48887600
C	0.03076200	-5.09601500	-2.71085400
H	1.08830600	-5.06171400	-2.42044700
H	-0.21341300	-6.13619300	-2.95961300
H	-0.08733200	-4.49917000	-3.62463600

TS5''

Ni	0.00374300	-1.54018200	0.05553900
C	6.38759000	2.50141900	1.12729700
C	5.70095000	1.31426400	1.25628400
C	4.69494500	0.95207000	0.32008400
C	4.40517000	1.84289700	-0.76381900
C	5.12963900	3.05806600	-0.86868900
C	6.09977300	3.38156200	0.05555700
H	4.20116300	-0.93825800	1.24176400
H	7.15474200	2.76747000	1.84922000
H	5.92081900	0.63685400	2.07810400
C	3.96761600	-0.26171200	0.42134800

C	3.39597300	1.46996900	-1.69621900
H	4.90701500	3.73173700	-1.69272000
H	6.64870900	4.31474800	-0.03510500
C	2.71215200	0.28581100	-1.57428500
C	2.99261900	-0.61476200	-0.49998900
H	3.17093000	2.14387100	-2.51947400
H	1.94271800	0.03501000	-2.29779800
C	2.29833000	-1.90282100	-0.35113900
H	2.58514900	-2.47948600	0.52612200
C	1.47083700	-2.49379300	-1.26858500
H	1.25897300	-2.04825200	-2.23396900
H	1.16711300	-3.52708200	-1.15189700
C	-4.01510800	4.90609300	-0.64567600
C	-2.82986300	4.20460100	-0.65744200
C	-2.64186000	3.08147400	0.19293200
C	-3.70740300	2.68757100	1.06550600
C	-4.91527900	3.43058300	1.05463400
C	-5.06738200	4.51600800	0.21834300
H	-0.63103600	2.64083400	-0.45966700
H	-4.14824600	5.76175900	-1.30200400
H	-2.02097600	4.49916100	-1.32181700
C	-1.43517400	2.33941500	0.20825600
C	-3.50822200	1.56118200	1.01258000
H	-5.72315800	3.12789800	1.71670200
H	-5.99835100	5.07640600	0.21770100
C	-2.32715700	0.86448300	1.90416400
C	-1.25535200	1.24627900	1.04200300
H	-4.31577900	1.25641100	2.57396700
H	-2.20928400	0.00905700	2.56166700
C	0.04403800	0.56420100	1.03751700
H	0.79214000	1.02287200	0.39291400
C	0.46417100	-0.45058800	1.87012800
H	-0.17681800	-0.83437400	2.65836200
H	1.52445300	-0.65076000	1.97726400
I	-1.94192300	-1.52615400	-1.65811900
C	-0.57186300	-3.81830800	1.35237500
C	0.62638000	-4.02771500	2.24041700
H	0.81922700	-3.17103500	2.89474900
H	0.46034400	-4.90081900	2.89846600
H	1.53483500	-4.24313700	1.66582800
C	-0.78673100	-4.84421900	0.27112600
H	-1.47619600	-4.48549200	-0.49885600
H	0.14944200	-5.15081600	-0.20886500
H	-1.22656300	-5.75786300	0.71126200
C	-1.82859200	-3.32401700	2.01991000
H	-2.30057900	-4.15309900	2.57917700
H	-1.63378100	-2.52755800	2.74584700
H	-2.56107600	-2.96485400	1.29058500

TS6-t''

Ni	-0.14415300	-1.45440500	-0.03763100
C	6.57681500	2.14557700	1.15358200
C	5.82122800	0.99389500	1.13618400
C	4.77898500	0.82422700	0.18520400
C	4.52578200	1.87153800	-0.75874200
C	5.32139800	3.04500400	-0.71511100
C	6.32505200	3.18049000	0.22009600
H	4.18559400	-1.14303300	0.85196700
H	7.37101100	2.26427700	1.88539300
H	6.01316000	0.19782900	1.85169400
C	3.98029300	-0.34727700	0.13796500
C	3.48159600	1.68915900	-1.70937400
H	5.12668300	3.83789300	-1.43328100

H	6.92829400	4.08373200	0.24428300
C	2.72806400	0.54207900	-1.73163300
C	2.96674800	-0.51127700	-0.79500600
H	3.28935100	2.47930900	-2.43134200
H	1.94284900	0.43257400	-2.47320000
C	2.20036700	-1.76501900	-0.80455400
H	2.51510800	-2.49726000	-0.06293900
C	1.24082800	-2.13647200	-1.69878300
H	0.94005600	-1.51063300	-2.53229000
H	0.86441100	-3.15293300	-1.71668300
C	-3.95081400	5.03649900	-0.60055400
C	-2.78293600	4.30970300	-0.66999400
C	-2.58197700	3.17626000	0.16358500
C	-3.61562600	2.79903400	1.08086400
C	-4.80634200	3.56796100	1.12865300
C	-4.97182300	4.66252900	0.30703700
H	-0.61191600	2.69714500	-0.58033700
H	-4.09427100	5.89994000	-1.24439200
H	-1.99800300	4.59237300	-1.36754200
C	-1.39297300	2.40710400	0.11954400
C	-3.40427100	1.66216200	1.91077400
H	-5.59032700	3.27764900	1.82405500
H	-5.88946100	5.24274600	0.35161500
C	-2.24109100	0.93903500	1.84472200
C	-1.20110200	1.30440200	0.93771900
H	-4.18911900	1.36867900	2.60367500
H	-2.11548900	0.07267400	2.48641100
C	0.08087000	0.59000900	0.86756000
H	0.80352400	1.02676300	0.18020300
C	0.52624900	-0.41412400	1.70266400
H	-0.07692200	-0.76500800	2.53492100
H	1.58343800	-0.65221900	1.74331500
I	-2.29504200	-1.75560800	-1.43555300
C	-0.23782900	-3.74641300	1.49278000
C	0.98602000	-3.74874900	2.36981900
H	1.00186500	-4.65815300	2.99904900
H	1.91571500	-3.76000400	1.78811800
H	1.01443900	-2.89383000	3.05372700
C	-0.26077800	-4.77382700	0.39218700
H	0.69898300	-4.83821000	-0.13489800
H	-0.45038300	-5.77754200	0.81724100
H	-1.05216800	-4.57466500	-0.33683900
C	-1.55193600	-3.49436800	2.18342300
H	-1.83723400	-4.37661900	2.78703600
H	-1.50079400	-2.64640500	2.87689400
H	-2.35964900	-3.31136300	1.46846300

CP9-t''

Ni	2.28408400	-0.59021500	-0.18870000
C	-5.20041300	-3.66486500	-0.82321300
C	-3.84656800	-3.86206500	-0.98306000
C	-2.91407400	-3.23825200	-0.11021200
C	-3.40397700	-2.39977400	0.94393600
C	-4.80442100	-2.21721100	1.08172500
C	-5.68380300	-2.83499100	0.21788800
H	-1.14607100	-4.06012000	-1.04263400
H	-5.90398300	-4.14681200	-1.49626600
H	-3.47273500	-4.49944300	-1.78088200
C	-1.51320900	-3.41559000	-0.24579400
C	-2.46188000	-1.77761500	1.81193500
H	-5.17373600	-1.58339000	1.88441200
H	-6.75407900	-2.68867400	0.33423700
C	-1.11262100	-1.96946800	1.65692100

C	-0.60861200	-2.80609900	0.61359800
H	-2.82958400	-1.13364900	2.60682600
H	-0.42118100	-1.46652500	2.32479400
C	0.82390500	-3.05131600	0.42622900
H	1.07598900	-3.67265000	-0.43311200
C	1.83963000	-2.61354000	1.20756200
H	1.67784100	-2.04251400	2.11642400
H	2.85479200	-2.94963600	1.02470900
C	-2.62641900	5.66106100	-0.25807800
C	-1.53311100	4.95821600	-0.71318200
C	-1.58178000	3.54328300	-0.83939100
C	-2.78649700	2.85413800	-0.48265000
C	-3.89538700	3.60722000	-0.01965100
C	-3.81812900	4.97939200	0.09047100
H	0.43802500	3.31601000	-1.56900100
H	-2.57837400	6.74219800	-0.16278000
H	-0.61470900	5.47598600	-0.97845100
C	-0.47759300	2.79060100	-1.30779100
C	-2.82303500	1.43632200	-0.60970500
H	-4.80970900	3.08366300	0.24942300
H	-4.67416500	5.54500300	0.44831500
C	-1.73613300	0.73434400	-1.06360400
C	-0.52974500	1.40852800	-1.42417600
H	-3.73523600	0.90889100	-0.34165400
H	-1.79931500	-0.34473800	-1.15499200
C	0.63798000	0.70662400	-1.95163500
H	1.43816700	1.35623400	-2.30479400
C	0.81899300	-0.63658400	-2.07975700
H	0.04571700	-1.34689100	-1.80305500
H	1.64602800	-1.01893900	-2.66600500
I	2.27958900	1.34707500	1.54113300
C	4.01562400	-1.11251200	-1.10766800
C	3.92743000	-2.46632700	-1.81541200
H	3.68458800	-3.28404700	-1.12415200
H	3.18185600	-2.48007700	-2.62096700
H	4.89480800	-2.72600000	-2.28041400
C	4.34039900	0.00622800	-2.10152400
H	5.32808000	-0.15979200	-2.56765000
H	3.61461600	0.06446500	-2.92388100
H	4.37712100	0.98676800	-1.61148400
C	5.08120900	-1.15703700	-0.00563600
H	6.07263900	-1.38024100	-0.43936600
H	5.16082200	-0.20315100	0.52620700
H	4.88260700	-1.93715900	0.74096400

CP10''

Ni	-1.44226000	0.41782600	0.27873900
I	-1.93580700	-1.99266500	-0.31941400
C	-2.60975400	1.77477500	-0.47555700
C	5.66272600	0.62950600	-1.29224800
C	4.47633200	1.28926200	-1.06300100
C	3.49199000	0.73344700	-0.20026300
C	3.75366000	-0.52684800	0.43075100
C	4.98607700	-1.18081400	0.17350400
C	5.91980900	-0.61673500	-0.66869900
H	2.06872900	2.34125300	-0.42111300
H	6.40761300	1.06221500	-1.95425600
H	4.27517300	2.24521100	-1.54071200
C	2.26103300	1.38294000	0.05785000
C	2.76422600	-1.07274600	1.29487500
H	5.18144000	-2.13762800	0.65138000
H	6.85952200	-1.12773400	-0.85905900
C	1.58118700	-0.41825300	1.52914200

C	1.30499700	0.83774900	0.90622200
H	2.95780200	-2.02986300	1.77241400
H	0.84581800	-0.86833000	2.18753400
C	0.05547400	1.57944000	1.12852800
H	0.03614300	2.56995600	0.68490700
C	-0.96324400	1.24626900	2.02614900
H	-0.87346200	0.39854700	2.70236800
H	-1.69806600	1.99053700	2.31352900
C	-3.98440300	1.39220000	0.06984800
H	-4.22112600	0.33968700	-0.10347600
H	-4.06874300	1.59407100	1.14360700
H	-4.75477000	1.99862700	-0.43636600
C	-2.29080400	3.24225200	-0.20554800
H	-1.33782900	3.55130200	-0.64785600
H	-3.07115800	3.86524800	-0.66914900
H	-2.28256800	3.49317800	0.86018200
C	-2.43471000	1.45010200	-1.96203400
H	-2.78129400	0.44686400	-2.21712600
H	-3.01894400	2.17527400	-2.55403000
H	-1.39079400	1.54841300	-2.28565300

TS15'

Ni	0.41621800	-0.52783000	0.97167900
I	0.89173500	-0.63480600	3.55245000
C	-2.28289100	0.08327000	0.09973100
C	-1.31611600	1.96594900	1.03039200
C	-2.45999100	2.72635900	0.80185800
C	-3.57782400	2.14341400	0.19174100
C	-3.45909300	0.79003700	-0.15663300
C	-2.08919400	-1.35078600	-0.22757400
C	-0.62147800	-3.13749000	-0.18295800
C	-1.56947000	-4.00088600	-0.72315000
C	-2.84855100	-3.52219100	-1.03618400
C	-3.08407100	-2.16604600	-0.77111400
H	-0.44110700	2.39564400	1.50771800
H	-2.45881900	3.76536600	1.10718000
H	-4.29206500	0.28522500	-0.63187500
H	0.37059800	-3.49389800	0.07814500
H	-1.29582700	-5.03610600	-0.88529900
H	-4.05869700	-1.74213700	-0.98159400
N	-0.85826200	-1.84278700	0.05974600
N	-1.21823000	0.67658700	0.68833400
C	-4.87905300	2.90851600	-0.09524900
C	-3.95896400	-4.40336900	-1.62839300
C	-4.80119900	4.37651300	0.36503000
H	-5.74710100	4.88166500	0.14118400
H	-4.63196300	4.45726300	1.44463400
H	-4.00448600	4.92464300	-0.15040300
C	-6.04872700	2.22425100	0.65248800
H	-6.98525300	2.75927200	0.45574000
H	-6.18685800	1.18518200	0.33480700
H	-5.87786600	2.22393200	1.73473100
C	-5.15722200	2.88902400	-1.61763600
H	-6.08568500	3.42904300	-1.83750000
H	-4.34435700	3.37072700	-2.17265700
H	-5.26775800	1.86910600	-2.00152400
C	-5.16689900	-4.41860100	-0.66060700
H	-5.57628500	-3.41570600	-0.49954600
H	-5.96887700	-5.04331800	-1.07098300
H	-4.88413200	-4.82608700	0.31631500
C	-4.39802300	-3.82206400	-2.99393600
H	-5.19429000	-4.43908100	-3.42632800
H	-4.78314200	-2.80106000	-2.90062800

H	-3.56166100	-3.80230600	-3.70182400
C	-3.49227400	-5.85522200	-1.84582700
H	-2.64941100	-5.91366900	-2.54398500
H	-3.19547400	-6.33412100	-0.90594400
H	-4.31237800	-6.44431700	-2.27023900
C	1.21892000	5.66868900	-2.82729300
C	1.09013500	4.29732800	-2.80977300
C	1.58722200	3.53067600	-1.71916300
C	2.22903500	4.21500600	-0.63470100
C	2.34479500	5.62812200	-0.68241600
C	1.85170800	6.34261300	-1.75358600
H	0.98764100	1.60929300	-2.49986100
H	0.83554800	6.24034900	-3.66854200
H	0.60594400	3.77924500	-3.63478000
C	1.47331100	2.11943900	-1.66954500
C	2.72337500	3.43982500	0.45151400
H	2.83268500	6.14078200	0.14365400
H	1.94823300	7.42468700	-1.77909000
C	2.60052400	2.07204400	0.47000100
C	1.96651000	1.37119600	-0.60598000
H	3.20581900	3.95086600	1.28171400
H	2.97106800	1.51551200	1.32491800
C	1.81642400	-0.08979300	-0.60778900
H	1.33885600	-0.49390900	-1.49947100
C	2.56621600	-0.97627600	0.17499000
H	3.09098000	-0.66126400	1.06762000
H	2.42802100	-2.04668500	0.06511000
C	6.51009300	-3.15020700	-1.98688500
C	5.72982600	-2.16840400	-2.87628000
C	4.39122500	-1.75654500	-2.21081400
C	4.63818400	-1.23664400	-0.82161500
C	5.39674400	-2.16811100	0.08404300
C	6.73767500	-2.58454000	-0.57567500
H	3.87100000	-1.01333100	-2.82652200
H	6.33792000	-1.26885700	-3.04710000
H	5.53791600	-2.61249200	-3.86246900
H	5.94743900	-4.09306800	-1.91103500
H	7.47224800	-3.39885200	-2.45327900
H	4.89611600	-0.17997700	-0.74900300
H	5.58109300	-1.71326000	1.06446000
H	4.80655700	-3.08120700	0.26274700
H	7.39582600	-1.70637200	-0.63703700
H	7.25144100	-3.32164200	0.05564800
H	3.74465500	-2.64829700	-2.16729900

TS7'-t

Ni	-0.25626300	-1.35195800	0.08655100
I	-0.53049000	-1.78741000	-2.60302500
C	3.18052500	-1.33421400	4.24948900
C	1.95241500	-0.43966300	4.48488300
C	0.95262000	-0.54182900	3.30441000
C	0.58427200	-1.98990200	3.06684900
C	1.77247700	-2.88836200	2.80408300
C	2.77893900	-2.79355000	3.97885900
H	0.06255000	0.06562300	3.51359900
H	1.44941600	-0.74923200	5.41237100
H	2.26161700	0.60519900	4.62798600
H	3.74439100	-0.95021200	3.38557100
H	3.85865100	-1.28176400	5.11137800
H	-0.01593200	-2.37934800	3.89364100
H	1.45835600	-3.93219400	2.66887100
H	2.28934500	-2.58514800	1.88627100
H	2.31829700	-3.21716800	4.88290600

H	3.66833800	-3.40203800	3.76415500	C	6.65499300	-0.82712800	-1.93270200
H	1.42969700	-0.11559700	2.41441500	H	6.84598300	-1.46090500	-1.05910500
C	-7.00620200	0.38976200	-1.77626600	H	6.25436800	-1.45669500	-2.73501200
C	-5.87346600	-0.39207600	-1.73895700	H	7.61989800	-0.43577100	-2.27256400
C	-5.10976700	-0.51520100	-0.54355100				
C	-5.54416400	0.19757000	0.62275300				
C	-6.71713300	0.99384900	0.55214200				
C	-7.43522100	1.08945000	-0.62006200				
H	-3.61477600	-1.83590300	-1.37183800				
H	-7.57829400	0.47354200	-2.69666300				
H	-5.54187400	-0.92749400	-2.62520700				
C	-3.94219400	-1.31380100	-0.47648000				
C	-4.76845400	0.07152500	1.80653000				
H	-7.04208300	1.52797100	1.44283000				
H	-8.33293100	1.70063400	-0.66268700				
C	-3.63598800	-0.70916300	1.83913100				
C	-3.18988100	-1.43355400	0.68796700				
H	-5.08827500	0.60192400	2.70155200				
H	-3.07317700	-0.77395900	2.76597700				
C	-2.00018300	-2.30853100	0.71101200				
H	-1.96395900	-3.03124300	-0.10265300				
C	-1.31539900	-2.66555000	1.90405400				
H	-1.75021600	-2.34645500	2.84291600				
H	-0.85213800	-3.64741300	1.93666600				
C	0.98535200	1.28975000	0.02444500				
C	-1.26305500	1.49822300	0.52036200				
C	-1.17597200	2.88790900	0.56263800				
C	0.05179300	3.51908100	0.33857300				
C	1.13893800	2.67582600	0.06716700				
C	2.09211500	0.35809200	-0.31186300				
C	2.72037600	-1.84761600	-0.56876500				
C	3.99330100	-1.49239000	-1.00388100				
C	4.34045500	-0.13991200	-1.10761500				
C	3.34700400	0.78326500	-0.75334700				
H	-2.20752900	0.99695600	0.69443900				
H	-2.07645300	3.45212900	0.77062900				
H	2.11618100	3.10666600	-0.11278100				
H	2.42425800	-2.89028800	-0.51624000				
H	4.68855700	-2.27903900	-1.26900200				
H	3.54826200	1.84354000	-0.84456700				
N	1.79080700	-0.95503000	-0.21175300				
N	-0.21386600	0.70763600	0.26726100				
C	0.23938200	5.04296300	0.37357100				
C	5.71298800	0.34480200	-1.59788900				
C	-1.07700700	5.78092900	0.68215200				
H	-0.89650300	6.86117000	0.69694300				
H	-1.84263400	5.58520700	-0.07684600				
H	-1.48267300	5.50135000	1.66108200				
C	0.75755400	5.52293900	-1.00382100				
H	0.89568800	6.61037400	-0.99386800				
H	1.71997000	5.06834400	-1.26189700				
H	0.04638500	5.27730400	-1.80013800				
C	1.27136000	5.40361100	1.46925100				
H	1.41865200	6.48934700	1.50262700				
H	0.92831600	5.07707300	2.45747700				
H	2.24698200	4.94202900	1.28285900				
C	5.52305500	1.19913800	-2.87470700				
H	4.89957300	2.08044400	-2.69044900				
H	6.49588600	1.55016200	-3.23831800				
H	5.05061200	0.61582800	-3.67250700				
C	6.37462000	1.20372100	-0.49341800				
H	7.35352900	1.56184700	-0.83265300				
H	5.77054600	2.08113700	-0.23869900				
H	6.52516500	0.62163200	0.42286800				