

Mechanistic Study of the Competitiveness Between Branched and Linear Polyethylene Production on *N*-Arylciano- β -diketiminato Nickel Hydride

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I. Experimental Section

Experimental. Electrospray Ionization Mass Spectrometry (ESI-MS) was applied to identify the catalytically active species, which are responsible for the ethylene polymerization; the catalytic system **c** was taken as representative (Scheme 1). The catalyst (4.23 μmol , 2.0 mg) and saturated solution of ethylene, in anhydrous and degassed toluene (5.0 mL), were mixed with anhydrous and degassed solution of $\text{B}(\text{C}_6\text{F}_5)_3$ (21.15 μmol , 11.0 mg) under Ar atmosphere using a dual-syringe pump operating at a flow rate of 1 μL -100 mL/min in an effective micromixer, that was coupled directly to the ion source of the mass spectrometer. The solution was fed continuously into the MS and the flow rate could be varied from 2.0 to 100 $\mu\text{L}/\text{min}$. By connecting the microreactor directly to the spray capillary, reaction times from 0.3 s to min could be covered. ESI-MS and ESI-MS/MS analyses were conducted in a Bruker Daltonics AmaZon SL ion trap mass spectrometer (Bruker Daltonics, Bremen, Germany). The ESI source and the mass spectrometer were operated in the positive-ion mode, and the capillary voltage and drying gas temperature set to +4.0 kV and 220 $^\circ\text{C}$, respectively, with a scan range of m/z 70-2000. Drying gas flow and nebulizing gas pressure were set to 5.0 L/min and 8.0 psi, respectively. MS/MS experiments were carried out by mass selection of a specific ion in the ion trap, which was then submitted to collision-induced dissociation (CID) with helium (He) in the collision chamber. Mass spectra of the poorly soluble product were carried out using Matrix-Assisted Laser Desorption Ionization Time-of-Flight (MALDI-TOF) technique. Mass spectra were recorded on a Bruker Autoflex Speed system equipped with a pulsed nitrogen laser (337 nm) (Bruker Daltonics Inc., Bremen Germany), operating in positive ion reflector mode, using 19 kV acceleration voltage and alpha-cyano-4-hydroxycinnamic acid as matrix.

Mass Spectrometry Experiments. MS/MS experiments were carried out by mass selection of a specific ion in the ion-trap, which was then submitted to collision-induced dissociation (CID) with helium (He) in the collision chamber. Mass spectra of the poorly soluble product were carried out using Matrix-Assisted Laser Desorption Ionization Time-of-Flight (MALDI-TOF) technique. Mass spectra were recorded on a Bruker Autoflex Speed system equipped with a pulsed nitrogen laser (337 nm) (Bruker Daltonics Inc., Bremen Germany), operating in positive ion reflector mode, using 19 kV acceleration voltage and alpha-cyano-4-hydroxycinnamic acid as matrix.

Polymer Characterization. By ESI-MS experiments we had not observed any different products of ethylene insertions into **c1** or **c** nickel species from those shown

in Figure 2 (main manuscript), presumably due to their short lifetimes and low solubility.

However, polymeric products formed during the ESI-MS experiments (see Figure 1-2 in the manuscript) were further analyzed by MALDI-TOF technique confirming the presence of polymer (see Figure 3 in the main manuscript). We were able to detect products of up to 36 insertions of ethylene.¹

II. Computational Studies

Computational Details. DFT calculations were carried out using Gaussian 16 package.² Geometries were optimized using the M06L³ functional and a mixed basis set of SDD^{4, 5} for Ni, and the def2-SVP^{6, 7} basis set for other atoms. Frequency calculations characterized the nature of the stationary points. Single-point energies were calculated with the M06L functional with Grimme D3⁸ dispersion corrections, SDD and def2-TZVP^{6, 7} basis sets were used for Ni and all other atoms, respectively. Solvation energy calculations by SMD⁹ continuum solvation model were performed on gas-phase optimized geometries. Toluene ($\epsilon=2.37$) was used in the SMD calculations for consistency with the experiment. All reported Gibbs free energies involve zero-point vibrational energy corrections, thermal corrections to the Gibbs free energy at 323.15, 333.15, and 343.15 K, were calculated in order to obtain a reasonable comparison of the stabilities and entropic effects of the catalytic systems involved in the production of linear or branched chains (experimental conditions).

Interaction energies were computed from optimized geometries in Gaussian 16 with the use of the second-generation energy decomposition analysis based on the absolutely localized molecular orbitals (ALMO-EDA2)^{10, 11} in Q-Chem 5.2 package¹² under the same level of theory. ALMO-EDA2 calculations were performed in gas-phase because their current implementation does not allow solvent corrections. Energies obtained through single-point calculations in Q-Chem 5.2 are in good agreement with the computed energies in Gaussian 16 (see Table S1).

The energetic span model (δG)¹³ was performed to characterize the selectivity of the catalytic cycles that follow the formation of linear or branched chain. This model provides a way to calculate the TOF from Gibbs free energy profiles based on DFT calculations. Using this model we were able to identify the energy states of one transition state and one intermediary of each reaction path; (i) the TOF determining transition state (TDTS) and (ii) the TOF determining intermediate (TDI) determine if

the catalytic cycle understudy is favorable or not. TDTS and TDI are the most important species that determine the catalytic activity (TOF) of a reaction pathway, which is not necessarily adjoining along the reaction pathway of a catalytic cycle, they are the states that maximize δG .

The δG can be calculated as the energetic difference between TDTS and TDI ($\delta G = \text{TDTS} - \text{TDI}$), where lower values of the δG indicate a more favorable catalytic cycle and where the catalytic activity by this model can be obtained as:

$$TOF = \frac{k_B T}{h} e^{-\delta G/RT}$$

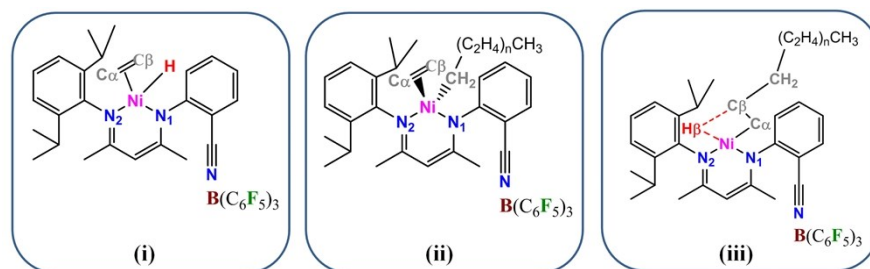
with k_B as the Boltzmann constant, T corresponds to the temperature (323.15, 333.15, and 343.15 K), h is the Planck constant and R is the gas constant. Therefore, the great advantage of the energetic span model is that by knowing the location of the determining states (TDTS and TDI) that gives insights on the species that must be modified to improve the course of a catalytic cycle.

The steric effects around the nickel center were measured by calculations of percent buried volumen ($\%V_{\text{bur}}$) with the SambVca 2.0 web tool developed by Cavallo et al.¹⁴ NCI (non-covalent interactions)¹⁵ plots were computed in the Multiwfn 3.7 program¹⁶ in order to characterize the interactions between the substrate and the second coordination sphere in the chain propagation and termination transition state structures. NCI is based on the electron density and the reduced density gradients (RDG) characterizing attractive or repulsive inter- and intramolecular non-covalent interactions by colors (red, strong repulsion; blue, strong attraction; and green, weak attractive interaction). Most important structures had been represented by using CYLView.¹⁷

Table S1. Summary of electronic energies computed in Gaussian and Q-Chem for chain propagation (c1b- c1b*) and termination (c1c-c1c*) pairwise.

System	<i>E</i> (Hartree) Gaussian M06L/SDD/def2-SVP	<i>E</i> (Hartree) Q-Chem M06L/SDD/def2-SVP
c1b-R	-3629.9171549	-3629.909955
c1b*-R	-3629.9187541	-3629.910526
c1b-TS	-3629.8926546	-3629.885774
c1b*-TS	-3629.8976328	-3629.891087
c1c-R	-3708.4794826	-3708.473362
c1c*-R	-3708.4706383	-3708.461221
c1c-TS	-3708.4583355	-3708.456621
c1c*-TS	-3708.454003	-3708.445936

Table S2. Optimized distances (Å) and angles (°) for **c1** and π -complexes **c1a-c1c** (i). H^C represents the exchange between H and C (ii) from new ethylene insertions in **c1b-c1c** (once C _{β} -H bond is formed in P_{c1a}). H _{β} represents the β -hydrogen in the agostic product structures for **c1b***, **c1c** and **c1c*** (iii).



System		Ni-N ₁	Ni-N ₂	Ni-C _{β}	Ni-C _{α}	C _{α} -C _{β}	Ni-H ^C	C _{β} -H ^C	\angle Ni-C _{α} -C _{β}	\angle N ₁ -Ni-N ₂
c1		1.88	1.93	-	-	-	H ^{1.48}	-	-	94.80
c1a	R _{c1a}	1.92	2.00	2.02	2.04	1.39	H ^{1.48}	H ^{2.32}	67.85	94.47
	TS _{c1a}	1.94	1.90	2.15	1.94	1.44	H ^{1.59}	H ^{1.43}	77.39	95.87
	P _{c1a}	1.94	1.86	2.21	1.90	1.49	H ^{1.76}	H ^{1.11}	80.42	97.18
c1b	R _{c1b}	2.02	2.01	1.97	2.02	1.40	C ^{1.93}	C ^{2.77}	67.34	90.86
	TS _{c1b}	1.92	1.99	2.00	1.93	1.44	C ^{2.05}	C ^{2.01}	71.06	93.96
	P _{c1b}	1.86	1.89	2.67	1.91	1.53	C ^{2.48}	C ^{1.53}	97.63	95.76
c1b*	R _{c1b*}	2.00	2.00	1.95	1.98	1.41	C ^{1.96}	C ^{2.73}	67.94	92.20
	TS _{c1b*}	2.01	1.94	1.99	1.94	1.44	C ^{2.08}	C ^{2.01}	70.40	93.34
	P _{c1b*}	1.94	1.87	2.12	1.90	1.48	H _{β} 1.67 / C ^{2.99}	H _{β} 1.18 / C ^{1.52}	76.45	97.06
	TS _{c1b*βH}	1.93	1.95	2.04	1.98	1.42	H _{β} 1.45 / C ^{1.84}	H _{β} 1.82 / C ^{1.51}	71.73	94.79
	P _{c1b*βH}	1.95	1.98	2.00	1.94	1.40	H _{β} 1.41 / C ^{3.03}	H _{β} 2.32 / C ^{1.51}	71.11	94.67
	cw	1.87	1.90	-	-	-	1.96	-	-	96.61
c1c	R _{c1c}	2.00	2.02	1.96	1.99	1.41	C ^{1.97}	C ^{2.72}	67.75	91.86
	TS _{c1c}	2.00	1.94	1.99	1.93	1.44	C ^{2.08}	C ^{2.02}	70.63	93.57
	P _{c1c}	1.95	1.88	2.14	1.91	1.47	H _{β} 1.65 / C ^{3.21}	H _{β} 1.18 / C ^{1.52}	77.62	96.84
	TS _{c1cβH}	1.93	1.96	2.04	1.98	1.42	H _{β} 1.44 / C ^{2.87}	H _{β} 1.86 / C ^{1.50}	71.91	94.56
c1c*	P _{c1cβH}	1.93	1.98	2.01	1.97	1.40	H _{β} 1.44 / C ^{3.32}	H _{β} 2.16 / C ^{1.50}	70.90	93.99
	R _{c1c*}	2.02	2.07	1.95	2.02	1.40	C ^{2.03}	C ^{2.96}	66.82	90.75
	TS _{c1c*}	2.01	1.95	2.01	1.94	1.43	C ^{2.13}	C ^{2.09}	71.60	93.02
	P _{c1c*}	1.95	1.89	2.15	1.90	1.47	H _{β} 1.66 / C ^{3.25}	H _{β} 1.18 / C ^{1.53}	77.90	97.01
	TS _{c1c*βH}	1.95	1.98	2.15	2.00	1.41	H _{β} 1.46 / C ^{3.09}	H _{β} 1.85 / C ^{1.51}	75.97	94.27
	P _{c1c*βH}	1.93	1.96	2.19	2.01	1.39	H _{β} 1.45 / C ^{3.20}	H _{β} 1.93 / C ^{1.51}	77.69	94.14

Table S3. Interaction energy (ΔE_{int}) decomposition in terms of ΔE_{Pauli} , ΔE_{elstat} , ΔE_{disp} , ΔE_{pol} and ΔE_{CT} energies for the ground state (R) and transition state (TS) geometries for the propagation and termination steps. ΔE is the difference in energy between the Ni-complex and the monomer. $\Delta\Delta E$ is the difference in energy between the ground state and transition state geometries. And $\Delta\Delta\Delta E$ is the difference in $\Delta\Delta E$ for pairwise combinations c1b-c1b* and c1c-c1c*, respectively. Energies are in kcal mol⁻¹.

Energy Term	c1b		c1b*		c1c		c1c*	
	R	TS	R	TS	R	TS	R	TS
ΔE_{int}	-42.4	-57.8	-46.6	-59.2	-42.0	-54.1	-35.9	-51.9
$\Delta\Delta E_{\text{int}}$	-15.4		-12.6		-12.0		-16.0	
$\Delta\Delta\Delta E_{\text{int}}$	-2.9				4.0			
ΔE_{Pauli}	173.6	314.3	203.7	320.4	202.3	320.8	204.3	302.7
$\Delta\Delta E_{\text{Pauli}}$	140.7		116.7		118.5		98.4	
$\Delta\Delta\Delta E_{\text{Pauli}}$	24.0				20.1			
ΔE_{disp}	-23.1	-36.2	-23.4	-41.0	-23.9	-37.6	-25.5	-36.3
$\Delta\Delta E_{\text{disp}}$	-13.1		-17.6		-13.7		-10.8	
$\Delta\Delta\Delta E_{\text{disp}}$	4.5				-2.9			
ΔE_{elstat}	-114.6	-177.8	-133.4	-179.5	-130.0	-170.1	-129.5	-172.5
$\Delta\Delta E_{\text{elstat}}$	-63.2		-46.1		-49.1		-42.9	
$\Delta\Delta\Delta E_{\text{elstat}}$	-17.1				-6.3			
ΔE_{pol}	-17.1	-47.3	-22.5	-47.0	-23.0	-47.4	-22.5	-43.8
$\Delta\Delta E_{\text{pol}}$	-30.2		-24.4		-24.5		-21.2	
$\Delta\Delta\Delta E_{\text{pol}}$	-5.8				-3.3			
ΔE_{CT}	-61.2	-110.3	-71.3	-112.2	-67.5	-110.7	-62.8	-102.2
$\Delta\Delta E_{\text{CT}}$	-49.1		-40.8		-43.3		-39.4	
$\Delta\Delta\Delta E_{\text{CT}}$	-8.3				-3.9			

Table S4. Summary of electronic energies of computed structures. E_{SMD} is the single-point energies corrected with a SMD solvation model in toluene.

System	E (Hartree) M06L/SDD/def2-SVP	E_{SMD} (Hartree) M06L-D3/SDD/def2-TZVP	Imaginary frequencies (cm^{-1})
cc	-3865.511870	-	-
c1	-3472.7988366	-3472.822819	-
c1a-R	-3551.3556915	-3551.394292	-
c1a-TS	-3551.339550	-3551.378246	-427.5675
c1a-P	-3551.3793586	-3551.402595	-
c1b-R	-3629.9171549	-3629.939705	-
c1b-TS	-3629.8926546	-3629.915559	-390.9608
c1b-P	-3629.9304679	-3629.968015	-
c1b*-R	-3629.9187541	-3629.941819	-
c1b*-TS	-3629.8976328	-3629.920868	-419.1167
c1b*-P	-3629.9483759	-3629.971884	-
c1b*-TS β H	-3629.9363703	-3629.959161	-414.125
c1b*-P β H	-3629.947333	-3629.975194	-
c1b*-I	-3629.9326007	-3629.957462	-
c1c-R	-3708.4794826	-3708.503954	-
c1c-TS	-3708.4583355	-3708.483363	-398.5403
c1c-P	-3708.5176867	-3708.543002	-
c1c-TS β H	-3708.499430	-3708.5240202	-395.9208
c1c-P β H	-3708.507130	-3708.541633	-
c1c*-R	-3708.4706383	-3708.494091	-
c1c*-TS	-3708.454003	-3708.478353	-351.9818
c1c*-P	-3708.5158489	-3708.540792	-
c1c*-TS β H	-3708.498842	3708.5227582	-238.3122
c1c*-P β H	-3708.507767	-3708.532066	-

Table S5. Summary of enthalpies and Gibbs free energies of computed structures. Enthalpies and free energies are at 323.15 K in toluene using M06L-D3/SDD/def2-TZVP method.

System	H (Hartree)	G (Hartree)
c1	-3472.122304	-3472.2917
c1a-R	-3550.637304	-3550.81395
c1a-TS	-3550.619535	-3550.7988
c1a-P	-3550.644407	-3550.8152
c1b-R	-3629.120407	-3629.3044

c1b-TS	-3629.098026	-3629.2753
c1b-P	-3629.137102	-3629.3182
c1b*-R	-3629.122695	-3629.306817
c1b*-TS	-3629.103458	-3629.279731
c1b*-P	-3629.152884	-3629.331933
c1b*-TSβH	-3629.132603	-3629.312038
c1b*-PβH	-3629.149739	-3629.323611
c1b*-I	-3629.13840	-3629.321885
c1c-R	-3707.62644	-3707.809316
c1c-TS	-3707.604325	-3707.789226
c1c-P	-3707.658561	-3707.853853
c1c-TSβH	-3707.635024	-3707.827003
c1c-PβH	-3707.642335	-3707.834056
c1c*-R	-3707.614975	-3707.805227
c1c*-TS	-3707.599728	-3707.784598
c1c*-P	-3707.659913	-3707.851831
c1c*-TSβH	-3707.636916	-3707.82907
c1c*-PβH	-3707.649444	-3707.839888

Table S6. Summary of enthalpies and Gibbs free energies of computed structures. Enthalpies and free energies are at 333.15 K in toluene using M06L-D3/SDD/def2-TZVP method.

System	<i>H</i>(Hartree)	<i>G</i>(Hartree)
c1	-3472.118528	-3472.296968
c1a-R	-3550.633335	-3550.819477
c1a-TS	-3550.615539	-3550.804436
c1a-P	-3550.64053	-3550.820504
c1b-R	-3629.116213	-3629.310132
c1b-TS	-3629.09390	-3629.280821
c1b-P	-3629.132995	-3629.323863
c1b*-R	-3629.118502	-3629.312579
c1b*-TS	-3629.099336	-3629.285249
c1b*-P	-3629.151884	-3629.336933
c1b*-TSβH	-3629.132006	-3629.317396
c1b*-PβH	-3629.145070	-3629.330131
c1b*-I	-3629.134255	-3629.328557
c1c-R	-3707.62214	-3707.815041
c1c-TS	-3707.600007	-3707.795014
c1c-P	-3707.654308	-3707.859559
c1c-TSβH	-3707.631024	-3707.833265
c1c-PβH	-3707.638125	-3707.840056
c1c*-R	-3707.610598	-3707.811181
c1c*-TS	-3707.595394	-3707.790385

c1c*-P	-3707.655584	-3707.857836
c1c*-TSβH	-3707.632599	-3707.834521
c1c*-PβH	-3707.645155	-3707.845663

Table S7. Summary of enthalpies and Gibbs free energies of computed structures. Enthalpies and free energies are at 343.15 K in toluene using M06L-D3/SDD/def2-TZVP method.

System	<i>H</i>(Hartree)	<i>G</i>(Hartree)
c1	-3472.114667	-3472.302381
c1a-R	-3550.629278	-3550.825124
c1a-TS	-3550.611453	-3550.810166
c1a-P	-3550.636564	-3550.825965
c1b-R	-3629.111924	-3629.316016
c1b-TS	-3629.089679	-3629.286494
c1b-P	-3629.128794	-3629.329654
c1b*-R	-3629.114214	-3629.318468
c1b*-TS	-3629.095120	-3629.290891
c1b*-P	-3629.155884	-3629.340933
c1b*-TSβH	-3629,136303	-3629,321496
c1b*-PβH	-3629,140774	-3629,335611
c1b*-I	-3629.130016	-3629.334556
c1c-R	-3707.617741	-3707,820896
c1c-TS	-3707.595589	-3707.800933
c1c-P	-3707.649956	-3707.864394
c1c-TSβH	-3707.627561	-3707.838521
c1c-PβH	-3707.634125	-3707.844876
c1c*-R	-3707.606122	-3707.817268
c1c*-TS	-3707.59096	-3707.796304
c1c*-P	-3707.651155	-3707.863972
c1c*-TSβH	-3707.628283	-3707.841522
c1c*-PβH	-3707.640468	-3707.852569

Cartesian Coordinates

cc
Ni 2.89689700 -0.48292600 1.58259100
N 1.32672300 -1.67931500 1.73622000
N 3.35514300 -0.93488000 -0.19108600
C 3.97816800 6.31830700 1.78793500
H 4.60459800 7.18277100 2.06014200
H 4.68208000 5.47086100 1.79157300
C 3.50505100 6.51800900 0.37323000
C 2.21641200 6.64496600 0.02644700
H 1.92750800 6.80584900 -1.00840600
H 1.41181300 6.61533700 0.75532200
C 4.59800400 6.59583700 -0.64829600
H 5.24219000 7.46727500 -0.46654400
H 4.20097400 6.67914400 -1.66321800
H 5.25226600 5.71467700 -0.60786900
C 0.17909200 -3.80406300 1.23954800
H 0.30025000 -4.63865500 0.54893600
H -0.88403400 -3.55076500 1.23649800
H 0.42382300 -4.14898400 2.24990100
C 1.09519700 -2.67335700 0.85624000
C 1.78102400 -2.77034200 -0.35075700
H 1.50818200 -3.61384100 -0.97636400
C 2.77812400 -1.91507500 -0.87894200
C 3.22594300 -2.19584400 -2.28696600
H 4.14405800 -2.79668600 -2.28611700
H 3.45486000 -1.27805100 -2.83619300
H 2.46223200 -2.75191300 -2.83170800
C 0.43482700 -1.41430400 2.76440400
C -0.94996800 -1.13051500 2.56762200
C -1.78679200 -0.77115200 3.64851400
H -2.83303300 -0.56584600 3.44469300
C 0.08333200 -0.95009700 5.14264100
H 0.49090000 -0.89626400 6.14849800
C 0.90483700 -1.32827800 4.09129900
C 4.31793000 -0.10943000 -0.85585300
C 3.93625200 1.17814500 -1.31528700
C 4.89709100 1.97689000 -1.94249200
H 4.61686800 2.96634200 -2.29469500
C 6.20634200 1.53391500 -2.10557000
C 6.57154800 0.28173100 -1.62561800
H 7.59729300 -0.05616300 -1.74636600
C 5.64687900 -0.55963900 -0.99400600
C 2.91177500 6.11056400 2.85596200
H 3.38147000 6.21708400 3.84282500
H 2.17981200 6.92686500 2.78914900
C 2.17600600 4.77262200 2.79057600
H 1.73796400 4.65084100 1.79117000
H 1.32823300 4.79196800 3.48866000
C 2.54106100 1.72331200 -1.09829800
H 2.18726300 1.30901200 -0.13910200
C 6.10360200 -1.88913600 -0.42464400
H 5.24525300 -2.57531100 -0.42875500

C	2.52380400	3.24231600	-0.97342300
H	2.72027300	3.74402900	-1.92965300
H	1.53930200	3.58630000	-0.63755900
H	3.26768900	3.60871100	-0.25280200
C	1.55149000	1.25523400	-2.16431000
H	0.55846700	1.68405000	-1.98356800
C	6.53758700	-1.73538700	1.03426500
H	7.34828500	-1.00133700	1.12170300
C	-1.26931100	-0.65717500	4.92571600
H	5.70455800	-1.39745500	1.65569200
H	6.90017900	-2.68682900	1.43768400
C	7.22135400	-2.54002000	-1.23480600
H	7.40842500	-3.55548700	-0.87403300
H	1.86797100	1.56066000	-3.16850700
H	1.44322000	0.16555800	-2.16438500
H	6.98012100	-2.59458000	-2.30161100
H	8.16609700	-1.99335300	-1.13477100
H	6.94028800	2.16738500	-2.59539500
H	1.94547900	-1.58592400	4.27230900
C	3.04635200	3.55820000	3.08470700
H	3.89031000	3.53588900	2.38041200
H	3.50406900	3.65013900	4.08150300
C	2.29293700	2.23658600	2.96857600
H	1.78901400	2.19778700	1.99063800
H	1.49953200	2.18191200	3.72713600
H	4.23390200	1.70493600	1.24340300
C	4.18184500	0.88028100	1.95677200
H	5.17256400	0.49221700	2.19450100
H	2.62522000	0.06736400	3.19808600
C	3.23426200	1.04237000	3.08947100
H	3.71055900	1.02304000	4.08300100
C	-1.61605300	-1.24592500	1.33655000
N	-2.32614600	-1.30086400	0.41993800
B	-3.39245400	-1.35234900	-0.77324300
C	-4.43452400	-0.09355400	-0.60079400
C	-4.51274600	0.83364100	0.44345200
C	-5.44483400	0.01638000	-1.56829700
C	-5.51147500	1.81330800	0.52534500
C	-6.45681400	0.97640000	-1.52913500
C	-6.48984200	1.88561100	-0.46653500
C	-4.23018600	-2.74966500	-0.47864100
C	-4.53481000	-3.73050200	-1.42994300
C	-4.73137600	-3.00113100	0.80946700
C	-5.25749200	-4.89065400	-1.12819400
C	-5.45310100	-4.14535100	1.15512900
C	-5.71769500	-5.10169000	0.17309000
C	-2.38587500	-1.32093800	-2.08028100
C	-2.24254800	-0.23078700	-2.94945400
C	-1.46413100	-2.36114700	-2.28977100
C	-1.27560400	-0.17400100	-3.96073000
C	-0.50377900	-2.35530600	-3.30136700
C	-0.39732400	-1.24202800	-4.13806300
F	-5.51081400	-5.79483200	-2.07834400
F	-6.40923700	-6.20103600	0.47587600
F	-5.89492000	-4.32898800	2.40380100

F	-4.51883100	-2.10567600	1.80093800
F	-4.13583800	-3.59304100	-2.70373900
F	-1.46422300	-3.43291400	-1.47101100
F	0.33932200	-3.38776600	-3.45252300
F	0.55252400	-1.19068700	-5.07393600
F	-1.15858900	0.91737500	-4.72239900
F	-3.02221000	0.85586300	-2.82544700
F	-7.38604900	1.03491400	-2.48613400
F	-5.44259000	-0.84122700	-2.60590200
F	-7.44662700	2.81289300	-0.40493700
F	-5.53580200	2.67640800	1.54733100
F	-3.60818600	0.82643500	1.44762900
H	-1.90770700	-0.35858700	5.74981600

c1

Ni	-0.30118900	0.46976200	0.62747400
N	0.17815400	-0.00557900	2.43931600
N	1.38320700	0.05129500	-0.09572600
C	1.67284700	-0.10655200	4.37602100
H	2.72653300	0.08192000	4.60992400
H	1.40315900	-1.08559800	4.79812200
H	1.05912900	0.63755200	4.90418300
C	1.42226600	-0.03143200	2.89827900
C	2.53326700	0.02106900	2.03552300
H	3.51720100	0.05158500	2.50273700
C	2.50957000	-0.02246200	0.64187100
C	-0.89031500	-0.41358900	3.27941300
C	-1.01478900	-1.76571900	3.67216500
C	-2.08135800	-2.10264700	4.51363500
H	-2.19730000	-3.13643300	4.84612500
C	-3.01109900	-1.15213800	4.92822400
H	-3.82883400	-1.44332900	5.59111500
C	-2.91595000	0.16101100	4.47341500
H	-3.66723000	0.89656500	4.76994300
C	-1.86593300	0.53977800	3.63792400
C	-0.08544200	-2.82442800	3.10545200
H	0.94091200	-2.42081700	3.10141200
C	-0.44619000	-3.10706800	1.64649600
H	0.24972200	-3.83375700	1.20088900
H	-0.41230800	-2.19227000	1.03255200
H	-1.46134700	-3.52462900	1.56498800
C	-0.05142000	-4.11025000	3.91550200
H	0.71631300	-4.79205500	3.52416000
H	-1.00766900	-4.65297800	3.87154000
H	0.17644800	-3.92600800	4.97561800
C	-1.74524200	1.90160100	3.00267000
H	-0.69754800	2.21845700	3.14272900
C	-2.64224600	2.97527200	3.58823900
H	-2.45219200	3.94477800	3.10918100
H	-2.47139200	3.09586500	4.66724400
H	-3.70889100	2.74898200	3.43943900
C	-1.95921700	1.76139600	1.48585600
H	-1.30186700	2.41352300	0.88881200
H	-2.98516600	2.01381000	1.17369800

H	-1.94643000	0.67450100	1.14001400
C	1.47556400	-0.09199200	-1.48961900
C	1.71761900	-1.32358400	-2.10445600
C	1.77621100	-1.42726800	-3.49206100
H	1.95357900	-2.40413500	-3.94770700
C	1.35910000	0.93177800	-3.72930100
H	1.20088900	1.82231900	-4.34029400
C	1.59674100	-0.30666900	-4.30859100
H	1.83737600	-2.20621900	-1.47226800
C	1.30683600	1.03842600	-2.32827100
C	1.02381500	2.28569000	-1.72996700
N	0.75795000	3.32453400	-1.29319100
C	3.82993800	-0.10496000	-0.06963000
H	3.96724400	-1.07261500	-0.57329500
H	3.91748600	0.66544300	-0.84998000
H	4.66011100	0.02425100	0.63234500
H	1.63309600	-0.40225200	-5.39451500
B	0.06821500	4.68198200	-0.87263100
H	-0.82862100	0.75084900	-0.72732000
C	0.89526900	5.84974300	-1.64720300
C	2.28366700	5.89599800	-1.50963500
C	0.33061500	6.86866700	-2.41380100
C	3.08307800	6.87075400	-2.10151300
C	1.09291000	7.86692600	-3.02136600
C	2.47673100	7.86699600	-2.86380000
C	-1.45543700	4.41207800	-1.40705700
C	-1.64311900	4.05772600	-2.74699900
C	-2.60841300	4.35802300	-0.62534600
C	-2.86196600	3.66222500	-3.28622700
C	-3.84962800	3.94951800	-1.11712400
C	-3.98079600	3.60177600	-2.45663100
C	0.21621600	4.89692400	0.73238200
C	0.80938300	4.02781400	1.64436900
C	-0.26610700	6.08835500	1.27883500
C	0.90094100	4.29559500	3.01088500
C	-0.19495200	6.40036400	2.63317700
C	0.39358500	5.48940400	3.51104200
F	0.51267900	8.81727900	-3.74457200
F	3.21285100	8.80924700	-3.43567200
F	4.40231800	6.86432200	-1.94397700
F	2.90586000	4.96473100	-0.77176900
F	-0.98907500	6.93541100	-2.59721300
F	-0.68766900	7.54146500	3.09831300
F	0.45897400	5.75635900	4.80764000
F	-0.87364100	6.96995600	0.47981000
F	1.44415500	3.40128700	3.83640400
F	1.31292800	2.84966100	1.24977900
F	-0.59461400	4.07066800	-3.58674100
F	-2.96780700	3.33120200	-4.56751000
F	-5.15066900	3.21194100	-2.93939000
F	-4.89664300	3.86845600	-0.30217300
F	-2.58709800	4.66560200	0.67761800

c1a-R

Ni	-0.24267800	0.08008700	0.34739000
N	0.03518700	-0.02162600	2.32394700
N	1.63002900	0.03766800	-0.06941100
C	1.38210200	-0.23764100	4.38406000
H	2.08112800	0.49510900	4.80989700
H	1.82462300	-1.22997300	4.56392900
H	0.44061800	-0.19238200	4.94060300
C	1.22414800	-0.00823100	2.90636900
C	2.43526200	0.17106200	2.19942600
H	3.32846700	0.29395800	2.81273100
C	2.63264400	0.16981900	0.82801900
C	-1.10258400	-0.37669600	3.10624900
C	-1.40643800	-1.75274000	3.24885500
C	-2.59121900	-2.10726100	3.89916000
H	-2.84835800	-3.16349300	4.00969400
C	-3.45033600	-1.13907800	4.41298500
H	-4.37574600	-1.43594800	4.91135100
C	-3.11206300	0.20419200	4.30954500
H	-3.77042700	0.96021000	4.74582000
C	-1.93644900	0.61476400	3.66800900
C	-0.48208000	-2.82483600	2.69492400
H	0.54217900	-2.41626300	2.69848100
C	-0.80891400	-3.16542900	1.24289000
H	-0.15390400	-3.96595100	0.86826700
H	-0.67796200	-2.29720300	0.57516400
H	-1.85034600	-3.50761100	1.13611000
C	-0.45911000	-4.08474100	3.55018800
H	0.33291100	-4.76694000	3.21049100
H	-1.40326800	-4.64651300	3.49188400
H	-0.27509800	-3.85836800	4.61047600
C	-1.56034400	2.08501100	3.67364000
H	-0.77069900	2.22322300	2.91484200
C	-0.97251500	2.48674600	5.02661300
H	-0.71047400	3.55439200	5.04257100
H	-0.06343400	1.92578100	5.27636600
H	-1.70278600	2.31629100	5.83275500
C	-2.72455200	3.01290100	3.33908000
H	-2.36399200	4.04014900	3.18062800
H	-3.45428200	3.05877700	4.16120900
H	-3.27415800	2.71612400	2.43516900
C	1.96624000	-0.09573500	-1.42555100
C	2.58226100	-1.24201700	-1.94106500
C	2.85059200	-1.36066500	-3.30153600
H	3.31650900	-2.27517900	-3.67585200
C	1.91508500	0.81535500	-3.71955200
H	1.63780000	1.62929800	-4.39227000
C	2.51861900	-0.33844500	-4.19667900
H	2.82113500	-2.05652200	-1.25364100

C	1.64856900	0.93845300	-2.34372300
C	1.03726000	2.11387700	-1.85482700
N	0.55799500	3.10549100	-1.49858200
C	4.03155200	0.39168900	0.32761500
H	4.44623000	-0.48797700	-0.18396400
H	4.05775200	1.21652800	-0.40117600
H	4.70611000	0.64677100	1.15140200
H	2.72474600	-0.44668300	-5.26221400
B	-0.13799300	4.47065400	-1.13603000
H	-0.44163000	0.00448400	-1.08477600
C	-1.91407200	1.15883400	0.28417000
H	-1.89141400	1.72517000	-0.65198500
H	-1.94280500	1.76030000	1.19609700
C	-2.26639500	-0.18617800	0.29714900
H	-2.61328100	-0.67210600	1.21263900
H	-2.52131500	-0.70173500	-0.63275500
C	0.72839600	5.60197500	-1.93322100
C	2.11593100	5.62343000	-1.77419800
C	0.19954600	6.61783600	-2.72959700
C	2.94596200	6.56817400	-2.37229400
C	0.99369300	7.58661900	-3.34460500
C	2.37437300	7.56094100	-3.16522700
C	-1.65866600	4.23929300	-1.67921300
C	-1.84501800	3.90789300	-3.02381900
C	-2.81890900	4.23333800	-0.90561200
C	-3.08184700	3.61143400	-3.58676300
C	-4.08129600	3.94001000	-1.42473600
C	-4.21398300	3.62552500	-2.77329000
C	0.02009700	4.75777100	0.45587400
C	0.69898600	3.96951600	1.37974200
C	-0.48112500	5.96092800	0.95768600
C	0.87492100	4.33305800	2.71514500
C	-0.34890400	6.35754200	2.28497000
C	0.33861800	5.53046000	3.17426200
F	0.44551900	8.53335200	-4.09654700
F	3.13961900	8.47475000	-3.74486200
F	4.26199700	6.53611400	-2.19179400
F	2.71077500	4.69685800	-1.00541900
F	-1.11436700	6.71149800	-2.93937000
F	-0.86482000	7.50366000	2.71207600
F	0.47092600	5.88034700	4.44769300
F	-1.14794600	6.77796700	0.13654700
F	1.53034500	3.52722000	3.54858800
F	1.23306500	2.79567400	1.02328500
F	-0.78299200	3.86201400	-3.84397300
F	-3.19359400	3.30616400	-4.87418300
F	-5.40281000	3.33543900	-3.28029200
F	-5.14796300	3.93062100	-0.63410100

F -2.77850700 4.46544700 0.40983000

c1a-TS

Ni -2.30942700 1.17614200 0.87869500
N -3.28790900 0.32631100 -0.51510000
N -1.53470000 2.56142900 -0.23879400
C -4.03685500 -0.09125400 -2.80523800
H -3.74732400 0.16593200 -3.83023800
H -5.10826400 0.13300800 -2.68415100
H -3.94306100 -1.17705200 -2.67680000
C -3.21290700 0.66116300 -1.80100900
C -2.43064400 1.72129200 -2.29874700
H -2.42726700 1.84677300 -3.38027200
C -1.68607400 2.64415600 -1.57165500
C -4.28593200 -0.61972300 -0.12162300
C -5.57554900 -0.12621800 0.18851300
C -6.51731900 -1.01296400 0.71761300
H -7.51443400 -0.64756500 0.97573200
C -6.20875800 -2.35521700 0.92170100
H -6.95392900 -3.03193300 1.34581100
C -4.95634700 -2.83301400 0.55783300
H -4.72866300 -3.89550400 0.68524600
C -3.97692600 -1.98799700 0.02122800
C -5.93068600 1.33734300 -0.02060700
H -5.30085100 1.71821400 -0.84241700
C -5.60350500 2.18464900 1.20693200
H -5.89149200 3.23508100 1.05006500
H -4.52457600 2.16968700 1.43476200
H -6.14026600 1.82130900 2.09768500
C -7.38073900 1.53972700 -0.44002800
H -7.55577900 2.58427900 -0.73449500
H -8.08571500 1.32097300 0.37593500
H -7.65601800 0.90083400 -1.29174300
C -2.65935100 -2.59131800 -0.43406800
H -2.00619800 -1.76813000 -0.77686200
C -2.90088000 -3.54407300 -1.60626500
H -1.97024100 -4.01782600 -1.94248200
H -3.34780300 -3.04727700 -2.47838300
H -3.58318800 -4.35684600 -1.31458900
C -1.92139500 -3.33757000 0.67476000
H -0.93784300 -3.68387500 0.32015700
H -2.47586400 -4.23158900 0.99853500
H -1.74740500 -2.71912600 1.56370000
C -0.85778800 3.58487200 0.43120100
C -1.42113600 4.84345700 0.68120000
C -0.72835200 5.79901100 1.41782400
H -1.19738900 6.76649500 1.61180700
C 1.14790900 4.31254900 1.68021000
H 2.15041300 4.08339700 2.04724200
C 0.55178100 5.53999200 1.92386200
H -2.42723100 5.04571000 0.30674000
C 0.44903600 3.34608900 0.93280600
C 1.04443000 2.10624500 0.62011500
N 1.55546700 1.10788300 0.33709300

C	-0.99844600	3.74480000	-2.32504400
H	-1.47895600	4.72023200	-2.15604800
H	0.05071100	3.85413100	-2.01408100
H	-1.01151700	3.54861100	-3.40263600
H	1.07962100	6.29792900	2.50404100
B	2.26960300	-0.25012900	-0.02924100
H	-1.49456800	1.86181100	2.05373300
C	-2.07809700	0.96986500	3.00211000
H	-2.54617500	1.73211400	3.63749800
H	-1.12618300	0.61031100	3.41238900
C	-2.92453500	0.03254500	2.31787300
H	-2.55819000	-0.98984400	2.18676800
H	-4.00792900	0.09949800	2.46628300
C	2.24256000	-1.07449200	1.37799500
C	1.01649000	-1.26315000	2.01418600
C	3.34025300	-1.63938700	2.02501500
C	0.86011600	-1.93986100	3.21838300
C	3.23129200	-2.33338900	3.23237500
C	1.98448800	-2.48539600	3.83409700
C	3.75204700	0.18458800	-0.53863000
C	4.50514200	1.10301800	0.19555800
C	4.37687100	-0.31799900	-1.68034000
C	5.78045900	1.52362400	-0.16550200
C	5.65576400	0.07466100	-2.08084200
C	6.35995400	1.00392400	-1.32149900
C	1.34404800	-0.93824800	-1.17803900
C	0.72712300	-0.19827600	-2.18816200
C	1.16967900	-2.31938300	-1.26436200
C	-0.04692400	-0.76980200	-3.19726700
C	0.42666700	-2.93437300	-2.26867200
C	-0.21099100	-2.15201800	-3.22740100
F	4.30702800	-2.85029400	3.81269700
F	4.56650800	-1.55045900	1.50620600
F	1.86950500	-3.13605800	4.98214600
F	-0.34180300	-2.06725200	3.77820200
F	-0.10176700	-0.77815400	1.44549200
F	1.76309100	-3.13856400	-0.38934100
F	0.31377500	-4.25917200	-2.30539200
F	-0.94537800	-2.71731800	-4.17594500
F	-0.60427400	-0.02093700	-4.14436200
F	0.90925500	1.12987100	-2.25627400
F	3.77885500	-1.22973500	-2.45147300
F	6.20466500	-0.43315000	-3.17741400
F	7.57354700	1.38753700	-1.68921700
F	6.44703000	2.40176900	0.57593400
F	4.01018700	1.60269400	1.34173800

c1a-P

Ni	-2.44976500	1.06737200	0.90513000
N	-3.30748000	0.03401800	-0.38483700
N	-1.65659200	2.35737900	-0.30604600
C	-3.87488100	-0.73205100	-2.62920000
H	-3.54981200	-0.59148800	-3.66637400
H	-4.96487900	-0.58110300	-2.58663800
H	-3.70441100	-1.78078100	-2.34991700

C	-3.16304200	0.20680300	-1.69829400
C	-2.41469400	1.24683900	-2.28615000
H	-2.38015300	1.25410000	-3.37641700
C	-1.75425900	2.29425300	-1.64290300
C	-4.29262400	-0.88644800	0.09172900
C	-5.60580500	-0.40146200	0.29336200
C	-6.53679000	-1.24795300	0.90156600
H	-7.55343100	-0.88852700	1.08015200
C	-6.19324300	-2.54234000	1.28334800
H	-6.93136400	-3.18532500	1.76801800
C	-4.91564400	-3.02015300	1.01894300
H	-4.65843200	-4.04920100	1.28681400
C	-3.94714300	-2.21471700	0.40813600
C	-5.99967500	1.00724200	-0.12049000
H	-5.33613200	1.30661600	-0.94970400
C	-5.77732500	2.01755300	1.00256100
H	-6.09156300	3.02622200	0.69431800
H	-4.71447100	2.07508300	1.29012300
H	-6.35306500	1.74864700	1.90230400
C	-7.42869900	1.08981000	-0.64099100
H	-7.62600000	2.08053300	-1.07458600
H	-8.17236700	0.94174200	0.15624200
H	-7.62706800	0.33812600	-1.41873000
C	-2.58714500	-2.80244800	0.08508900
H	-2.01834200	-2.04724700	-0.48289000
C	-2.71202600	-4.04774100	-0.78924100
H	-1.71949600	-4.40237200	-1.09898900
H	-3.29559100	-3.86237500	-1.70238900
H	-3.20345400	-4.87138300	-0.24957700
C	-1.78841300	-3.12895800	1.34163000
H	-0.82075600	-3.58255200	1.08188000
H	-2.32585900	-3.84265500	1.98557800
H	-1.58558300	-2.23387600	1.94294000
C	-1.07409800	3.46140600	0.31843700
C	-1.76203400	4.66291800	0.54211600
C	-1.17317200	5.69498200	1.26504500
H	-1.73436800	6.61688000	1.43432400
C	0.83397700	4.39992800	1.57856200
H	1.84418400	4.27446600	1.97224300
C	0.11960800	5.56853600	1.78957100
H	-2.77850500	4.75758200	0.15254100
C	0.24367200	3.35673700	0.84082000
C	0.93089000	2.15479800	0.57219400
N	1.45103300	1.15290500	0.32255000
C	-1.09673800	3.35250800	-2.47791700
H	-1.43933000	4.36046100	-2.20296700
H	-0.00405300	3.34546000	-2.33921300
H	-1.29428500	3.20610000	-3.54456900
H	0.56394100	6.38363000	2.36219300
B	2.07409300	-0.20875100	-0.16170200
C	-3.04093000	0.23473700	2.50971800
H	-2.61161700	-0.75812900	2.69397800
H	-4.12894200	0.22843100	2.65716600
C	1.84881800	-1.31599900	1.00734600
C	1.00718500	-1.19306300	2.10885700

C	2.56012800	-2.51617900	0.94081500
C	0.88883300	-2.16603400	3.09942800
C	2.47057300	-3.51944900	1.90188400
C	1.62652100	-3.33942300	2.99783000
C	3.66428900	0.10236400	-0.33809600
C	4.36016000	0.73157000	0.69478600
C	4.42996400	-0.25268600	-1.44817700
C	5.72322900	1.01389800	0.64631600
C	5.79737900	0.00753200	-1.53863400
C	6.44734800	0.64632200	-0.48521800
C	1.25132300	-0.47196300	-1.54543100
C	1.24138200	0.52492800	-2.52493100
C	0.46309100	-1.58565200	-1.83103600
C	0.49836200	0.45447700	-3.69637100
C	-0.31276600	-1.69148200	-2.98820600
C	-0.30233600	-0.66170700	-3.92003700
F	3.16764600	-4.64259300	1.78280600
F	3.34492500	-2.75385100	-0.11485000
F	1.51434200	-4.28545400	3.91903600
F	0.03441700	-1.99537500	4.10541400
F	0.21545100	-0.11560000	2.26561100
F	0.40471500	-2.62766400	-0.99666000
F	-1.08561500	-2.75444100	-3.18876100
F	-1.08128700	-0.71884900	-4.99334800
F	0.49232300	1.45874100	-4.56877100
F	1.97572100	1.63478700	-2.34316900
F	3.87578400	-0.88114700	-2.48621000
F	6.48565900	-0.35093500	-2.61559200
F	7.74577300	0.90178800	-0.55843800
F	6.33221100	1.62220400	1.65887600
F	3.70775700	1.09740200	1.81092300
C	-2.28776600	1.38741500	3.09058300
H	-1.75331400	1.91309000	2.32708600
H	-2.90118900	2.14032300	3.53973900
H	-1.49038700	1.10736700	3.74683000

c1b-R

Ni	0.40322600	-0.78585200	0.64023900
N	0.01016000	0.47898800	2.17103800
N	2.26933400	-0.06248200	0.48172400
C	0.58564800	1.56877000	4.30680200
H	1.46504000	1.96417500	4.82491500
H	0.09127200	0.87387600	5.00072200
H	-0.11979600	2.39520800	4.13536700
C	0.97119000	0.90900500	3.01197100
C	2.32735100	0.84390300	2.71643500
H	2.99848400	1.24998000	3.47182100
C	2.92099400	0.52532200	1.47386700
C	4.35781900	0.94465600	1.34137400
H	4.53054800	1.90540800	1.84249100
H	4.69021500	1.02668600	0.30079200
H	5.00317700	0.21048400	1.84946900
C	-1.31817200	0.66729200	2.53275300
C	-1.91959000	-0.17082000	3.51019100
C	-3.27642800	-0.05015600	3.86253900

C	-3.48284500	1.72648100	2.24813300
H	-4.10045200	2.47619900	1.74806100
C	-2.13996300	1.61099700	1.90227500
C	2.83377100	-0.10171700	-0.82897900
C	3.85772300	-1.00667600	-1.19373100
C	4.26423800	-1.04072400	-2.53432300
H	5.04778800	-1.74387100	-2.83127100
C	3.69902500	-0.20759600	-3.48991000
C	2.71767000	0.70432200	-3.11047500
H	2.29310000	1.37708500	-3.85932300
C	2.27281400	0.77867500	-1.78880500
C	1.34404100	-3.11311800	1.18821000
H	2.03255700	-2.48260400	1.77903100
H	1.85810800	-4.08417100	1.05690500
C	0.98608600	-2.46178300	-0.11497400
H	0.20215100	-2.99580300	-0.66964400
H	1.83383500	-2.28416500	-0.78563400
C	4.56217800	-1.92678800	-0.20924200
H	4.11762200	-1.76706900	0.78946900
C	1.27093400	1.83729700	-1.36782600
H	0.67132500	1.40827600	-0.54686400
C	4.39975600	-3.40571200	-0.55606100
H	4.91167100	-3.65041500	-1.49915700
H	4.84712600	-4.03520700	0.22671000
H	3.35105600	-3.70745300	-0.67023300
C	6.05628000	-1.60837900	-0.13319700
H	6.54882600	-2.21947900	0.63520100
C	0.31025300	2.25140800	-2.47168100
H	0.80852200	2.82756500	-3.26605100
C	-4.05533800	0.90558500	3.22852500
H	-0.17255200	1.38552200	-2.94755100
H	-0.48385600	2.89865500	-2.07036700
C	1.98807700	3.05541700	-0.78853100
H	1.26833700	3.80789300	-0.43179800
H	6.55031200	-1.83308500	-1.09054200
H	6.26171700	-0.55456500	0.09313000
H	2.63225200	2.79027400	0.06143000
H	2.62497500	3.53777800	-1.54626800
H	4.02971900	-0.25901000	-4.52961500
H	-1.69571800	2.25668700	1.14046200
C	-1.49149700	-1.45350500	0.38630700
H	-1.50262700	-2.54436100	0.31675100
H	-2.20304700	-1.04974600	1.10934200
C	-1.05038300	-0.66422500	-0.68175000
H	-1.35519000	0.38819100	-0.74215000
H	-0.71333600	-1.09720700	-1.62959500
C	-1.12822400	-1.20035600	4.05632000
N	-0.50359600	-2.07649800	4.48198100
B	0.22479300	-3.30014100	5.14856000
H	-5.10966500	1.00956700	3.48767200
C	-0.59022500	-4.64868800	4.73689600
C	-1.55922100	-4.77887800	3.74379700
C	-0.30974300	-5.81720200	5.44847200
C	-2.22296000	-5.97737200	3.47705200
C	-0.94226500	-7.03405000	5.21581000

C	-1.91658200	-7.11148100	4.22187100
C	0.04577800	-3.02406600	6.75104700
C	1.06672800	-3.09928900	7.69887900
C	-1.22035900	-2.72916800	7.26100900
C	0.85538700	-2.88099800	9.06050600
C	-1.47672700	-2.50021900	8.61079500
C	-0.42418200	-2.57818800	9.51936000
C	1.75492200	-3.22100100	4.58997800
C	2.47893300	-2.03540900	4.74360900
C	2.41784700	-4.22899900	3.89008100
C	3.76112000	-1.83932500	4.24014800
C	3.70203600	-4.07599400	3.36524400
C	4.36972800	-2.86837200	3.52476700
F	-2.53625700	-8.25797500	3.98074300
F	-0.62659500	-8.11422200	5.91919000
F	-3.14071500	-6.04128100	2.51761700
F	-1.90407400	-3.73999400	2.96127000
F	0.65380500	-5.80175400	6.37589400
F	1.83105100	-5.39827800	3.62222200
F	4.25689400	-5.05522200	2.65792600
F	5.57632100	-2.69047400	2.99912300
F	4.41417100	-0.69572900	4.42820100
F	1.93542900	-1.01719800	5.42659700
F	2.31449700	-3.40257800	7.33789100
F	1.86100400	-2.96453900	9.92279000
F	-0.63908400	-2.36723200	10.80983000
F	-2.70351600	-2.21519900	9.03459900
F	-2.27773900	-2.65627800	6.43180900
H	0.46128400	-3.31837700	1.81585300
H	-3.69517200	-0.71867300	4.61730200

c1b-TS

Ni	3.80872300	1.03881600	-1.27007700
N	3.54796200	2.69680000	-0.34119700
N	4.84820400	0.21357800	0.21080400
C	3.43842900	4.23896200	1.56185200
H	3.84475200	4.35676200	2.57237300
H	2.33948400	4.27181200	1.64236400
H	3.72907300	5.11739000	0.96745300
C	3.89739100	2.95397700	0.93450400
C	4.65597400	2.08683100	1.71206500
H	4.90473900	2.43494200	2.71424800
C	5.15899500	0.81541300	1.35125400
C	6.09129600	0.15410200	2.32849500
H	6.28791500	0.79630000	3.19338900
H	7.04905900	-0.11132600	1.86062700
H	5.67558200	-0.79266200	2.69650600
C	2.83008300	3.65230100	-1.07028900
C	1.41180400	3.63431900	-1.06040900
C	0.64925400	4.51754500	-1.84909500
C	2.70061200	5.49698600	-2.64303000
H	3.21285500	6.23763400	-3.26169400
C	3.45270200	4.62208700	-1.86689700
C	5.55317200	-0.98295200	-0.10174400
C	5.06934100	-2.25196400	0.29413200

C	5.88348200	-3.36693000	0.05758500
H	5.54118300	-4.35304400	0.38298100
C	7.11218300	-3.25240200	-0.58098000
C	7.53636900	-2.00767600	-1.03605500
H	8.48718200	-1.92723200	-1.56922100
C	6.77251400	-0.85794500	-0.81548000
C	1.65880100	-0.75165900	-2.63697800
H	1.03467700	0.12818800	-2.41955500
H	1.07038100	-1.63235800	-2.33723500
C	2.95879800	-0.72489500	-1.88218000
H	3.56880300	-1.63019900	-2.00412700
H	2.73921500	-0.62410400	-0.80233000
C	3.69926200	-2.46052400	0.92466300
H	3.13875600	-1.52060000	0.81156600
C	7.26229100	0.48935300	-1.32695700
H	6.36965400	1.13092900	-1.45417000
C	2.93166400	-3.56364100	0.19839000
H	3.42865100	-4.53988300	0.29493900
H	1.92820200	-3.69309700	0.62211800
H	2.82096800	-3.36336900	-0.87733000
C	3.73133400	-2.76158100	2.42111800
H	2.70930500	-2.92617200	2.79592100
C	7.95187300	0.37982600	-2.68272800
H	8.94486800	-0.08801100	-2.60512800
C	1.30120600	5.44419100	-2.64702500
H	7.37159200	-0.21465900	-3.40389900
H	8.10933700	1.37695100	-3.11874800
C	8.17508900	1.21336700	-0.33883400
H	8.58788000	2.12692700	-0.79182900
H	4.31484200	-3.66874200	2.64263500
H	4.15209900	-1.93675000	3.00994900
H	7.65001400	1.52070700	0.57438300
H	9.02616700	0.57985100	-0.04327900
H	7.73108800	-4.13747400	-0.74427100
H	4.54429400	4.66062400	-1.87519600
C	3.60195600	1.68815300	-3.07721200
H	2.60553800	1.87155900	-3.50166900
H	4.29066900	2.53253400	-3.19206600
C	4.12724800	0.34885800	-3.11932000
H	5.21266600	0.21317100	-3.01943800
H	3.73714700	-0.36711000	-3.84798400
C	0.77583600	2.72474900	-0.19108700
N	0.23054400	2.03391900	0.56064700
B	-0.48374900	1.21528600	1.69238600
H	0.72447200	6.13178000	-3.26694700
C	-0.49828700	-0.34315400	1.20444800
C	-0.91539600	-0.63568100	-0.09534800
C	-0.19708200	-1.45291100	1.99619600
C	-0.99913900	-1.92741200	-0.60931400
C	-0.27797000	-2.76173000	1.52412200
C	-0.66359700	-3.00162400	0.20842200
C	-2.03365000	1.69554100	1.80493000
C	-2.81017600	1.08221800	2.79013000
C	-2.71191200	2.59972500	0.99148800
C	-4.16238300	1.34300900	2.98350100

C	-4.06916300	2.88939600	1.14352100
C	-4.79888000	2.25727200	2.14509100
C	0.44957900	1.53985900	2.99108100
C	0.10090300	2.39104400	4.04103500
C	1.72841900	0.98486400	3.07762900
C	0.93881300	2.63655600	5.13111700
C	2.58215100	1.17641200	4.15801000
C	2.18656400	2.02340800	5.19067500
F	-0.68736400	-4.23972000	-0.26410500
F	0.06361200	-3.78254800	2.30474500
F	-1.36868900	-2.13886900	-1.86932600
F	-1.26701900	0.36203000	-0.92190500
F	0.19399100	-1.31465800	3.26378200
F	2.17030200	0.19790800	2.08857500
F	3.76513100	0.57028100	4.22036700
F	2.99177100	2.23929400	6.22115800
F	0.55730300	3.45317900	6.10611200
F	-1.07304500	3.02749900	4.05534200
F	-2.22906900	0.20825100	3.62028400
F	-4.84690200	0.73645000	3.94535300
F	-6.08742600	2.52451900	2.30323600
F	-4.66699000	3.76240500	0.33920900
F	-2.08507800	3.25343800	-0.00075000
H	1.77705500	-0.81466200	-3.72884600
H	-0.43991600	4.46319000	-1.81613500

c1b-P

Ni	3.74847100	0.80045700	-0.87591300
N	3.59494400	2.57389500	-0.35058600
N	5.06559500	0.33850100	0.39844300
C	3.63608300	4.42138600	1.24867100
H	4.12079000	4.71395500	2.18595700
H	2.54691200	4.48829000	1.40257900
H	3.88815600	5.17070400	0.48442100
C	4.04422700	3.03628900	0.83561500
C	4.84278800	2.30298900	1.71233500
H	5.09703600	2.78349100	2.65726100
C	5.39635300	1.02476400	1.47730800
C	6.38744600	0.46873800	2.45392200
H	6.36740600	1.01820200	3.40131200
H	7.41326200	0.51727400	2.05700800
H	6.18633600	-0.59209400	2.65980600
C	2.93150000	3.42277300	-1.24739700
C	1.52305400	3.56137900	-1.20269200
C	0.82513000	4.35082100	-2.13610600
C	2.93164000	4.90767000	-3.16375700
H	3.49062200	5.43948600	-3.93708900
C	3.61990300	4.12119500	-2.24583800
C	5.78668000	-0.79709300	-0.04202100
C	5.14922600	-2.06069900	-0.05419700
C	5.88370900	-3.16273400	-0.50387800
H	5.42250700	-4.15216700	-0.50631100
C	7.19157600	-3.02316200	-0.95648000
C	7.77803500	-1.76194800	-1.01086100
H	8.78749200	-1.65846400	-1.41499000

C	7.08843000	-0.62698000	-0.57821900
C	3.70883000	-2.21913500	0.40438200
H	3.15816400	-1.29985600	0.09829400
C	7.65678900	0.76277800	-0.79765400
H	7.33637500	1.40852900	0.03558700
C	3.01265800	-3.40191100	-0.25205800
H	3.41097600	-4.36246800	0.10670200
H	1.94299800	-3.41028500	-0.01380900
H	3.11221400	-3.39319700	-1.34762300
C	3.60340600	-2.29590200	1.92400400
H	2.55516700	-2.39295300	2.24273900
C	7.05515600	1.36384800	-2.06868500
H	7.33470800	0.77402900	-2.95522400
C	1.53646700	5.02248500	-3.11760200
H	5.95241400	1.38950800	-2.02012600
H	7.40609500	2.39488700	-2.22705600
C	9.17616900	0.80720600	-0.83937500
H	9.53082500	1.84657500	-0.87733300
H	4.15170900	-3.16980000	2.30812900
H	4.00899600	-1.39823200	2.40741900
H	9.62679000	0.33313200	0.04481000
H	9.58331600	0.30326200	-1.72862500
H	7.74779000	-3.89967900	-1.29620100
H	4.70602800	4.01854400	-2.29488000
C	2.40907700	0.61703600	-2.21849600
H	1.45620400	0.42092600	-1.68289900
H	2.22677100	1.44878700	-2.91838300
C	0.82767600	2.86181700	-0.19855900
N	0.23748000	2.30303700	0.62384500
B	-0.53632000	1.42633000	1.66520600
H	1.00892200	5.63458600	-3.85028500
C	-0.56016300	-0.06199300	0.98630600
C	-0.94989200	-0.18575800	-0.34885700
C	-0.23682900	-1.25814700	1.62639000
C	-0.98466500	-1.39612000	-1.03555300
C	-0.26327200	-2.49256800	0.97875500
C	-0.61774100	-2.55960000	-0.36625600
C	-2.07155200	1.94369200	1.77363300
C	-2.92226100	1.22843200	2.61843100
C	-2.67399000	2.97150900	1.05247400
C	-4.27675700	1.50592500	2.76615900
C	-4.03046700	3.28272400	1.16278700
C	-4.83686700	2.54453400	2.02310700
C	0.37476100	1.56636400	3.01058900
C	-0.01460200	2.18764100	4.19720300
C	1.68161200	1.07049300	2.99892200
C	0.81828000	2.28023000	5.31517300
C	2.53835100	1.12756100	4.09258800
C	2.10186800	1.74765000	5.26186200
F	-0.58510800	-3.71838200	-1.01057000
F	0.08958000	-3.60090400	1.62372300
F	-1.33510100	-1.44461100	-2.31610300
F	-1.30583600	0.90457100	-1.04548500
F	0.13055400	-1.27541400	2.90942700
F	2.14649000	0.47885500	1.88899100

F	3.76047200	0.60029900	4.04940500
F	2.90575000	1.82702900	6.31281700
F	0.39715900	2.88019400	6.42207200
F	-1.22287100	2.73883800	4.32740400
F	-2.41550800	0.23112900	3.35235800
F	-5.03502600	0.79858600	3.59476500
F	-6.12648000	2.82903200	2.13874900
F	-4.55565900	4.27460400	0.45070000
F	-1.96901000	3.72817100	0.19568500
H	-0.26246500	4.41822200	-2.07406000
C	2.89770700	-0.61913500	-2.97103800
H	3.53572400	-1.33072600	-2.38934100
C	1.76372400	-1.49240700	-3.51429800
H	1.19354800	-1.89903300	-2.66120100
H	1.04582200	-0.85773300	-4.06058600
C	2.24954000	-2.62455600	-4.39320100
H	1.42107900	-3.25655000	-4.74087100
H	2.77369900	-2.24913400	-5.28466700
H	2.95631100	-3.27762900	-3.85814400
H	3.55799300	-0.30181900	-3.79617800

c1b*-R

Ni	-1.87761100	-2.61115600	-0.68452700
N	-1.91082200	-2.70919200	1.32081300
N	0.10748000	-2.85809300	-0.74065100
C	-1.00710600	-2.64723100	3.60945900
H	-0.04577400	-2.73499000	4.12748600
H	-1.67447800	-3.44224700	3.97033100
H	-1.47597500	-1.70396500	3.92720300
C	-0.84090100	-2.69185600	2.11481100
C	0.48369000	-2.73416300	1.63521300
H	1.26054600	-2.75688200	2.39962200
C	0.93350900	-2.84176900	0.31864100
C	-3.17539900	-2.83696800	1.96485800
C	-3.74883100	-4.12415600	2.07029500
C	-4.98496800	-4.24841500	2.71329700
H	-5.44614500	-5.23474400	2.80703100
C	-5.63953600	-3.13674200	3.23417900
H	-6.60092600	-3.25406800	3.73917300
C	-5.07096600	-1.87344900	3.10033600
H	-5.59688800	-1.00369600	3.50139500
C	-3.83817300	-1.69552500	2.46509900
C	-3.04427900	-5.33645300	1.48512200
H	-2.45478100	-4.97407800	0.62136700
C	-4.00778700	-6.39551600	0.96688200
H	-3.46499400	-7.17248300	0.40939200
H	-4.76904600	-5.97205500	0.29509900
H	-4.53885900	-6.90913100	1.78233700
C	-2.04759400	-5.95465500	2.46281000
H	-1.57953200	-6.85234000	2.03235200
H	-2.54523300	-6.25746600	3.39727000
H	-1.23578600	-5.26371300	2.72600400
C	-3.25389200	-0.31145400	2.25803000
H	-2.15549800	-0.40816500	2.26229200
C	-3.62395900	0.68962800	3.33964600

H	-3.06934500	1.62669700	3.19541800
H	-3.38613900	0.31582000	4.34621500
H	-4.69453100	0.94298300	3.32073300
C	-3.63798100	0.19835000	0.87295000
H	-3.13804300	1.14958300	0.63138200
H	-4.72556800	0.35523300	0.79588800
H	-3.35867700	-0.53776100	0.10636900
C	0.64374800	-2.98268500	-2.02308500
C	0.47291400	-4.15754900	-2.76819400
C	0.95852200	-4.26223500	-4.06665800
H	0.81775600	-5.19619100	-4.61547800
C	1.80078200	-2.01019100	-3.98266200
H	2.29421600	-1.15019200	-4.43944700
C	1.62506800	-3.19373800	-4.67972100
H	-0.04661800	-4.99257200	-2.29431900
C	1.31575600	-1.90417600	-2.66425100
C	1.41682400	-0.68001000	-1.97397700
N	1.45907600	0.32863500	-1.40851600
C	2.41467800	-3.00229700	0.11336900
H	2.63731800	-3.88032200	-0.51094600
H	2.86713600	-2.13809800	-0.39443100
H	2.93892600	-3.11512700	1.06890700
H	1.99622500	-3.28640900	-5.70113900
B	1.42905000	1.63699700	-0.54297200
C	-3.06308800	-0.57425600	-2.62586400
H	-3.55020500	-1.28393900	-3.31061400
H	-3.82113700	-0.21214200	-1.91862800
C	-1.83952600	-1.14000600	-1.97168200
H	-1.09345200	-1.40159100	-2.73391500
H	-1.39176000	-0.44329800	-1.23612300
C	-3.74453000	-3.10363800	-1.10054600
H	-4.37632500	-2.26337000	-1.39801500
H	-4.16236300	-3.70061400	-0.28586900
C	-2.82945700	-3.67920800	-2.00819100
H	-2.49907700	-4.71622100	-1.85695900
H	-2.73661200	-3.32929500	-3.04243500
C	0.13467800	2.52557000	-0.97088200
C	-0.68423900	2.33914000	-2.08409500
C	-0.15158000	3.65887500	-0.20663100
C	-1.76145600	3.17519300	-2.38387800
C	-1.21706600	4.51548500	-0.46340100
C	-2.03486500	4.26593700	-1.56497700
C	2.76907600	2.48976800	-0.91200300
C	3.11204900	2.68975200	-2.25023500
C	3.59049900	3.12826400	0.01803200
C	4.20173400	3.45287900	-2.66195000
C	4.68930500	3.90565900	-0.34977800
C	4.99721100	4.06810700	-1.69801200
C	1.41489200	1.00789200	0.96601000
C	2.52143000	0.25386100	1.36677900
C	0.38678800	1.08401900	1.90484900
C	2.64030100	-0.35445500	2.60957600
C	0.47564200	0.51314100	3.17694400
C	1.60243800	-0.22003700	3.52675700
F	3.35851300	3.01849500	1.32747100

F	5.44319200	4.48952800	0.57364500
F	6.03820100	4.80299000	-2.06197000
F	4.48391400	3.60205500	-3.95169900
F	2.36476000	2.13343800	-3.21762100
F	-2.51865400	2.94126600	-3.45261200
F	-0.47075500	1.33595300	-2.94932200
F	-3.05293300	5.06890000	-1.83811500
F	-1.45601000	5.56378600	0.31433000
F	0.61808700	3.93905500	0.84993600
F	-0.75783000	1.72067700	1.63848700
F	-0.52677700	0.63328700	4.04309600
F	1.67143400	-0.82737100	4.70428800
F	3.69212900	-1.11251800	2.90657500
F	3.54792300	0.09066500	0.51791500
H	-2.77187500	0.29168500	-3.24278200

c1b*-TS

Ni	-2.78037300	1.26108400	0.77881500
N	-3.33823500	-0.09132200	-0.48875700
N	-1.69132100	2.25485800	-0.58236400
C	-3.34338300	-1.40182300	-2.56628100
H	-3.01710100	-1.30283700	-3.60742200
H	-4.43367500	-1.53133000	-2.55287500
H	-2.93129700	-2.34453400	-2.17480500
C	-2.89652100	-0.22661100	-1.73744600
C	-2.01933100	0.67997600	-2.36707400
H	-1.78129800	0.46678900	-3.40925400
C	-1.47135900	1.84874800	-1.84357300
C	-4.33593300	-1.01934900	-0.06238000
C	-5.69478600	-0.65435700	-0.18921600
C	-6.66702300	-1.57045000	0.22500800
H	-7.72468900	-1.30992900	0.13818800
C	-6.31026100	-2.80826400	0.74997400
H	-7.08309600	-3.51290100	1.06526400
C	-4.96643400	-3.14680800	0.87353300
H	-4.69802100	-4.12251300	1.28440200
C	-3.95429700	-2.26841300	0.47100400
C	-6.08934900	0.70714900	-0.73927200
H	-5.27162700	1.40471600	-0.47424100
C	-7.37197900	1.24663000	-0.11914600
H	-7.53029700	2.29522800	-0.40908800
H	-7.35479200	1.20184200	0.97997400
H	-8.26074700	0.69137200	-0.45480500
C	-6.19664000	0.71835500	-2.26264900
H	-6.54867400	1.69689700	-2.62129900
H	-6.91292800	-0.03946600	-2.61676800
H	-5.23429900	0.52544300	-2.75399000
C	-2.49003900	-2.64517600	0.61438400
H	-1.95480400	-2.21691600	-0.25032200
C	-2.24658000	-4.14623900	0.59669100
H	-1.17112800	-4.35795100	0.53775300
H	-2.72785800	-4.63080500	-0.26544200
H	-2.62243100	-4.63633200	1.50753500
C	-1.87185400	-2.00664600	1.85486800
H	-0.81756800	-2.29993300	1.96708600

H	-2.40709900	-2.30679600	2.76995000
H	-1.90959800	-0.90756700	1.79044100
C	-1.08131200	3.41618400	-0.11895100
C	-1.81425400	4.59067100	0.10797000
C	-1.21155400	5.72014800	0.64920600
H	-1.80710000	6.62330600	0.80151900
C	0.90219000	4.57829200	0.79816900
H	1.95825800	4.54146600	1.07276800
C	0.14558200	5.72063400	0.99855400
H	-2.87276900	4.59341700	-0.16158400
C	0.29446200	3.43463500	0.24277300
C	1.03617100	2.24595500	0.09477700
N	1.63292100	1.25804300	0.01154300
C	-0.63361000	2.69521900	-2.75967200
H	-0.99723900	3.73342600	-2.78457600
H	0.41808300	2.74375100	-2.44070600
H	-0.63701800	2.30196300	-3.78218700
H	0.60518700	6.61158500	1.42830700
B	2.36264000	-0.12499400	-0.11834600
C	-1.57236400	1.24235400	3.73205900
H	-2.23416900	1.69942600	4.48197400
H	-1.81661400	0.17267800	3.68200400
C	-1.63652800	1.91697900	2.38852000
H	-1.31961300	2.96760600	2.43182800
H	-0.95963800	1.38544000	1.68846200
C	-4.16249500	0.98445100	2.10791700
H	-3.98445200	0.25303400	2.90602700
H	-5.12938000	0.85989800	1.61790800
C	-3.60836700	2.30406300	2.25526500
H	-3.99597100	3.08328800	1.57832700
H	-3.42276100	2.74500800	3.23998800
C	2.30763100	-0.88685800	1.31792700
C	1.82902200	-0.38143100	2.52429900
C	2.85683000	-2.16869600	1.38816900
C	1.83159500	-1.11291100	3.71303900
C	2.87853200	-2.93712300	2.54739500
C	2.35725100	-2.40076300	3.72478500
C	3.92121900	0.20464000	-0.46396500
C	4.60708600	1.16189800	0.28518800
C	4.67969100	-0.45791800	-1.42963800
C	5.95073000	1.47337700	0.09322700
C	6.02935200	-0.18218300	-1.65185000
C	6.66744600	0.79154200	-0.88771000
C	1.51809700	-0.81688400	-1.33265800
C	1.49785900	-0.16761700	-2.57004500
C	0.73184100	-1.96542100	-1.26056500
C	0.77410400	-0.61151900	-3.66899800
C	-0.00042500	-2.45681200	-2.34394400
C	0.01085100	-1.76960900	-3.55133100
F	4.13578300	-1.40362200	-2.19696500
F	6.70919100	-0.83779000	-2.58449600
F	7.94770300	1.06749400	-1.09034900
F	6.55054800	2.40148000	0.83117200
F	3.96406100	1.83225800	1.25669500
F	1.34578600	-0.58246000	4.83256500

F	1.33523000	0.86495000	2.61034600
F	2.36877100	-3.10913600	4.84472400
F	3.39138700	-4.16080900	2.54786200
F	3.36160200	-2.71694500	0.27875800
F	0.63424300	-2.67454200	-0.13201600
F	-0.73431400	-3.55917700	-2.21661000
F	-0.72584700	-2.18798900	-4.57214700
F	0.74577000	0.08759600	-4.80038000
F	2.20685700	0.96040900	-2.73236700
H	-0.54854000	1.30787400	4.12534100

c1b*-P

Ni	2.99634000	1.28771900	-0.74392500
N	3.38078100	0.05743100	0.61702700
N	1.80235600	2.41455400	0.28419900
C	3.34763000	-0.87934400	2.88322800
H	3.13408600	-0.53044400	3.89997900
H	4.41846800	-1.11044600	2.80686900
H	2.82237100	-1.83823400	2.75127200
C	2.91663000	0.13726700	1.86134600
C	2.03241400	1.14581100	2.30607300
H	1.76430000	1.10965800	3.36256200
C	1.48352000	2.19669500	1.57268600
C	4.29050600	-0.98850600	0.27615700
C	5.66564600	-0.67552500	0.18061000
C	6.55020100	-1.69187600	-0.19186200
H	7.61813200	-1.47638400	-0.26956000
C	6.09207900	-2.97456800	-0.47324600
H	6.79714800	-3.75754600	-0.76132200
C	4.73300800	-3.25703500	-0.39472700
H	4.38767300	-4.26590300	-0.62752000
C	3.80245600	-2.27884200	-0.02295600
C	6.15995900	0.73398200	0.44792900
H	5.38196200	1.41604700	0.04877500
C	7.46153400	1.06160800	-0.26877900
H	7.69010000	2.13320300	-0.18067700
H	7.42036300	0.81514300	-1.33986500
H	8.31968100	0.52177700	0.15969300
C	6.28638500	1.03533400	1.93944300
H	6.67792200	2.05050000	2.10129200
H	6.97882000	0.33299900	2.42923500
H	5.32366900	0.97607500	2.46369100
C	2.31639900	-2.60179900	0.01277200
H	1.87916700	-2.07142300	0.87645900
C	2.03758200	-4.08496400	0.20867400
H	0.96824200	-4.25698600	0.37814200
H	2.58153800	-4.49366900	1.07277700
H	2.32082600	-4.67630500	-0.67487300
C	1.58327800	-2.07338800	-1.22033100
H	0.52997100	-2.38764100	-1.20380600
H	2.03008000	-2.45628800	-2.15241400
H	1.60089900	-0.97167000	-1.26327600
C	1.14635500	3.38841500	-0.46516200
C	1.82128200	4.52674100	-0.93734300
C	1.18411700	5.45619800	-1.74952900

H	1.73575800	6.33623500	-2.08824300
C	-0.84985500	4.17303900	-1.70020200
H	-1.88604500	4.00111600	-1.99826500
C	-0.15313600	5.28766600	-2.13408400
H	2.86422800	4.66137900	-0.64103000
C	-0.20721400	3.22777800	-0.87391900
C	-0.90566100	2.06254200	-0.50071700
N	-1.50738300	1.10895600	-0.23976600
C	0.56494400	3.15437100	2.27434100
H	0.92416600	4.18926400	2.16811200
H	-0.45640300	3.13930200	1.86805100
H	0.48344900	2.92338800	3.34173400
H	-0.64204600	6.02280400	-2.77447100
B	-2.34151000	-0.15405500	0.18368000
C	1.85053600	0.35135400	-4.68583200
H	2.42954700	0.81608200	-5.49772300
H	2.33389300	-0.60739400	-4.44751700
C	1.76246200	1.24546000	-3.46820900
H	1.23673300	2.18302100	-3.71776100
H	1.13802800	0.75642300	-2.70366600
C	3.87529200	0.47330800	-2.22235600
H	3.55063700	-0.55256100	-2.43488900
H	4.96961500	0.56574200	-2.21351800
C	3.11005300	1.57628900	-2.83942500
H	2.90005900	2.37953300	-2.00460600
H	3.72401400	2.24549200	-3.47077600
C	-2.32604600	-1.24223100	-1.02368100
C	-1.74679400	-1.10276500	-2.28219900
C	-3.01063400	-2.44077600	-0.81355900
C	-1.79184100	-2.10015200	-3.25713700
C	-3.08202700	-3.46359400	-1.75323300
C	-2.46512600	-3.28797900	-2.99206000
C	-3.87062000	0.38233900	0.36702900
C	-4.45390300	1.14043300	-0.64935000
C	-4.69973200	0.09132200	1.45020900
C	-5.76515900	1.60699900	-0.60836100
C	-6.02080500	0.53309100	1.53076300
C	-6.55585200	1.29640800	0.49590000
C	-1.57595000	-0.59434600	1.55697000
C	-1.52538700	0.31894300	2.61359300
C	-0.83869100	-1.75962700	1.75539600
C	-0.79835100	0.11677500	3.77975100
C	-0.08700400	-2.00286900	2.90734500
C	-0.05403100	-1.05174100	3.91902800
F	-4.25444100	-0.63560400	2.47566400
F	-6.77133500	0.23301000	2.58346200
F	-7.80805900	1.72546300	0.56105200
F	-6.26510700	2.33374800	-1.60224700
F	-3.73440300	1.45190200	-1.74190100
F	-1.19488700	-1.92117700	-4.43269900
F	-1.08432600	0.01271700	-2.62435600
F	-2.51864500	-4.24599900	-3.90629600
F	-3.72864500	-4.59246100	-1.49044200
F	-3.59861100	-2.64960300	0.36908700
F	-0.80606800	-2.72601000	0.83352100

F	0.62740700	-3.11964200	3.02216800
F	0.70101100	-1.23571600	4.99386600
F	-0.74215400	1.05019600	4.72641300
F	-2.19746700	1.47556800	2.51409500
H	0.85060200	0.12066000	-5.07611100

c1b*-TSβH

Ni	3.12087400	1.42674500	-0.80486200
N	3.38956700	0.06514400	0.56872000
N	1.84341300	2.44705900	0.22710500
C	3.34702000	-0.86288400	2.84726500
H	3.13630600	-0.49876000	3.85933700
H	4.41645600	-1.10087200	2.77329200
H	2.81747500	-1.82121700	2.73074400
C	2.92250700	0.14191100	1.81034300
C	2.03846700	1.15532700	2.24586100
H	1.76106300	1.12386400	3.29996300
C	1.50327500	2.20801400	1.50796400
C	4.29804700	-0.98858600	0.25302700
C	5.67502100	-0.67945700	0.16357800
C	6.56171500	-1.70147200	-0.18757400
H	7.63049600	-1.48765600	-0.25807000
C	6.10538500	-2.98732800	-0.45675300
H	6.81196900	-3.77401800	-0.73044900
C	4.74585400	-3.26799600	-0.38286400
H	4.40183800	-4.27980000	-0.60397600
C	3.81340900	-2.28462100	-0.02907100
C	6.17367400	0.73032200	0.42437200
H	5.40163600	1.41592500	0.01907000
C	7.47861800	1.05059300	-0.28926600
H	7.70855700	2.12229700	-0.20748500
H	7.44203900	0.79735700	-1.35891400
H	8.33392900	0.51192500	0.14623300
C	6.29517600	1.03748100	1.91496400
H	6.69069800	2.05138100	2.07455200
H	6.98175200	0.33356800	2.41072600
H	5.32984200	0.98451300	2.43524800
C	2.32723900	-2.60814900	0.00757600
H	1.89455300	-2.09251900	0.88234300
C	2.04658200	-4.09369000	0.17864500
H	0.97730000	-4.26702100	0.34651100
H	2.59022300	-4.51746100	1.03550100
H	2.32893800	-4.67011400	-0.71500800
C	1.58887200	-2.05596500	-1.21092200
H	0.53148700	-2.35587300	-1.18924600
H	2.02124300	-2.43174300	-2.15256700
H	1.61816200	-0.95495000	-1.23728000
C	1.15447000	3.40350800	-0.51970800
C	1.77690500	4.56695600	-1.00240300
C	1.08889400	5.47859800	-1.79003200
H	1.60236300	6.37954300	-2.13360500
C	-0.89975500	4.13112300	-1.69859100
H	-1.93704200	3.92299700	-1.96907300
C	-0.25168100	5.26741400	-2.14619800
H	2.82038000	4.73879600	-0.73044800

C	-0.20476000	3.20474800	-0.89025800
C	-0.87171400	2.02763500	-0.50349500
N	-1.46834600	1.07271600	-0.23358100
C	0.57000400	3.15485000	2.20734700
H	0.89952900	4.19658100	2.07791800
H	-0.45804800	3.10604900	1.82260300
H	0.51312400	2.93633200	3.27916100
H	-0.77893500	5.98806300	-2.77247300
B	-2.31808700	-0.17556600	0.19564200
C	1.61262700	0.43741500	-4.54561700
H	2.13893200	0.91537900	-5.38454600
H	2.04070200	-0.56788300	-4.41984100
C	1.73332400	1.24871200	-3.26520100
H	1.24199000	2.22841700	-3.38699600
H	1.17745100	0.73403500	-2.46538800
C	3.96501800	0.43378900	-2.29008800
H	3.59491900	-0.59527700	-2.25292000
H	5.05580500	0.52657000	-2.31910100
C	3.16388400	1.45871800	-2.84122000
H	3.38817200	2.68040000	-1.48274500
H	3.67788600	2.27878700	-3.36000200
C	-2.32956800	-1.26642300	-1.00871700
C	-1.76206500	-1.13541500	-2.27324700
C	-3.03060900	-2.45379300	-0.79043200
C	-1.83504700	-2.13116700	-3.24824600
C	-3.12998800	-3.47456900	-1.72967200
C	-2.52529600	-3.30766400	-2.97574600
C	-3.83796000	0.38522900	0.38467600
C	-4.41031600	1.16620500	-0.62051900
C	-4.67027300	0.09278900	1.46496500
C	-5.71390200	1.65298000	-0.57102700
C	-5.98422500	0.55377000	1.55334900
C	-6.50825500	1.33970500	0.52981700
C	-1.55404800	-0.62569700	1.56613200
C	-1.48927900	0.28705300	2.62213700
C	-0.82264900	-1.79552500	1.75774300
C	-0.75057300	0.08190300	3.78044500
C	-0.06079500	-2.04271100	2.90211500
C	-0.01193800	-1.09112400	3.91308700
F	-4.23406100	-0.65393500	2.48001300
F	-6.73818400	0.25104900	2.60284300
F	-7.75343900	1.78758900	0.60245200
F	-6.20307700	2.40151500	-1.55401900
F	-3.68837900	1.48126100	-1.71099600
F	-1.25026400	-1.96123600	-4.43117500
F	-1.08436400	-0.03036300	-2.62023600
F	-2.60551300	-4.26390300	-3.88986700
F	-3.79132300	-4.59319100	-1.45994100
F	-3.60796300	-2.65241700	0.39911400
F	-0.80402000	-2.76111600	0.83422500
F	0.65041900	-3.16240800	3.00946500
F	0.75033700	-1.28069800	4.98184400
F	-0.67760600	1.01698300	4.72426800
F	-2.15569700	1.44726100	2.52911700
H	0.56061400	0.31236300	-4.83226500

c1b*-PβH

Ni	3.01352800	1.26850800	-0.86812200
N	3.45912900	0.03478400	0.61604100
N	1.69005600	2.26886300	0.14937600
C	3.38953600	-0.84914800	2.92014800
H	3.68960800	-0.30599800	3.82733200
H	4.21297300	-1.50397700	2.61470400
H	2.54753700	-1.49112100	3.21909300
C	2.97346200	0.11518000	1.84311000
C	2.04190400	1.11349000	2.23433200
H	1.78237500	1.11800900	3.29508500
C	1.45049700	2.11658700	1.46750300
C	4.35256500	-1.00396200	0.23754100
C	5.72922400	-0.72197500	0.08416900
C	6.56133400	-1.73590200	-0.40096800
H	7.62819300	-1.53911400	-0.52864900
C	6.05745200	-2.99089800	-0.72509000
H	6.72441400	-3.76915700	-1.10239600
C	4.70098700	-3.25347100	-0.56252800
H	4.31563900	-4.24386100	-0.81301900
C	3.82478300	-2.27575400	-0.08101600
C	6.28581700	0.63848600	0.45031300
H	5.51252500	1.37828400	0.17285500
C	7.55697100	1.00284600	-0.30101900
H	7.82747400	2.05211200	-0.11590600
H	7.45109400	0.87162600	-1.38784500
H	8.41741900	0.39647500	0.02022200
C	6.49942000	0.76885400	1.95624500
H	6.84108800	1.78001500	2.22234100
H	7.26107000	0.05652800	2.30963300
H	5.57975100	0.57522200	2.52381900
C	2.33951100	-2.55535900	0.05758000
H	1.98993800	-2.07481700	0.98761800
C	2.01157000	-4.03594300	0.17843900
H	0.95748800	-4.17506900	0.44672600
H	2.61841900	-4.52448400	0.95422800
H	2.17935700	-4.57452700	-0.76635000
C	1.54742500	-1.91807300	-1.08130700
H	0.48147800	-2.16974700	-1.00000100
H	1.90434300	-2.26946000	-2.06275600
H	1.61838500	-0.81352400	-1.07181400
C	1.07138900	3.26964200	-0.59361600
C	1.79345900	4.35651600	-1.11669600
C	1.18047000	5.30722800	-1.91969800
H	1.77200900	6.14235000	-2.30194900
C	-0.92749900	4.16240700	-1.75503300
H	-1.98470800	4.04697700	-2.00291200
C	-0.18168000	5.21771700	-2.24593000
H	2.85589200	4.42672200	-0.87368500
C	-0.30826500	3.19509500	-0.93402600
C	-1.04809600	2.07889900	-0.50885300
N	-1.65802300	1.14352800	-0.20559900
C	0.54350300	3.09242200	2.16128300
H	0.75681700	4.12468700	1.84781100

H	-0.51886000	2.91305400	1.93950700
H	0.65103700	3.03071100	3.24960400
H	-0.64813500	5.96790800	-2.88550000
B	-2.45033400	-0.14524300	0.20074900
C	1.59418100	0.25196600	-4.13293700
H	2.42406400	-0.18540600	-4.70673700
H	1.36756500	-0.43207800	-3.30450600
C	1.92459500	1.65487600	-3.66744200
H	2.10077800	2.29028200	-4.55421900
H	1.03907600	2.11450500	-3.18917600
C	4.02777300	0.73728700	-2.43862800
H	3.80072100	-0.29902800	-2.72327400
H	5.09287100	0.92774700	-2.26526400
C	3.15028800	1.79574600	-2.79433900
H	3.90654100	2.34313800	-0.67544900
H	3.58132100	2.80504500	-2.81502200
C	-2.34042800	-1.23114100	-1.00488900
C	-1.62878700	-1.10333400	-2.19593100
C	-3.03910500	-2.43025500	-0.85350600
C	-1.58017100	-2.10801800	-3.16347400
C	-3.02034600	-3.45848300	-1.78999800
C	-2.28226600	-3.29167500	-2.96148400
C	-4.00194400	0.32806700	0.35384800
C	-4.59037400	1.10052400	-0.64858100
C	-4.84164100	-0.02858700	1.40874400
C	-5.91857200	1.51827500	-0.61929500
C	-6.17873200	0.36356400	1.47690000
C	-6.71938000	1.14326800	0.45708900
C	-1.69500200	-0.55398300	1.59138600
C	-1.65486200	0.38830400	2.62250500
C	-0.94784900	-1.70671600	1.82234000
C	-0.90910000	0.23772500	3.78494700
C	-0.19327000	-1.90811100	2.98012300
C	-0.16089300	-0.92387300	3.96024700
F	-4.38899000	-0.77611700	2.41643700
F	-6.93981800	0.00135000	2.50227200
F	-7.98708200	1.52592600	0.50986900
F	-6.42429700	2.26015700	-1.59893500
F	-3.86302300	1.47688100	-1.71510600
F	-0.85276000	-1.94943000	-4.26572200
F	-0.90537400	-0.00389500	-2.46341600
F	-2.24508100	-4.25494400	-3.87086600
F	-3.68778600	-4.58659900	-1.58261700
F	-3.72463000	-2.64099600	0.27490900
F	-0.90517900	-2.70036300	0.92938400
F	0.53242900	-3.01479700	3.12666600
F	0.60688400	-1.06613100	5.03268900
F	-0.85461000	1.20278100	4.69798400
F	-2.34719500	1.53056700	2.49391300
H	0.70915200	0.25062400	-4.78093000

c1b*-cw

Ni	-2.89552200	1.06524100	-0.13043000
N	-3.34507000	-0.69849900	-0.63834000
N	-1.88027200	1.47161800	-1.64140500

C	-3.38749100	-2.77108700	-1.94482800
H	-3.33168100	-3.04766000	-3.00439600
H	-4.40898900	-2.95159100	-1.58226700
H	-2.73818900	-3.47102100	-1.39449600
C	-2.96073600	-1.35228100	-1.71730100
C	-2.13395900	-0.72011600	-2.67460200
H	-1.85880100	-1.31078600	-3.54939200
C	-1.64499700	0.58633700	-2.63787200
C	-4.26670100	-1.19388600	0.31568000
C	-5.60615800	-0.73111100	0.25785100
C	-6.49616800	-1.16410600	1.24515600
H	-7.53456300	-0.82660500	1.22023900
C	-6.08001800	-2.01376000	2.26537800
H	-6.79163900	-2.34261700	3.02606100
C	-4.75372800	-2.43137400	2.32781600
H	-4.43507600	-3.07978800	3.14670400
C	-3.82127800	-2.02597200	1.36935000
C	-6.05770500	0.20378600	-0.84965600
H	-5.20392400	0.87851100	-1.06584800
C	-7.23888000	1.07691400	-0.45361000
H	-7.41094400	1.85773300	-1.20790800
H	-7.08192900	1.57527900	0.51432000
H	-8.17322200	0.50014200	-0.37810700
C	-6.35909400	-0.55289700	-2.14068400
H	-6.68970400	0.13552600	-2.93208500
H	-7.16174800	-1.29064800	-1.98612000
H	-5.48187100	-1.09059700	-2.52359700
C	-2.35353400	-2.37244800	1.51114000
H	-1.92817400	-2.47816400	0.49799400
C	-2.10673600	-3.67802500	2.25099600
H	-1.04534900	-3.95070200	2.20661500
H	-2.68218500	-4.50806500	1.81587000
H	-2.37533600	-3.60664700	3.31553400
C	-1.61867200	-1.20987900	2.17922100
H	-0.55799200	-1.44912400	2.33678900
H	-2.06035900	-0.96787400	3.15920900
H	-1.66222100	-0.29347000	1.55893600
C	-1.29609900	2.74524200	-1.68510000
C	-1.94257600	3.85363700	-2.24274100
C	-1.36003900	5.11697600	-2.19671200
H	-1.89151200	5.96621600	-2.63236200
C	0.58103600	4.23271700	-1.08183600
H	1.57074100	4.34784300	-0.63532700
C	-0.10810200	5.31644700	-1.60476300
H	-2.91639100	3.70296500	-2.71237200
C	-0.00632000	2.95531800	-1.13301500
C	0.71527900	1.83466600	-0.67526400
N	1.34966900	0.93257700	-0.32768100
C	-0.79982600	1.04717200	-3.79150100
H	-1.24642600	1.92000200	-4.29048200
H	0.20448100	1.35772300	-3.46769400
H	-0.67362400	0.25420000	-4.53524400
H	0.33191000	6.31370500	-1.56557500
B	2.21305200	-0.31575100	0.07134500
C	-2.17473200	2.18887900	3.26164700

H	-1.31367600	1.61597000	2.89795000
H	-2.47643400	1.75167700	4.22367000
C	-3.30940200	2.20121400	2.26421300
H	-3.70951200	1.15478300	2.15228800
C	-2.96984800	2.75198900	0.86644400
H	-2.04462600	3.35585200	0.88359500
C	2.16132600	-0.49405900	1.68515900
C	1.54168000	0.35612400	2.59835300
C	2.84324000	-1.57544000	2.24482000
C	1.53618300	0.12392800	3.97416400
C	2.86529000	-1.84870700	3.60867300
C	2.20099500	-0.98753500	4.48254700
C	3.74296500	0.04775200	-0.35989000
C	4.28590400	1.28104700	0.00392500
C	4.61144800	-0.81752700	-1.02531200
C	5.59505200	1.66084500	-0.28019400
C	5.93163200	-0.48041800	-1.32653700
C	6.42553400	0.76686800	-0.95250300
C	1.49791500	-1.48906200	-0.81414500
C	1.44953600	-1.33114000	-2.20245900
C	0.81231100	-2.60117000	-0.32963600
C	0.77860300	-2.19384600	-3.05969200
C	0.11400700	-3.48800000	-1.15260200
C	0.08420900	-3.27501900	-2.52463700
F	4.20695600	-2.02892800	-1.40998400
F	6.71934600	-1.33597600	-1.96663000
F	7.67650000	1.10207700	-1.23409600
F	6.05584900	2.85315300	0.08274600
F	3.52952400	2.17132500	0.66910300
F	0.89483400	0.95169200	4.79376600
F	0.88677300	1.45298700	2.19159000
F	2.20650900	-1.22622200	5.78636200
F	3.50820700	-2.90782900	4.08512300
F	3.47903200	-2.42789300	1.43458200
F	0.78109000	-2.88783600	0.97539000
F	-0.55715700	-4.50956900	-0.62419200
F	-0.62417900	-4.06957600	-3.31629000
F	0.72537900	-1.95995400	-4.36851400
F	2.06657800	-0.28200900	-2.76726800
C	-4.12689800	3.51783800	0.26873200
H	-5.05323600	2.91787000	0.26663200
H	-4.36424300	4.43438400	0.84243400
H	-3.94966400	3.83969800	-0.76683400
H	-4.18827100	2.73862500	2.66701900
H	-1.81681200	3.20957600	3.46075800

c1c-R

Ni	-2.91908500	1.39234100	-0.41457000
N	-3.47518800	-0.54406800	-0.30277900
N	-1.73750600	1.02985100	-1.98974500
C	-3.36130100	-2.96808300	-0.73207600
H	-3.01826900	-3.64649300	-1.52074400
H	-4.44673700	-3.08382600	-0.61552000
H	-2.92523100	-3.31668200	0.21748100
C	-2.96279000	-1.54464500	-1.01732700

C	-2.04159500	-1.35904300	-2.06748200
H	-1.75923100	-2.25914400	-2.61332000
C	-1.48243000	-0.17081400	-2.53594300
C	-4.48834900	-0.90086800	0.63463100
C	-5.84079100	-0.80415300	0.23787200
C	-6.83008500	-1.16424800	1.15862100
H	-7.88251200	-1.09623600	0.87180100
C	-6.49608400	-1.60553300	2.43471300
H	-7.28101300	-1.88733500	3.14006300
C	-5.15874400	-1.68397000	2.81236100
H	-4.90799800	-2.03141300	3.81696600
C	-4.13105600	-1.33676400	1.92914800
C	-6.20873900	-0.30624300	-1.15007700
H	-5.38676400	0.35742500	-1.47580900
C	-7.49387000	0.51128000	-1.16785300
H	-7.63630700	0.98622200	-2.14932900
H	-7.49141100	1.30731500	-0.40868900
H	-8.38410500	-0.11019000	-0.98893600
C	-6.28562800	-1.43884800	-2.17153200
H	-6.60244100	-1.05952800	-3.15426200
H	-7.01480000	-2.20370800	-1.86188000
H	-5.31913500	-1.93907300	-2.31676200
C	-2.67467700	-1.39850300	2.35531700
H	-2.08548300	-1.72849800	1.48170500
C	-2.40656200	-2.38558600	3.47981900
H	-1.32685500	-2.49125800	3.64770800
H	-2.80518300	-3.38510700	3.25378300
H	-2.84948600	-2.05526000	4.43141000
C	-2.16669400	-0.00641100	2.71464600
H	-1.08937200	-0.01169000	2.94247000
H	-2.69850600	0.39791600	3.59044700
H	-2.33025500	0.69383200	1.88222800
C	-1.10393000	2.16280000	-2.50193000
C	-1.82128800	3.14385600	-3.20016100
C	-1.20844200	4.32044200	-3.61602500
H	-1.79473600	5.06361600	-4.16133000
C	0.88660300	3.62393700	-2.66055300
H	1.93937100	3.78899300	-2.42126400
C	0.14351200	4.56974900	-3.34650200
H	-2.87854900	2.96058600	-3.40079400
C	0.26840500	2.42807500	-2.24413700
C	1.01364400	1.49036600	-1.50380900
N	1.64042300	0.73904200	-0.88659100
C	-0.59993700	-0.26452300	-3.75018000
H	-0.97535400	0.38080700	-4.55858100
H	0.43325000	0.05383500	-3.55499700
H	-0.54666100	-1.29335600	-4.12337700
H	0.60933000	5.50137500	-3.67006300
B	2.42798200	-0.32008800	-0.04357900
H	0.40268900	4.56374400	0.45292100
C	0.04173400	5.03112200	1.38068600
H	-0.58223100	5.89166000	1.09224800
H	0.92676600	5.42193100	1.90154600
C	-0.71940300	4.05484100	2.25302100
H	-0.05011100	3.23715200	2.56167300

H	-1.02010200	4.55117200	3.19051700
C	-1.96917100	3.44522700	1.61414700
H	-2.70647800	4.24462000	1.41925200
H	-2.42921400	2.78340300	2.36302200
C	-1.66406900	2.70472200	0.33673200
H	-1.38557900	3.41469100	-0.45414200
H	-0.83796100	1.97670200	0.47453200
C	-4.49581300	2.19629600	0.50373400
H	-4.27145200	2.64093500	1.47460600
H	-5.31637300	1.47756600	0.52653500
C	-4.17377500	2.86909700	-0.68895000
H	-4.71129400	2.62473600	-1.61552700
H	-3.71031600	3.86229000	-0.68725800
C	2.56989000	0.21403500	1.48611400
C	2.31170500	1.50479100	1.94457600
C	3.12350900	-0.65294300	2.43038400
C	2.54759100	1.90665800	3.26055100
C	3.36410100	-0.30081300	3.75446300
C	3.06786800	0.99575400	4.17406500
C	3.93332800	-0.39774700	-0.67123500
C	4.62936100	0.77938200	-0.95224200
C	4.64758300	-1.57844600	-0.88021600
C	5.93908800	0.80820800	-1.42472100
C	5.96242300	-1.59614800	-1.34704500
C	6.61167000	-0.39538500	-1.62202100
C	1.51726800	-1.65314100	-0.27979000
C	1.43799100	-2.17899900	-1.57174100
C	0.72694000	-2.29979400	0.66895000
C	0.67888900	-3.29103000	-1.91198400
C	-0.03551600	-3.43295700	0.37547600
C	-0.06640500	-3.92636900	-0.92339100
F	4.09061100	-2.76719800	-0.64166400
F	6.59864700	-2.74592800	-1.53386800
F	7.85967100	-0.39711300	-2.06759100
F	6.54890600	1.96075500	-1.68012700
F	4.03394900	1.96853400	-0.75733300
F	2.28112700	3.15259900	3.64397000
F	1.82886100	2.45053400	1.12512500
F	3.29304700	1.36006300	5.42816100
F	3.87390500	-1.17441100	4.61366700
F	3.43664300	-1.89890700	2.06061600
F	0.65947800	-1.86406300	1.93061700
F	-0.76210500	-4.02382100	1.32057700
F	-0.82310000	-4.97244900	-1.22798500
F	0.59902600	-3.70785300	-3.17309100
F	2.12387500	-1.59399600	-2.56508800

c1c-TS

Ni	-2.99610300	1.32656800	-0.52863400
N	-3.45364800	-0.54422900	-0.33160100
N	-1.73879900	0.98760700	-2.05138500
C	-3.28191500	-2.97520400	-0.64801800
H	-2.97097400	-3.67601500	-1.43062300
H	-4.35477800	-3.10894900	-0.46288000
H	-2.78271700	-3.28109600	0.28501800

C	-2.92243800	-1.55856000	-1.00966300
C	-2.00800500	-1.40141700	-2.07163500
H	-1.71632200	-2.31598100	-2.58772100
C	-1.46231400	-0.22042900	-2.57005100
C	-4.44146700	-0.87071200	0.64649600
C	-5.80287300	-0.85910800	0.26865500
C	-6.76078300	-1.16431500	1.24105100
H	-7.82027100	-1.15828800	0.97324800
C	-6.38876100	-1.47697800	2.54423800
H	-7.15112600	-1.71329200	3.28999000
C	-5.04226400	-1.49641500	2.89388100
H	-4.76120600	-1.75757800	3.91637400
C	-4.04280700	-1.20320900	1.95954700
C	-6.22450400	-0.52349100	-1.15394500
H	-5.44509500	0.14021200	-1.57226100
C	-7.55196500	0.22313900	-1.21493500
H	-7.73701100	0.60124400	-2.23050000
H	-7.58273500	1.08106300	-0.52693700
H	-8.40353300	-0.42640400	-0.96268300
C	-6.27838100	-1.75400100	-2.05776000
H	-6.67079700	-1.48911000	-3.05062900
H	-6.93912300	-2.52859900	-1.63813500
H	-5.29073400	-2.20550200	-2.21534900
C	-2.57465000	-1.24186200	2.35144200
H	-2.00892000	-1.60832800	1.47650400
C	-2.28438900	-2.19124800	3.50403300
H	-1.20197200	-2.30452200	3.64533200
H	-2.70140300	-3.19296800	3.32581700
H	-2.69580600	-1.82195300	4.45542600
C	-2.03976400	0.15511700	2.65111900
H	-0.96111600	0.12962800	2.87105500
H	-2.55244900	0.60291300	3.51764600
H	-2.19250700	0.82723200	1.79299400
C	-1.10463000	2.12047900	-2.55037000
C	-1.79953300	3.07837400	-3.30469300
C	-1.18794000	4.25973400	-3.70682700
H	-1.75533700	4.98037800	-4.30042100
C	0.86593500	3.61754300	-2.63040300
H	1.90441500	3.80318300	-2.34765200
C	0.14236900	4.54023600	-3.36658200
H	-2.83775000	2.86633500	-3.56930400
C	0.24881000	2.41540300	-2.22771800
C	0.98719000	1.48328600	-1.47212800
N	1.61943100	0.73911300	-0.85124000
C	-0.56528500	-0.32407500	-3.77124700
H	-0.94888000	0.28837700	-4.60136000
H	0.45604100	0.03026400	-3.57211200
H	-0.47827900	-1.36054900	-4.11596100
H	0.60842900	5.47489700	-3.68099200
B	2.43953100	-0.31018600	-0.02337900
H	0.34376100	4.51091400	0.48315100
C	0.07106900	4.87640700	1.48470500
H	-0.41114300	5.85781600	1.35519600
H	1.01162000	5.03399000	2.02841300
C	-0.83322900	3.90562400	2.21604100

H	-0.30891200	2.95078900	2.37448300
H	-1.04537300	4.28694400	3.22830400
C	-2.16100300	3.63758000	1.51794100
H	-2.73066200	4.58149300	1.45360100
H	-2.76139200	2.97286900	2.15717100
C	-2.00384600	3.03226900	0.13847500
H	-1.63859200	3.75843100	-0.60055400
H	-1.26455900	2.20225700	0.18539500
C	-4.56011500	2.06805500	0.33535400
H	-4.56488900	2.17912400	1.42635600
H	-5.44803100	1.56562700	-0.04915400
C	-3.93216900	3.08277400	-0.46661900
H	-4.17170200	3.08666700	-1.54150300
H	-3.84012500	4.11430100	-0.11338600
C	2.57828100	0.20841700	1.51108500
C	2.23745600	1.46792100	1.99710300
C	3.17009500	-0.64826900	2.44088800
C	2.42202400	1.84788200	3.32741000
C	3.37058400	-0.31597400	3.77670000
C	2.98874300	0.94848400	4.22459500
C	3.93831500	-0.34887300	-0.67069800
C	4.60547400	0.84491400	-0.95155000
C	4.67513900	-1.51193100	-0.90062300
C	5.90695800	0.90610400	-1.44322300
C	5.98277700	-1.49734500	-1.38742400
C	6.60223700	-0.28071500	-1.66145100
C	1.55195800	-1.65953200	-0.25040700
C	1.47256500	-2.19940300	-1.53633500
C	0.77173300	-2.30401200	0.70780100
C	0.72163800	-3.32161800	-1.86102400
C	0.01356100	-3.44297900	0.42945800
C	-0.01856400	-3.95008400	-0.86397400
F	4.14846000	-2.71435600	-0.66344100
F	6.64035000	-2.63171400	-1.59369200
F	7.84307100	-0.25151000	-2.12575900
F	6.48725700	2.07424800	-1.69718100
F	3.98914500	2.02051500	-0.73901300
F	2.06533000	3.06216500	3.73961700
F	1.70660600	2.39964800	1.19109000
F	3.17068700	1.29159300	5.49166100
F	3.91860300	-1.17929000	4.62254300
F	3.54380400	-1.87032400	2.04900700
F	0.70939300	-1.85999400	1.96737700
F	-0.70960600	-4.02201200	1.38471200
F	-0.77125900	-5.00249900	-1.15594200
F	0.64275100	-3.75451300	-3.11665400
F	2.14860100	-1.61831400	-2.53828400

c1c-P

Ni	-3.47006200	0.58624700	-1.19598000
N	-3.62793000	-1.02476800	-0.24012600
N	-2.29566600	-0.08881400	-2.59630000
C	-3.21500600	-3.38424100	0.28850100
H	-2.81924300	-4.27882200	-0.20539100
H	-4.27621100	-3.54982900	0.51882000

H	-2.70910900	-3.29414900	1.26195300
C	-3.00743500	-2.15814700	-0.55875000
C	-2.16054200	-2.30249000	-1.67934300
H	-1.76038600	-3.30361200	-1.84319200
C	-1.82211200	-1.34828500	-2.63683400
C	-4.51736700	-1.02714000	0.87667000
C	-5.90633600	-1.11041100	0.63116800
C	-6.77258400	-1.08588300	1.72842400
H	-7.85088400	-1.14962500	1.56571100
C	-6.28506900	-0.97689100	3.02686600
H	-6.97686500	-0.96185100	3.87207700
C	-4.91530500	-0.88114400	3.24637800
H	-4.54475400	-0.78875700	4.26945200
C	-4.00357800	-0.90234600	2.18455400
C	-6.43895300	-1.20451200	-0.78723800
H	-5.76494800	-0.58871500	-1.41532000
C	-7.84488200	-0.64204900	-0.93880900
H	-8.12148900	-0.57629100	-2.00067900
H	-7.93981700	0.36427800	-0.50499100
H	-8.60176200	-1.27932000	-0.45672000
C	-6.37510700	-2.62659600	-1.33979500
H	-6.80432500	-2.67232900	-2.35164800
H	-6.94566900	-3.32495900	-0.70776300
H	-5.34647100	-3.00357200	-1.41127400
C	-2.51504700	-0.74626300	2.44311300
H	-1.97468700	-1.33985000	1.68601300
C	-2.08506000	-1.26330100	3.80824000
H	-0.99028800	-1.27477300	3.88532000
H	-2.44297600	-2.28696600	3.99243300
H	-2.45690800	-0.62812700	4.62611700
C	-2.06573600	0.69941300	2.24582600
H	-1.00218400	0.80354700	2.50245700
H	-2.63501700	1.39163900	2.88688200
H	-2.19168900	1.02341900	1.20030500
C	-1.89001000	0.84381300	-3.54968800
C	-2.80294800	1.39655500	-4.46307300
C	-2.40690300	2.36302500	-5.37949900
H	-3.13999600	2.76134100	-6.08480600
C	-0.16086500	2.32612500	-4.52025200
H	0.86722200	2.69413800	-4.49688000
C	-1.08552800	2.82820200	-5.41986000
H	-3.83349000	1.03414000	-4.43780100
C	-0.55963600	1.34594400	-3.58953800
C	0.33049500	0.94253300	-2.57745600
N	1.03139600	0.66510700	-1.70035400
C	-0.95243500	-1.78590500	-3.78150000
H	-1.35781300	-1.44657200	-4.74611700
H	0.07194200	-1.38966000	-3.71606900
H	-0.86141100	-2.87729000	-3.81071300
H	-0.78823500	3.58895300	-6.14277600
B	1.96153300	0.24839800	-0.50634900
H	0.66145100	4.48287200	-2.19265900
C	0.07095800	5.41233500	-2.13459700
H	-0.24463500	5.66258100	-3.15978100
H	0.75366800	6.20531200	-1.80072300

C	-1.11352500	5.24496500	-1.20557900
H	-0.75568900	4.96234300	-0.20286000
H	-1.63247900	6.20884600	-1.06645900
C	-2.10094000	4.19743700	-1.69234700
H	-1.53386300	3.31651900	-2.04357100
H	-2.63517900	4.56876800	-2.58756400
C	-3.09442700	3.72814300	-0.64605000
H	-2.54566600	3.34227100	0.22815600
H	-3.69658800	4.57233600	-0.26996000
C	-4.61597900	1.71050500	-0.16784600
H	-4.33146500	1.85241900	0.88308000
H	-5.67478300	1.44364500	-0.27768200
C	-4.04657700	2.65145000	-1.14770000
H	-3.40470100	2.05215100	-1.94023700
H	-4.78780800	3.05200900	-1.86327300
C	1.71753300	1.27201800	0.73194700
C	0.69165000	2.20421900	0.85453400
C	2.59158400	1.20320000	1.81822500
C	0.52622000	3.01360800	1.97784600
C	2.47239200	1.99725500	2.95470600
C	1.42847900	2.91892800	3.03175100
C	3.47561200	0.42873300	-1.08050400
C	3.82851400	1.60072100	-1.75110000
C	4.50157100	-0.50103900	-0.91534000
C	5.10546000	1.84712200	-2.25002600
C	5.79521100	-0.29419500	-1.39385300
C	6.09795400	0.88723700	-2.06698800
C	1.46958900	-1.28328900	-0.23152200
C	1.51914700	-2.19792700	-1.28659400
C	0.85834300	-1.75505600	0.92927600
C	0.98508300	-3.47878500	-1.22890700
C	0.31301700	-3.03713500	1.03412400
C	0.36288700	-3.89742500	-0.05566900
F	4.28093800	-1.64748100	-0.27098700
F	6.73965200	-1.20882600	-1.21166000
F	7.32185600	1.09735700	-2.52979800
F	5.38261100	2.97764400	-2.89124900
F	2.91064500	2.56547000	-1.94474900
F	-0.51303000	3.84237700	2.06501700
F	-0.24444600	2.33381800	-0.10025300
F	1.28342000	3.67720000	4.10870400
F	3.32659700	1.88072500	3.96347500
F	3.56536800	0.28742700	1.81335600
F	0.75369400	-0.99211300	2.02231900
F	-0.28343000	-3.42750300	2.15719800
F	-0.20572500	-5.09437000	0.00488500
F	0.99770100	-4.27812400	-2.29172500
F	2.08635400	-1.83100200	-2.44650900

c1c-TSβH

Ni	-3.31063100	0.91798900	-1.03330100
N	-3.46814300	-0.84553800	-0.20042000
N	-1.94147200	0.37642100	-2.28154700
C	-3.24804300	-3.29271800	-0.06604400
H	-3.01782400	-4.10859200	-0.76100700

H	-4.30478500	-3.36126400	0.22300100
H	-2.67135600	-3.48217600	0.85269700
C	-2.91373100	-1.95613200	-0.67186100
C	-2.01056000	-1.96961700	-1.76048800
H	-1.66713000	-2.95336800	-2.08169700
C	-1.52181900	-0.88698100	-2.48663700
C	-4.35663400	-0.94431800	0.90989200
C	-5.74645200	-0.86033700	0.66561100
C	-6.61413000	-0.90021900	1.76090300
H	-7.69237100	-0.84097500	1.59679000
C	-6.12697700	-1.00501100	3.05918600
H	-6.81890600	-1.03309400	3.90385800
C	-4.75576000	-1.06762600	3.28124700
H	-4.38976100	-1.14265300	4.30638000
C	-3.84045700	-1.03921600	2.22159300
C	-6.27768000	-0.70743300	-0.74821800
H	-5.55879600	-0.05389600	-1.28327500
C	-7.63825300	-0.02937200	-0.81097700
H	-7.90144900	0.20947100	-1.85102300
H	-7.66500900	0.90773000	-0.23582500
H	-8.44181300	-0.67424500	-0.42390300
C	-6.31242100	-2.03362300	-1.50393200
H	-6.73407300	-1.89914300	-2.51089000
H	-6.93826600	-2.77290800	-0.98010900
H	-5.31388700	-2.47169000	-1.63060300
C	-2.34231200	-1.08176300	2.48832500
H	-1.89966500	-1.79254900	1.76807700
C	-2.00141900	-1.59001000	3.88090200
H	-0.92127600	-1.74429700	3.98172600
H	-2.49344200	-2.54850000	4.09956400
H	-2.30083800	-0.87462500	4.66159500
C	-1.66027400	0.25939900	2.22060200
H	-0.58539400	0.19681400	2.44492500
H	-2.08203300	1.06483300	2.84487900
H	-1.75798700	0.56000000	1.16534800
C	-1.28013400	1.45268900	-2.87250200
C	-1.90572900	2.30195600	-3.80100700
C	-1.25164100	3.40955500	-4.32082400
H	-1.76765500	4.03809600	-5.05026100
C	0.71099900	2.92164400	-3.02254900
H	1.72578500	3.14443000	-2.68600300
C	0.05776800	3.73152600	-3.93277300
H	-2.92483400	2.06045200	-4.10974600
C	0.04995500	1.78997000	-2.49515500
C	0.73013100	1.02070500	-1.53318600
N	1.35533000	0.44432600	-0.74705100
C	-0.55117500	-1.16130800	-3.59968200
H	-0.91389900	-0.72866000	-4.54414800
H	0.44166200	-0.72636300	-3.42232800
H	-0.40247700	-2.23702400	-3.74213800
H	0.55764000	4.61021000	-4.34204200
B	2.28812500	-0.36324800	0.22361200
H	0.37771300	4.46642600	-0.12185500
C	0.13348300	5.29799400	0.55532700
H	-0.15634300	6.15693400	-0.07027500

H	1.06722700	5.56433600	1.07001200
C	-0.95353800	4.92875400	1.54460400
H	-0.60787600	4.08717300	2.16618400
H	-1.11334200	5.76301900	2.24676300
C	-2.28790000	4.55521600	0.91744600
H	-2.72064700	5.41957700	0.38224100
H	-3.00792400	4.31215600	1.71708000
C	-2.19562100	3.36426300	-0.03725900
H	-1.63135100	3.65089800	-0.94065000
H	-1.61025600	2.56444900	0.44825000
C	-4.28586900	1.93509100	0.35173500
H	-3.90024200	1.61896400	1.32688300
H	-5.37433700	1.87867900	0.24750800
C	-3.55141900	2.85270700	-0.43045700
H	-3.64569400	1.90881300	-2.03160000
H	-4.11722900	3.53503000	-1.07911400
C	2.37461400	0.39102700	1.66023000
C	1.80356700	1.61230600	2.00729300
C	3.18827600	-0.18718300	2.63604600
C	2.01463800	2.22554200	3.24311200
C	3.41545300	0.37867900	3.88605600
C	2.82274400	1.60413300	4.18969500
C	3.77058700	-0.28130000	-0.45562800
C	4.26966800	0.95705300	-0.86320100
C	4.64478000	-1.35791100	-0.60533300
C	5.53832400	1.13787900	-1.40771800
C	5.92627700	-1.22222700	-1.14046300
C	6.37510700	0.03260000	-1.54529700
C	1.57851600	-1.83002400	0.21622200
C	1.49562300	-2.53442900	-0.98687100
C	0.89409300	-2.40577400	1.28377000
C	0.78559500	-3.71840400	-1.14250500
C	0.15810200	-3.58715000	1.17168100
C	0.09281900	-4.24063900	-0.05324300
F	4.28341200	-2.58752400	-0.23774900
F	6.72157000	-2.27702100	-1.26777900
F	7.58884800	0.17352900	-2.05838300
F	5.95403100	2.34170200	-1.78708200
F	3.50790500	2.05903900	-0.73275000
F	1.44944000	3.39753800	3.52306400
F	1.00050300	2.26874100	1.15588600
F	3.02751000	2.17200600	5.36958000
F	4.18591300	-0.22479000	4.78243000
F	3.76841900	-1.36409200	2.37819800
F	0.89779800	-1.83679200	2.49295200
F	-0.51855900	-4.06247500	2.21432700
F	-0.64142700	-5.33636600	-0.19336600
F	0.69345900	-4.31340300	-2.32934100
F	2.10918400	-2.05105900	-2.07639800

c1c-PβH

Ni	-3.29574900	0.96545000	-1.24205900
N	-3.44900700	-0.75985400	-0.28159000
N	-1.87875200	0.35174600	-2.39494300
C	-3.24941300	-3.20114600	-0.02529600

H	-3.09123300	-4.04637000	-0.70551200
H	-4.28753600	-3.22026500	0.32979100
H	-2.62218200	-3.38552400	0.86101400
C	-2.90267100	-1.89770400	-0.69234600
C	-1.99111200	-1.96727400	-1.77355700
H	-1.65898900	-2.96868900	-2.04907500
C	-1.47885200	-0.92508800	-2.54361700
C	-4.34045200	-0.77846200	0.82885300
C	-5.72849700	-0.67344100	0.57891400
C	-6.59505900	-0.61986300	1.67437200
H	-7.67155300	-0.54319700	1.50614400
C	-6.11027600	-0.65484900	2.97746500
H	-6.80218900	-0.60895700	3.82133500
C	-4.74145800	-0.74364800	3.20402900
H	-4.37533700	-0.76594500	4.23172100
C	-3.82757500	-0.80769500	2.14499500
C	-6.26049400	-0.61490100	-0.84118800
H	-5.52754900	-0.02699500	-1.42853600
C	-7.60209500	0.09303000	-0.95636200
H	-7.86024400	0.25847700	-2.01184700
H	-7.60249300	1.07174200	-0.45479800
H	-8.42242500	-0.49805300	-0.52156300
C	-6.33331400	-1.99636600	-1.48694500
H	-6.74717300	-1.93212600	-2.50400300
H	-6.98220700	-2.67167200	-0.90770300
H	-5.34789100	-2.47294300	-1.57092600
C	-2.33137400	-0.86706200	2.41471600
H	-1.89865700	-1.61418900	1.72601600
C	-1.99867100	-1.32137600	3.82762100
H	-0.92217400	-1.49637300	3.93400600
H	-2.51164600	-2.25871100	4.08648900
H	-2.28027700	-0.56711200	4.57763500
C	-1.63780000	0.45389600	2.08595400
H	-0.56470000	0.40126900	2.32232600
H	-2.06430100	1.29469200	2.65774800
H	-1.72497700	0.69455800	1.01475800
C	-1.21422300	1.40866800	-3.01065000
C	-1.83408000	2.24431300	-3.95555700
C	-1.17439200	3.34020200	-4.49172200
H	-1.68657900	3.95764900	-5.23320600
C	0.78217700	2.87028700	-3.17847200
H	1.79694700	3.09481200	-2.84300000
C	0.13483400	3.66570100	-4.10500100
H	-2.85410200	2.00369900	-4.26077600
C	0.11644500	1.74987800	-2.63288900
C	0.79264800	0.99781300	-1.65577000
N	1.41574100	0.43402700	-0.85843500
C	-0.51409700	-1.26295900	-3.64365200
H	-0.30411500	-2.33714800	-3.67694100
H	-0.92634800	-0.95649600	-4.61691900
H	0.45234800	-0.75143200	-3.54436900
H	0.63845000	4.53576400	-4.52781500
B	2.34126700	-0.36401300	0.12625400
H	0.50680600	4.56176100	-0.25730500
C	0.23575900	5.33979200	0.47148000

H	-0.06591600	6.23278600	-0.09806800
H	1.15666800	5.59022100	1.01601500
C	-0.85502100	4.88079800	1.41783700
H	-0.49726300	4.01023800	1.99021500
H	-1.04570200	5.66438600	2.16918600
C	-2.17136800	4.51756600	0.74928600
H	-2.61455500	5.40255300	0.25838800
H	-2.89830000	4.21383000	1.52125900
C	-2.04839000	3.38564500	-0.27423100
H	-1.44538500	3.72223700	-1.13371600
H	-1.48250100	2.55737000	0.18786600
C	-4.26698200	2.13154300	0.01822600
H	-3.99437900	1.84089200	1.04039000
H	-5.34304000	2.14346400	-0.18361700
C	-3.39071500	2.91843900	-0.75675900
H	-3.89075300	1.60372600	-2.39079600
H	-3.82500200	3.52727400	-1.55868500
C	2.46985000	0.43425000	1.53559000
C	1.94138400	1.68404700	1.84591400
C	3.27273500	-0.13797400	2.52363400
C	2.18322400	2.33084200	3.05891400
C	3.52951500	0.46129000	3.75214100
C	2.97957700	1.71487100	4.01906300
C	3.81749700	-0.34770700	-0.57209500
C	4.34467700	0.86127100	-1.02984700
C	4.66334600	-1.45119500	-0.68705100
C	5.61276300	0.98883100	-1.59050200
C	5.94339200	-1.36849900	-1.23619200
C	6.42018500	-0.14176200	-1.69186000
C	1.59338600	-1.81045700	0.18280200
C	1.49297300	-2.56919400	-0.98532400
C	0.89398100	-2.31592100	1.27608800
C	0.76246500	-3.74722100	-1.08086400
C	0.13650800	-3.48751300	1.22286700
C	0.05981900	-4.20083600	0.03245700
F	4.27475500	-2.65656800	-0.26939500
F	6.71139700	-2.44684700	-1.32885300
F	7.63312500	-0.05109300	-2.21789300
F	6.05598500	2.16629900	-2.01829600
F	3.61402100	1.98730900	-0.93352000
F	1.65933100	3.52901500	3.30556100
F	1.15283200	2.33559800	0.97759000
F	3.21331500	2.31514700	5.17732200
F	4.28752500	-0.13734600	4.66232900
F	3.81045400	-1.34212500	2.30158400
F	0.90226000	-1.68275100	2.45297300
F	-0.55365800	-3.89463200	2.28570900
F	-0.69633500	-5.28702000	-0.05382100
F	0.65667100	-4.39848300	-2.23695900
F	2.10704300	-2.14804800	-2.09958300
c1c*-R			
Ni	-2.71081700	1.42156400	0.16758900
N	-3.40560600	-0.42262800	-0.46604100
N	-1.56686700	1.58861000	-1.48712100

C	-3.41841400	-2.50817700	-1.77207500
H	-3.06766900	-2.88138500	-2.74014700
H	-4.51105800	-2.60145200	-1.73366300
H	-3.03898100	-3.18873200	-0.99450000
C	-2.96429800	-1.09501700	-1.52376000
C	-2.07258700	-0.55977000	-2.47501200
H	-1.85095400	-1.19870500	-3.33024400
C	-1.46603400	0.69325100	-2.48622100
C	-4.35273100	-1.09874500	0.36104500
C	-5.73982700	-0.95759700	0.12782700
C	-6.63271500	-1.57499700	1.01208000
H	-7.70825900	-1.46531500	0.84447600
C	-6.18101400	-2.32650200	2.08860500
H	-6.89306500	-2.79434900	2.77199500
C	-4.81284600	-2.50339500	2.27480600
H	-4.46497000	-3.12762000	3.10015600
C	-3.87944400	-1.91316900	1.41786800
C	-6.30398100	-0.19301800	-1.05722500
H	-5.46096300	0.29963600	-1.56987400
C	-7.30484700	0.87881800	-0.63160300
H	-7.60151100	1.50167400	-1.48857000
H	-6.90605600	1.54473200	0.14552300
H	-8.22669800	0.42988600	-0.23176300
C	-6.96318400	-1.13123200	-2.06695200
H	-7.35921000	-0.56891700	-2.92525300
H	-7.80748500	-1.67255500	-1.61318700
H	-6.26846100	-1.88401000	-2.46249200
C	-2.39226500	-2.15739400	1.60469600
H	-1.95096800	-2.28340800	0.60077500
C	-2.07851400	-3.42192800	2.38911700
H	-1.00363000	-3.63774200	2.35001800
H	-2.60659300	-4.29676900	1.98279500
H	-2.35261200	-3.32939500	3.45085200
C	-1.70673300	-0.94698700	2.21905700
H	-0.64494200	-1.14191500	2.43018800
H	-2.19166200	-0.63202000	3.15531800
H	-1.74279800	-0.08632900	1.52711400
C	-0.99730100	2.84593900	-1.70325400
C	-1.71902700	3.89799800	-2.28322000
C	-1.13997700	5.14990600	-2.46087300
H	-1.72451500	5.95038900	-2.92023800
C	0.92525200	4.38313300	-1.48639200
H	1.95737700	4.54579200	-1.17048000
C	0.17479400	5.40266600	-2.05010000
H	-2.75077400	3.70634400	-2.58815200
C	0.34749600	3.10868300	-1.33100000
C	1.10114200	2.01900900	-0.84604300
N	1.69777400	1.09845800	-0.47816500
C	-0.65811900	1.04617600	-3.70432900
H	-1.08149000	1.92111300	-4.21997800
H	0.37907000	1.31198900	-3.45428700
H	-0.62353200	0.21671200	-4.41799300
H	0.61221600	6.39349000	-2.17957400
B	2.45381700	-0.21741500	-0.07139000
C	-0.89883300	3.29774700	3.67424200

H	0.08602200	3.62270200	3.30823900
H	-0.74213800	2.85881600	4.66849100
C	-1.54014500	2.27731500	2.74080000
H	-0.93405800	1.36409900	2.77893200
C	-1.66106900	2.74201400	1.28789900
H	-0.68816000	2.56867500	0.79918100
C	-4.34460000	1.91982000	1.23922300
H	-4.12955100	2.52085800	2.12504700
H	-4.95578900	1.03271600	1.42738900
C	-4.30695800	2.52676200	-0.02454000
H	-4.83807800	2.09190300	-0.87738400
H	-4.05347200	3.58445600	-0.13799300
C	2.45350400	-0.36039400	1.54666000
C	1.98310100	0.56858800	2.47140800
C	3.03116000	-1.50698400	2.09453100
C	2.02348800	0.35690000	3.85049800
C	3.09015300	-1.76362500	3.46007600
C	2.57665400	-0.81858700	4.34810200
C	3.99632100	-0.02973200	-0.56660300
C	4.67741700	1.14924200	-0.25870900
C	4.74912000	-1.00219600	-1.22563500
C	6.01074500	1.37903600	-0.58848100
C	6.08858600	-0.81682000	-1.56986600
C	6.72226500	0.38150400	-1.25105400
C	1.59594500	-1.34416500	-0.88864700
C	1.55327200	-1.26219600	-2.28355100
C	0.82260000	-2.36609500	-0.34053300
C	0.82528800	-2.12727000	-3.09046900
C	0.07400300	-3.25859100	-1.11186600
C	0.06744300	-3.13182600	-2.49471700
F	4.20980800	-2.17529800	-1.56157100
F	6.76430200	-1.77117600	-2.19792700
F	7.99314000	0.57138800	-1.57538600
F	6.60495800	2.52602800	-0.27674100
F	4.03953600	2.13345400	0.39604600
F	1.53969300	1.26955200	4.68823300
F	1.45379700	1.73499000	2.07444000
F	2.62220100	-1.03623500	5.65462600
F	3.62770000	-2.88479000	3.92404100
F	3.52153100	-2.43972000	1.27156200
F	0.75596000	-2.55855200	0.98043800
F	-0.65685600	-4.20441800	-0.52647700
F	-0.67970700	-3.93265900	-3.24319100
F	0.78956500	-1.97117800	-4.41132500
F	2.24954300	-0.29895300	-2.90616400
C	-2.04266800	4.19530400	1.16379600
H	-2.98299500	4.42747100	1.69058100
H	-1.27371000	4.84631800	1.61348300
H	-2.15183600	4.53103900	0.12525900
H	-2.51788900	1.99049400	3.16121500
H	-1.52014300	4.19443600	3.80855800

c1c*-TS

Ni	-2.96676000	1.37189800	-0.66811800
N	-3.46163800	-0.49885200	-0.39784800

N	-1.68326600	0.92913100	-2.14654700
C	-3.35638900	-2.95219600	-0.65958300
H	-3.36101200	-3.61561600	-1.53352300
H	-4.32859700	-3.01689600	-0.15902400
H	-2.61988500	-3.37307100	0.04205100
C	-2.97512700	-1.54882500	-1.05358800
C	-2.07438500	-1.44695500	-2.13386700
H	-1.82054900	-2.38323700	-2.63250400
C	-1.48964800	-0.29755000	-2.66038600
C	-4.41216000	-0.73546000	0.64215600
C	-5.79398900	-0.66808000	0.34816500
C	-6.70251600	-0.79207900	1.40428400
H	-7.77446400	-0.73277400	1.19903000
C	-6.26845900	-1.00096500	2.70860400
H	-6.99250600	-1.08546100	3.52207800
C	-4.90883500	-1.14091700	2.96691200
H	-4.58083600	-1.35730400	3.98590200
C	-3.95624600	-1.03493600	1.94717300
C	-6.30449000	-0.52641100	-1.07742300
H	-5.50853600	-0.03798500	-1.66655400
C	-7.56571800	0.32501000	-1.18127700
H	-7.79473300	0.55169600	-2.23245700
H	-7.47868500	1.27980900	-0.64262200
H	-8.44609300	-0.19583500	-0.77598900
C	-6.55525200	-1.88760100	-1.72547000
H	-6.97372100	-1.76656800	-2.73559800
H	-7.27503800	-2.47907000	-1.13851900
H	-5.63949700	-2.48315400	-1.82418500
C	-2.48382100	-1.28235300	2.24562300
H	-2.04143800	-1.75140900	1.35056800
C	-2.26647100	-2.24737100	3.40268500
H	-1.20648600	-2.52276100	3.47295200
H	-2.84465300	-3.17472400	3.27893200
H	-2.54763500	-1.80468900	4.36995500
C	-1.70867900	0.00948700	2.46933500
H	-0.66509500	-0.19610300	2.74861500
H	-2.15697600	0.61397000	3.27347700
H	-1.69505700	0.61788000	1.55208100
C	-1.04488900	2.01398800	-2.73552800
C	-1.70865400	2.86909600	-3.62945900
C	-1.07012000	3.98118600	-4.16650900
H	-1.61152200	4.62365800	-4.86495400
C	0.94688700	3.46680500	-2.95696600
H	1.98139400	3.67572400	-2.67603300
C	0.25431300	4.29130500	-3.82798600
H	-2.74068400	2.63008700	-3.89670100
C	0.30472800	2.33254800	-2.42171800
C	1.01211400	1.46913500	-1.56375600
N	1.61341200	0.76511600	-0.86991300
C	-0.62522400	-0.45274000	-3.87972300
H	-1.00682800	0.15861300	-4.71156800
H	0.40935900	-0.12307400	-3.70668000
H	-0.58089100	-1.49515100	-4.21222400
H	0.74033400	5.17214000	-4.24945800
B	2.41811900	-0.25594100	0.00602600

C	-1.20059200	3.37916600	2.61773300
H	-0.57552300	2.47857100	2.65673000
H	-1.55928000	3.56981400	3.63861200
C	-2.36444000	3.20749000	1.65985200
H	-2.97480300	2.35414500	1.98948000
C	-1.93652700	3.02052600	0.21371200
C	-4.62813100	2.18116200	-0.09352800
H	-4.87333500	2.24227800	0.97312700
H	-5.40748600	1.71825000	-0.69826500
C	-3.81255000	3.19624500	-0.68616200
H	-3.84315100	3.32195900	-1.77898600
H	-3.71834900	4.17243400	-0.20196100
C	2.46824600	0.27669600	1.54008500
C	2.03003700	1.51083900	2.01688100
C	3.09622000	-0.53920500	2.48285500
C	2.17137000	1.90334300	3.34944100
C	3.24365200	-0.19763200	3.82293500
C	2.77316900	1.04010900	4.25959900
C	3.94181400	-0.24862700	-0.58071400
C	4.58602900	0.96608400	-0.82133800
C	4.71219900	-1.38966100	-0.80852200
C	5.89966700	1.06753100	-1.27194200
C	6.03285400	-1.33476600	-1.25577700
C	6.62993700	-0.09848200	-1.48936900
C	1.58232600	-1.63190100	-0.26399100
C	1.51116500	-2.11172700	-1.57491700
C	0.82891600	-2.34766700	0.66423000
C	0.76591400	-3.21931500	-1.95763900
C	0.07100400	-3.47069500	0.32536300
C	0.02469400	-3.89867600	-0.99519500
F	4.20683600	-2.60757500	-0.60791400
F	6.72354600	-2.44913100	-1.46319300
F	7.88280300	-0.03108700	-1.91601500
F	6.45780700	2.25363500	-1.49003800
F	3.93122600	2.12161900	-0.61259800
F	1.74119600	3.09457100	3.75598900
F	1.44323700	2.40348200	1.20256000
F	2.90921300	1.39583800	5.52890000
F	3.82952700	-1.02301700	4.68084400
F	3.56648000	-1.72950500	2.09681100
F	0.78982300	-1.99503400	1.95254000
F	-0.64794700	-4.10237500	1.25091700
F	-0.74532100	-4.91998600	-1.34582000
F	0.69345700	-3.59432300	-3.23201600
F	2.18692500	-1.47650100	-2.54451500
H	-0.54136800	4.21357500	2.34049200
C	-1.31218500	4.26698800	-0.37052800
H	-0.25933400	4.35877900	-0.06097000
H	-1.32873700	4.30268800	-1.46614000
H	-1.83156600	5.17011300	-0.01320400
H	-1.22505600	2.17018400	0.13963500
H	-3.02653400	4.08920900	1.72539600

c1c*-P

Ni	-2.78440400	0.93174000	-0.82336800
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N	-3.25625600	-0.76928200	-0.18219700
N	-1.66719900	0.32813500	-2.29828100
C	-3.25106500	-3.21907400	-0.07359300
H	-3.02802000	-4.06381400	-0.73498900
H	-4.32406000	-3.22809400	0.15969100
H	-2.73523300	-3.40528200	0.88143500
C	-2.81616400	-1.91722800	-0.68979100
C	-1.95902800	-2.00317100	-1.80910200
H	-1.72856100	-3.01286500	-2.15044700
C	-1.42037000	-0.96724300	-2.56993700
C	-4.17813300	-0.80995800	0.90701200
C	-5.55216200	-0.62939700	0.63275900
C	-6.44569700	-0.63598600	1.70817500
H	-7.51358600	-0.49948500	1.52294600
C	-5.99736400	-0.80798900	3.01372100
H	-6.71017100	-0.81291400	3.84141600
C	-4.63878500	-0.96791000	3.26402600
H	-4.29873800	-1.09533800	4.29372800
C	-3.70086900	-0.97099000	2.22488900
C	-6.03678200	-0.41120400	-0.78911100
H	-5.24608400	0.17085400	-1.30205900
C	-7.32293100	0.39894700	-0.86582700
H	-7.54265900	0.67598700	-1.90667600
H	-7.26669300	1.32646400	-0.27719100
H	-8.19352000	-0.16762600	-0.50192600
C	-6.18910300	-1.72002000	-1.56074300
H	-6.58092600	-1.53397200	-2.57165800
H	-6.89142900	-2.40082900	-1.05484900
H	-5.23555300	-2.25087800	-1.67982800
C	-2.21657700	-1.09952800	2.52392300
H	-1.75641000	-1.67794000	1.70421300
C	-1.93040800	-1.84767100	3.81762000
H	-0.85606500	-2.04806400	3.91491200
H	-2.45530800	-2.81330700	3.85947100
H	-2.22853300	-1.26698200	4.70342200
C	-1.52072600	0.26057600	2.52373300
H	-0.46677900	0.14742600	2.81513900
H	-1.99300300	0.95756400	3.23527600
H	-1.54213700	0.72876200	1.52588900
C	-1.07481000	1.33797600	-3.05358000
C	-1.85284200	2.21062200	-3.83383300
C	-1.27183000	3.25299100	-4.54476000
H	-1.90596900	3.90336700	-5.15164800
C	0.91012700	2.65522500	-3.72864800
H	1.98583500	2.82343900	-3.64704800
C	0.11076800	3.47852200	-4.50286700
H	-2.93107900	2.03693400	-3.87083700
C	0.32418200	1.59620700	-3.00620400
C	1.10401400	0.84021900	-2.11196400
N	1.70829900	0.26175900	-1.31361600
C	-0.60161200	-1.33833800	-3.77403300
H	-0.95089800	-0.80609200	-4.67152100
H	0.46454300	-1.09406200	-3.66210300
H	-0.65367400	-2.41528800	-3.96887900
H	0.55455700	4.30175400	-5.06397900

B	2.44928000	-0.49177600	-0.15220600
C	-1.91314000	5.68238700	2.18842800
H	-1.36492800	5.03266900	2.88509200
H	-2.51941400	6.37106300	2.79214700
C	-2.77641200	4.87656400	1.24054200
H	-3.55776800	4.34832700	1.81269000
C	-2.01935600	3.84995700	0.39698400
H	-1.50436100	3.15355400	1.08300700
C	-3.81441400	2.01990700	0.34652400
H	-3.59081600	1.91230500	1.41689300
H	-4.89082700	1.95699600	0.14199900
C	-3.03100800	3.02144100	-0.39726000
H	-2.38299800	2.48790400	-1.22396800
H	-3.63943800	3.65856400	-1.06717300
C	2.30416400	0.40886500	1.19705700
C	1.49046800	1.52499500	1.37658100
C	3.07028200	0.05150100	2.30887500
C	1.44212700	2.25269800	2.56495900
C	3.04695700	0.74106100	3.51749900
C	2.22497100	1.86068000	3.64449700
C	4.01083800	-0.54731800	-0.61566600
C	4.64082700	0.62107000	-1.04679100
C	4.81526800	-1.68613700	-0.58448300
C	5.97617300	0.67705700	-1.43875200
C	6.15722400	-1.67592900	-0.96546900
C	6.74046800	-0.48661300	-1.39619600
C	1.66428700	-1.92069300	-0.12412800
C	1.58632400	-2.66242800	-1.30568400
C	0.94590500	-2.44491600	0.94877300
C	0.83467000	-3.82203400	-1.44540800
C	0.18373000	-3.61206100	0.85619900
C	0.11387400	-4.29460100	-0.35195200
F	4.32431200	-2.85666000	-0.17418900
F	6.88284300	-2.78657000	-0.91968900
F	8.01355900	-0.46117700	-1.76346300
F	6.52242900	1.81759100	-1.84715500
F	3.94869000	1.77258700	-1.09794200
F	0.62556400	3.29907400	2.67771400
F	0.66328100	1.95372100	0.40787400
F	2.18326900	2.53590200	4.78405000
F	3.79047700	0.34705800	4.54362300
F	3.84151000	-1.03824300	2.24606100
F	0.94910400	-1.84971800	2.14545300
F	-0.50128000	-4.05645200	1.90673300
F	-0.65439500	-5.36901000	-0.47415800
F	0.73714700	-4.44114000	-2.61878000
F	2.25399100	-2.24101700	-2.39098400
H	-1.16806800	6.29337600	1.65884100
H	-3.32446500	5.55517400	0.56051700
C	-0.97100800	4.48497100	-0.50076800
H	-1.41205000	5.25634800	-1.15391800
H	-0.16973800	4.95866000	0.08276900
H	-0.48668500	3.73895500	-1.14853200

c1c*-TSβH

Ni	-2.92218300	1.08828100	-0.89100700
N	-3.27032000	-0.71019600	-0.14808400
N	-1.73219900	0.44022200	-2.28811900
C	-3.22536000	-3.17205300	-0.07886600
H	-2.96629500	-3.99802300	-0.75077500
H	-4.30237900	-3.21577600	0.13037700
H	-2.72761900	-3.36491100	0.88409400
C	-2.81386800	-1.84642000	-0.66414500
C	-1.96014400	-1.90646500	-1.78641400
H	-1.70893100	-2.90720600	-2.13797900
C	-1.45500600	-0.85582100	-2.54308500
C	-4.19900300	-0.83127300	0.92877600
C	-5.57761700	-0.71410900	0.64299800
C	-6.48355400	-0.80951700	1.70412100
H	-7.55486400	-0.72359400	1.50802200
C	-6.04361600	-1.00623600	3.00881500
H	-6.76531600	-1.07854000	3.82554900
C	-4.68170100	-1.10817800	3.27199400
H	-4.34886900	-1.26128100	4.30044300
C	-3.73248800	-1.02546700	2.24640100
C	-6.06020700	-0.47122000	-0.77679500
H	-5.28749800	0.15108900	-1.27025400
C	-7.37258300	0.29774500	-0.83902500
H	-7.59354400	0.60048100	-1.87236600
H	-7.35392400	1.20773600	-0.22099200
H	-8.22620400	-0.30888600	-0.50064800
C	-6.16498800	-1.76121300	-1.58699300
H	-6.56380700	-1.55915500	-2.59202100
H	-6.84183600	-2.48199100	-1.10211600
H	-5.19283800	-2.25315000	-1.72154500
C	-2.24690700	-1.11436700	2.55350100
H	-1.77354900	-1.69690500	1.74417700
C	-1.94572500	-1.83607700	3.85806500
H	-0.86728500	-2.01170100	3.95776900
H	-2.44766300	-2.81309100	3.91327700
H	-2.25850600	-1.24941700	4.73497000
C	-1.57494300	0.25613700	2.52671600
H	-0.51770900	0.16249700	2.81190300
H	-2.04851900	0.95910100	3.23196300
H	-1.60646300	0.70484600	1.52104900
C	-1.09808500	1.42041000	-3.06305500
C	-1.80983100	2.24432400	-3.94984700
C	-1.17128600	3.23504300	-4.68274100
H	-1.75637400	3.84843500	-5.37182000
C	0.94463900	2.67153200	-3.69192100
H	2.01613700	2.82835800	-3.55181400
C	0.20782300	3.45765500	-4.55861000
H	-2.88441600	2.07856700	-4.05013600
C	0.29827500	1.65914000	-2.95124700
C	1.03864400	0.91884900	-2.01171900
N	1.64756800	0.34432200	-1.21374200
C	-0.62553500	-1.21742400	-3.74502100
H	-0.98008400	-0.69441500	-4.64556500
H	0.43642400	-0.95753900	-3.63418800

H	-0.66239700	-2.29608900	-3.93311300
H	0.69596900	4.24506400	-5.13414200
B	2.42965600	-0.43623100	-0.09986200
C	-1.65559000	5.67992100	2.13223500
H	-1.01236200	5.05388800	2.76498000
H	-2.12739600	6.42810700	2.78341500
C	-2.70024400	4.85831000	1.40620200
H	-3.40327300	4.42270000	2.13575000
C	-2.14309900	3.71873400	0.53427500
H	-1.63107800	3.00131100	1.19937000
C	-4.02611900	1.98468700	0.51964600
H	-3.70004600	1.61914500	1.49810800
H	-5.08312000	1.82249700	0.28888900
C	-3.33278600	3.03441800	-0.08547300
H	-2.88374500	2.27602300	-1.73716700
H	-3.88849000	3.67267200	-0.78714300
C	2.32691700	0.41191400	1.28322400
C	1.47307900	1.48111400	1.53905200
C	3.13655300	0.03011900	2.35505600
C	1.41481600	2.13373900	2.76918400
C	3.11607700	0.65558700	3.59810700
C	2.24374500	1.72372900	3.80674900
C	3.97443200	-0.47675700	-0.61882400
C	4.58417600	0.69217600	-1.07631400
C	4.78669100	-1.61040200	-0.60492700
C	5.90626000	0.75222300	-1.51096000
C	6.11570900	-1.59607800	-1.02795700
C	6.67812800	-0.40671100	-1.48552300
C	1.64946100	-1.86916900	-0.08373700
C	1.55915900	-2.59274300	-1.27542900
C	0.94365200	-2.41050400	0.98910000
C	0.81219200	-3.75437600	-1.42275600
C	0.18326500	-3.57813500	0.88785400
C	0.10501800	-4.24541200	-0.32841200
F	4.31542700	-2.77939900	-0.16809500
F	6.84900200	-2.70221100	-0.99614600
F	7.93887700	-0.37664700	-1.89302100
F	6.43326500	1.89343000	-1.94248900
F	3.88721300	1.84164200	-1.11059300
F	0.53522300	3.11515400	2.96213700
F	0.60357600	1.91973900	0.61466600
F	2.19425200	2.32824400	4.98513100
F	3.90165400	0.24282900	4.58478100
F	3.94011000	-1.02982800	2.22116500
F	0.95632500	-1.83248000	2.19481800
F	-0.49174800	-4.03724400	1.93867400
F	-0.65702200	-5.32357800	-0.45668300
F	0.70370200	-4.35697900	-2.60379400
F	2.20819200	-2.14981500	-2.36316900
H	-1.00095900	6.22731600	1.43943600
H	-3.31593600	5.51895100	0.76837500
C	-1.14604900	4.21303400	-0.49897200
H	-1.58982400	4.98406700	-1.15059600
H	-0.25365900	4.64286600	-0.02463800
H	-0.80508900	3.38981100	-1.14127000

c1c*-PβH

Ni	-2.20173700	0.93233800	-1.00952000
N	-3.11359800	-0.62551000	-0.24190400
N	-1.42902200	-0.06397200	-2.46974500
C	-3.42921900	-3.01383200	0.21396700
H	-4.50532700	-2.91131000	0.41381000
H	-2.96102400	-3.02448000	1.20777600
H	-3.24187500	-3.98643700	-0.25429700
C	-2.89555500	-1.88296500	-0.62295600
C	-2.18804400	-2.23376300	-1.79308500
H	-2.12832100	-3.29881300	-2.01824200
C	-1.56569100	-1.37929500	-2.70128400
C	-3.97353500	-0.42332500	0.87775300
C	-5.33693400	-0.12749800	0.64367200
C	-6.16119700	0.12487600	1.74495000
H	-7.21568800	0.36246100	1.58258200
C	-5.66210000	0.08202900	3.04270600
H	-6.32030300	0.28369400	3.89072300
C	-4.32225100	-0.22337300	3.25639400
H	-3.93959100	-0.25859200	4.27903600
C	-3.45400800	-0.48562800	2.19036100
C	-5.89779600	-0.06601100	-0.76747300
H	-5.05156100	0.15423600	-1.44036100
C	-6.93471800	1.03684800	-0.94438300
H	-7.17934400	1.17172400	-2.00799800
H	-6.58632600	2.00499200	-0.55612500
H	-7.88084300	0.80191300	-0.43390500
C	-6.47645500	-1.40563300	-1.21793700
H	-6.91919500	-1.32221700	-2.22147800
H	-7.26911500	-1.74863600	-0.53499700
H	-5.71365500	-2.19343900	-1.27022300
C	-1.98884800	-0.78496400	2.45568700
H	-1.61525200	-1.40801000	1.62577500
C	-1.76734900	-1.56738900	3.74278300
H	-0.72142400	-1.88758500	3.82648700
H	-2.39494600	-2.46990600	3.78575900
H	-1.98986100	-0.96684100	4.63716500
C	-1.15973700	0.49493900	2.43709300
H	-0.10492200	0.28479300	2.65756100
H	-1.52236600	1.21589100	3.18609700
H	-1.20247100	0.98091700	1.44522900
C	-0.93895900	0.77343700	-3.47752300
C	-1.70008000	1.10375500	-4.60917200
C	-1.20348200	1.97130800	-5.57473400
H	-1.82541500	2.22197200	-6.43727700
C	0.85974400	2.21816500	-4.36029300
H	1.86169700	2.63515700	-4.24454800
C	0.07236700	2.53789200	-5.45477000
H	-2.70331100	0.68040000	-4.70008200
C	0.36439700	1.33562700	-3.38298600
C	1.14040100	0.93123600	-2.28199200
N	1.72871200	0.53200800	-1.36971800
C	-0.96978300	-1.96856200	-3.94550200
H	-1.47575000	-1.60454200	-4.85145000

H	0.09170200	-1.69527300	-4.05053900
H	-1.03956300	-3.06077900	-3.94165400
H	0.44646300	3.22360100	-6.21587500
B	2.43480300	-0.21256600	-0.18204700
C	-2.63043300	3.74309800	3.29665500
H	-1.61049600	3.40727000	3.54110300
H	-3.30076600	3.35871700	4.07840500
C	-3.06168800	3.27070000	1.92323700
H	-3.25862100	2.18623600	1.95575600
C	-2.05101600	3.55517600	0.81333900
H	-1.11288400	3.03591900	1.06866300
C	-3.66538500	2.28801000	-0.74137600
H	-4.32075000	2.01625700	0.08772700
H	-4.12144100	2.26704400	-1.73840000
C	-2.52167300	3.04175500	-0.52870600
H	-1.13984600	1.89229800	-1.24432600
H	-2.11260500	3.58943600	-1.38397800
C	2.24900600	0.67625700	1.16852300
C	1.61982000	1.91537300	1.27607400
C	2.83199000	0.20419500	2.34653400
C	1.53123400	2.62303100	2.47522400
C	2.75393900	0.86668900	3.56798700
C	2.08646900	2.08987000	3.63296500
C	4.01646900	-0.26430000	-0.56830300
C	4.66304900	0.91654800	-0.93578100
C	4.82204600	-1.40117900	-0.51577100
C	6.01731500	0.98612200	-1.25228800
C	6.18350500	-1.37693200	-0.82077300
C	6.78343900	-0.17622400	-1.19245700
C	1.66093900	-1.65667600	-0.21967500
C	1.64330100	-2.37512000	-1.42016800
C	0.92729400	-2.24020100	0.81157300
C	0.95063000	-3.56586900	-1.60581900
C	0.19422200	-3.42064000	0.66413200
C	0.19835100	-4.08377500	-0.55513100
F	4.31487400	-2.58338500	-0.16147100
F	6.91095400	-2.48597600	-0.75978600
F	8.07484300	-0.13835300	-1.48876500
F	6.58084100	2.13663300	-1.60502900
F	3.96440700	2.06131800	-0.99546200
F	0.90363100	3.79781400	2.51878100
F	1.05058300	2.50763700	0.21578500
F	1.99543400	2.74443800	4.78207800
F	3.30884900	0.35608500	4.66041000
F	3.48388100	-0.96240200	2.32444600
F	0.88483600	-1.69480300	2.02995600
F	-0.52633000	-3.89380200	1.67730800
F	-0.53006500	-5.17900800	-0.73177100
F	0.96139700	-4.18953000	-2.78124300
F	2.32725100	-1.91245600	-2.47881600
H	-2.63178800	4.83911800	3.38267300
H	-4.03224500	3.72749100	1.65577800
C	-1.69749600	5.03273700	0.69311200
H	-2.58232300	5.64602300	0.46032800
H	-1.25861300	5.41317300	1.62434700

H -0.95480100 5.19832000 -0.10121000

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