

DFT Study of Mechanism and Stereochemistry of Nickel-Catalyzed *trans*-Arylative Desymmetrizing Cyclization of Alkyne-tethered Malononitriles

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1. Computational methods

DFT calculations were performed by Gaussian 16.¹ All the minima and transition states were optimized using B3LYP functional² with D3³(BJ)⁴ dispersion correction at 298 K in the gas phase. Def2-SVP basis set⁵ was used for all atoms. Vibrational frequencies as well as free energy corrections were computed at the same level. Single-point energy of each structure was calculated using the same functional and dispersion correction with the basis set of def2-TZVP.⁶ Solvent effect was also considered by computing solvation energies in toluene using SMD model.⁷ Unscaled harmonic frequency calculations at the same level were performed to validate each structure as either a minimum or a transition state. Standard state concentrations of 1.0 M⁸ were used for all the species. The configurations of key intermediates were explored using Molclus⁹ and xTB-6.3.3¹⁰, all conformations of each structure were carefully explored and the structures with the lowest energy were applied. 3D structures were prepared with CYLview20.¹¹

2. Alkyne substrates' coordination and insertion

At the beginning, we discovered the coordination mode of substrate to metal center. There are four possible configurations of **INT4** (Figure S1.a), whose relative energies are affected by coordination mode as well as steric effect. **INT4** is more stable than **INT4'** due to the *trans*-effect of phosphine discussed in the text. Another complex **INT4'-2** is even higher in energy than **INT4'**, suggesting that the phenyl group of the substrate tends to stand above the P–Ni–N plane.

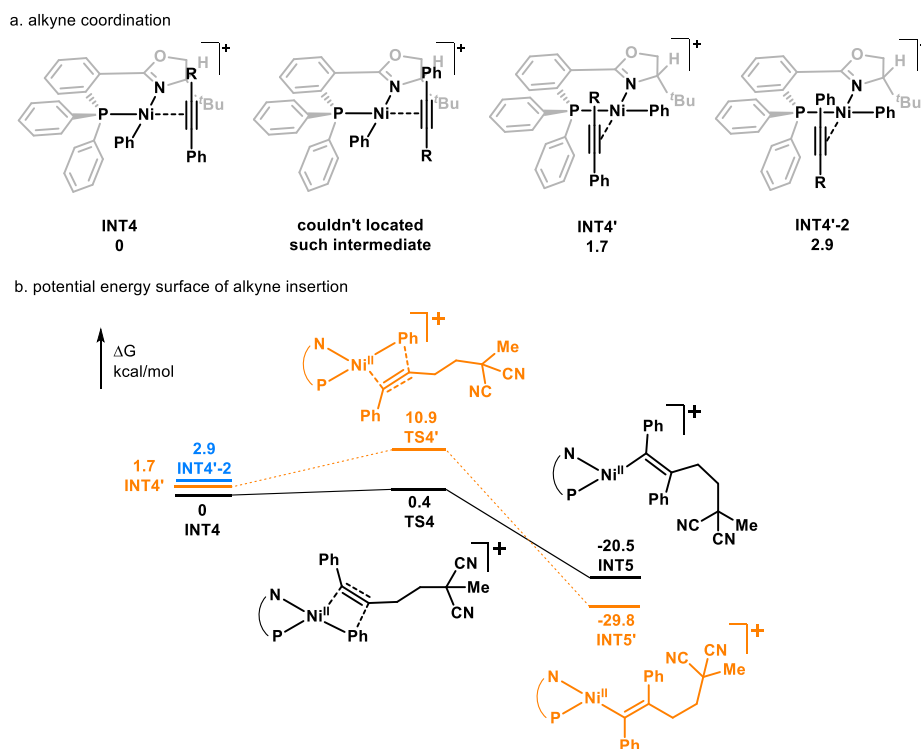


Figure S1. Structural diagram and relative Gibbs free energy profiles for alkyne coordination and insertion steps. Gibbs free energies were calculated at the B3LYP-D3(BJ)/def2-TZVP//SMD_{toluene}//B3LYP-D3(BJ)/def2-SVP level.

3. Interconversions of INT5 to INT5' and INT6 to INT6'

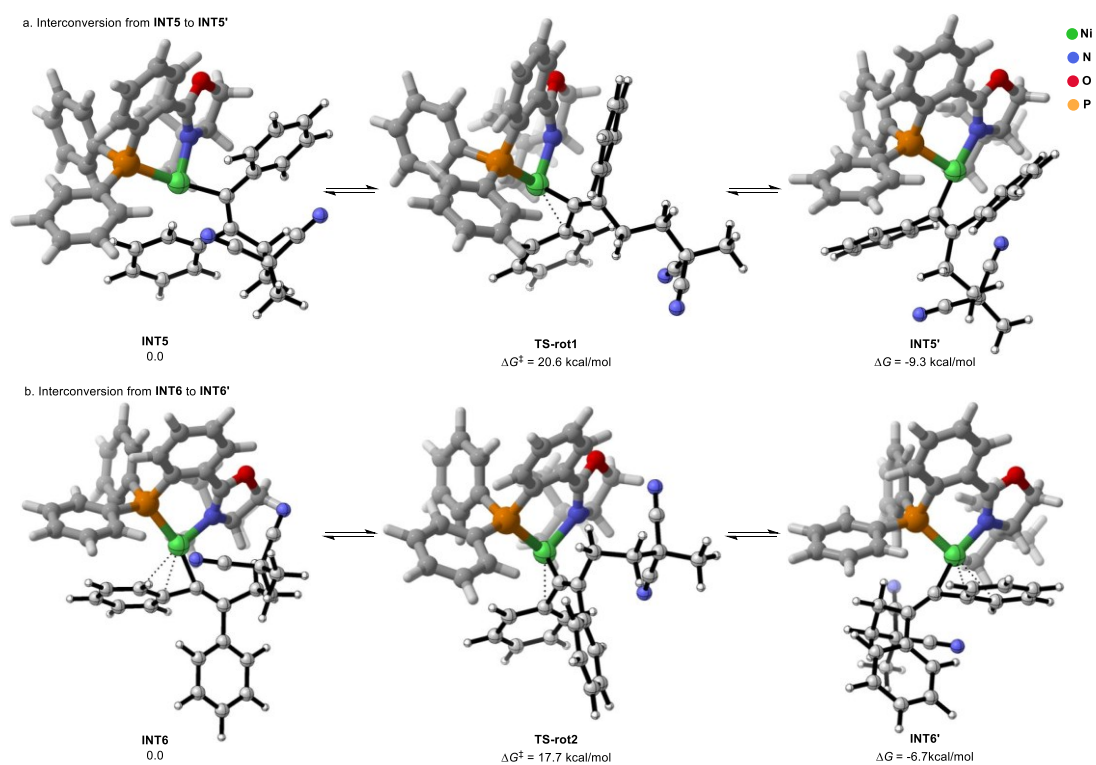


Figure S2. Interconversion of INT5 to INT5' (a) and INT6 to INT6' (b).

4. Cyano insertion step of INT6' and the origin of enantioselectivity

We have also considered the followed CN insertion step of **INT6'** and found that the enantioselectivity rises from the conformation of six-member-ring cyano-insertion transition state (orange and purple line in Figure S3). In general, intermediates that alkene group stand on the opposite of nitrogen atom are more stable. For the subsequent cyano insertion step, **TS7'** and **TS8'** keep the same enantioselectivity with **TS7** and **TS8** but respectively slightly more stable in energy (Figure S3). The only structural difference of **TS7'** and **TS8'** lies on the cyano-linked quaternary carbon, which is located in the formal six-membered ring. In **TS8'**, the more steric hindered methyl group stands on the *pseudo*-axial position, resulting in a congested transition state, while the cyano group lies in the *pseudo*-axial position in **TS7'**. According to the reported experimental data, a methyl group is about eight times larger than a cyano group.¹² When the cyano group stays in the *pseudo*-axial position in **TS7'**, A^{1,3} repulsions are effectively reduced. In a word, both paths from **INT6** and **INT6'** give the same enantioselectivity, which was also observed in experiments.

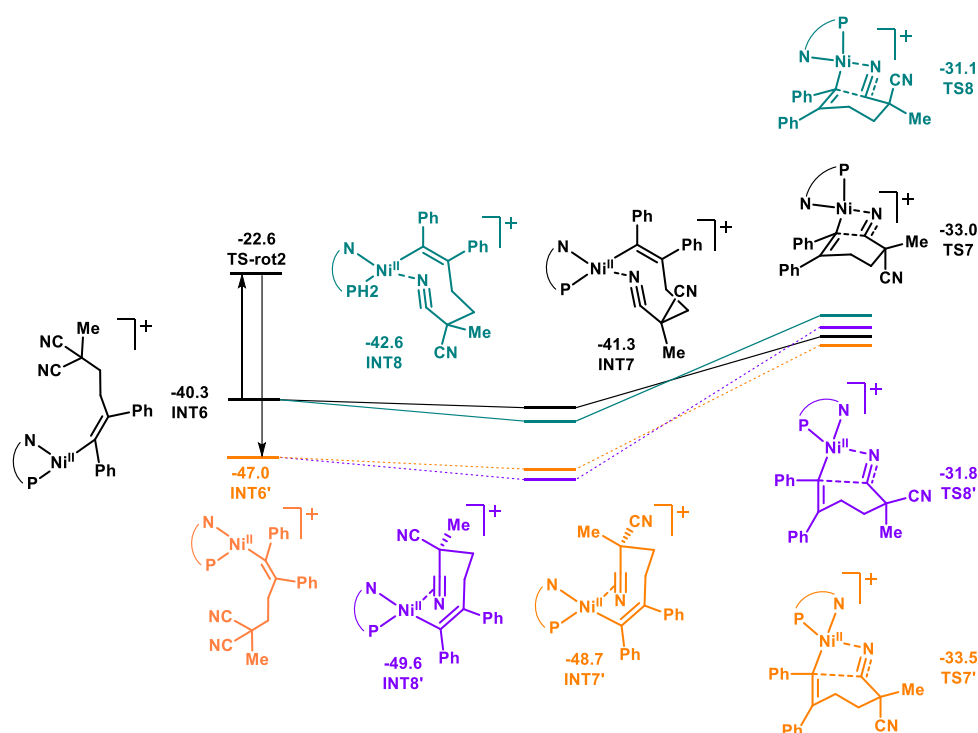


Figure S3. Relative Gibbs free energy profiles for cyano insertion step at the B3LYP-D3(BJ)/def2-TZVP//SMD_{toluene}//B3LYP-D3(BJ)/def2-SVP level.

5. Selection of functional

We tested several widely-used DFT functionals for the nickel systems by computing the energy barrier difference of the stereo-determining transition states of **TS7** and **TS8**, and comparing the results with experimental outcomes to select a suitable functional for single point energy calculations. Both **TS7** and **TS8** are the energy-lowest transition states for the generation of two enantiomers. As shown in Table S1, when using def2-TZVP as basis set, the energy barrier differences between **TS7** and **TS8** calculated by recently popular functionals like M06-L¹³, M06-2X¹⁴-D3, BP86¹⁵-D3, B3PW91^{2a,15a,16}-D3(BJ), and PBE0¹⁷-D3(BJ) are not so consistent with experimental data (ee: 83%). B3LYP-D3(BJ) and M06¹⁴ achieved satisfying outcomes. We further explored their application in the energy barrier differences between **TS7-Bn** and **TS8-Bn**. In this case, result from B3LYP-D3(BJ) is close to experimental result (ee: 90%). Based on the above consideration, we finally chose B3LYP-D3(BJ) as the functional in all discussions.

Table S1.

The reaction scheme shows the asymmetric hydroboration of alkyne **1a** (Ph-C≡C-CH₂-CH₂-C(CN)₂-Me) with Ph-B(OH)₂ (2) catalyzed by [Ni-L*] in H₂O and toluene. The reaction proceeds via two transition states, **TS7** and **TS8**, to yield product **3a** (Ph-C≡C-CH₂-CH₂-C(CN)₂-Me). The energy difference between the transition states is $\Delta\Delta G^\ddagger_1 = \Delta G^\ddagger_{TS8} - \Delta G^\ddagger_{TS7}$, leading to an enantiomeric excess (ee) of 83%.

The reaction scheme also shows the asymmetric hydroboration of alkyne **1b** (Ph-C≡C-CH₂-CH₂-C(CN)₂-Bn) with Ph-B(OH)₂ (2) catalyzed by [Ni-L*] in H₂O and toluene. The reaction proceeds via two transition states, **TS7-Bn** and **TS8-Bn**, to yield product **3b** (Ph-C≡C-CH₂-CH₂-C(CN)₂-Bn). The energy difference between the transition states is $\Delta\Delta G^\ddagger_2 = \Delta G^\ddagger_{TS8-Bn} - \Delta G^\ddagger_{TS7-Bn}$, leading to an enantiomeric excess (ee) of 90%.

functional ^a	$\Delta\Delta G^\ddagger_1$ ^b	ee (%)	$\Delta\Delta G^\ddagger_2$ ^c	ee (%)
B3LYP-D3(BJ)	1.9	92	2.8	98
M06	1.3	80	1.4	83
M06-L	0.6	47		
M06-2X-D3	6.8	99.9		
BP86-D3	-2.7	-98		
B3PW91-D3(BJ)	-0.1	-8		
PBE0-D3(BJ)	-0.5	-40		

^a Computed at the basis set of def2-TZVP in gas phase.

^b $\Delta\Delta G^\ddagger_1 = \Delta G^\ddagger_{TS7} - \Delta G^\ddagger_{TS8}$

^c $\Delta\Delta G^\ddagger_2 = \Delta G^\ddagger_{TS7-Bn} - \Delta G^\ddagger_{TS8-Bn}$

6. Computed energies of the stationary points

Thermal corrections to Gibbs energies (TCGs), single-point energies (SPEs) in gas phase and solvent.

	Imaginary Frequencies (cm ⁻¹)	SPEs (Hartree) ^a	TCGs (Hartree) ^b	$\Delta G_{\text{solvation}}$ (Hartree) ^c
B(OH)₃	-	-252.611099	0.021896	-0.007762
1a	-	-650.420873	0.174855	-0.016060
INT1	-	-3432.841746	0.528089	-0.063873
TS1	-289.29	-3432.831822	0.525639	-0.063052
INT2	-	-3432.859409	0.524553	-0.063837
INT3	-	-3830.708023	0.684385	-0.070966
TS3	-176.94	-3830.674475	0.688818	-0.067226
INT4	-	-3830.685204	0.685522	-0.073127
INT4'	-	-3830.683633	0.684398	-0.070792
TS4'	-184.68	-3830.674759	0.686483	-0.067102
TS4	-91.00	-3830.685204	0.682985	-0.069980
INT5	-	-3830.725425	0.688150	-0.068136
INT5'	-	-3830.739748	0.688626	-0.069116
TS-rot1	-48.08	-3830.685917	0.683961	-0.070659
TS5	-19.17	-3830.694077	0.688066	-0.068916
TS5'	-17.40	-3830.682981	0.687202	-0.068663
INT6	-	-3830.727576	0.688553	-0.067819
INT6'	-	-3830.736519	0.688305	-0.069312
TS-rot2	-33.01	-3830.697107	0.686662	-0.068161
INT7	-	-3830.724747	0.686912	-0.070699
INT8	-	-3830.725606	0.685977	-0.070841
TS7	-103.16	-3830.713277	0.687518	-0.069503
TS8	-81.77	-3830.712082	0.689214	-0.069389
Pro-S	-	-3830.745118	0.693095	-0.071651
Pro-R	-	-3830.747587	0.693482	-0.072450
Ni-OH	-	-3024.342726	0.405990	-0.061437
H₂O	-	-76.463448	0.003569	-0.020243
3a	-	-882.860936	0.281125	-0.004394
INT4'-2	-	-3830.679387	0.682048	-0.070730
INT7'	-	-3830.741660	0.691045	-0.069592
INT8'	-	-3830.743072	0.690440	-0.068975
TS7'	-134.95	-3830.721343	0.692765	-0.067391
TS8'	-205.91	-3830.716969	0.692058	-0.068383
TS7-Bn	-71.49	-4061.875797	0.763016	-0.074306
TS8-Bn	-90.11	-4061.871843	0.763755	-0.074473

^a Computed at the B3LYP-D3(BJ)/def2-TZVP level in gas phase

^b Computed at the B3LYP-D3(BJ)/def2-SVP level at 298 K in gas phase

^c Computed by $\text{SPE}_{\text{SMD}(\text{toluene})/\text{M05-2X}/6\text{-}31\text{G(d)}} - \text{SPE}_{\text{M05-2X}/6\text{-}31\text{G(d)}}$ at 298 K

Single point energy in gas phase for **TS7**, **TS8**, **TS7-Bn** and **TS8-Bn** using different functionals.^a

	TS7	TS8	TS7-Bn	TS8-Bn
M06	-3828.821611	-3828.821411	-4059.770570	-4059.768872
M06-L	-3830.079870	-3830.080659		
M06-2X-D3	-3829.487322	-3829.478218		
BP86-D3	-3830.804051	-3830.810128		
B3PW91-D3(BJ)	-3829.847154	-3829.849140		
PBE0-D3(BJ)	-3827.791467	-3827.794110		

^a All structures were computed at the basis set of def2-TZVP.

7. Cartesian coordinates of the stationary points

B(OH)₃				C	1.48854200	-0.41729500	1.72010200
O	-1.24392200	-0.61011400	0.00003600	C	0.33704200	-0.85946900	2.41455800
H	-1.94379600	0.05313000	0.00031900	C	0.41569200	-1.13366900	3.78762900
B	-0.01115600	-0.03247000	0.00020300	C	-0.94798400	-1.06587100	1.73284100
O	1.06571600	-0.87699300	-0.00016600	P	1.42813200	-0.12844000	-0.08363900
H	1.92537200	-0.44565300	0.00061700	N	-1.31356100	-0.60388600	0.57781400
O	0.06774900	1.34280600	-0.00029400	C	-2.63695500	-1.17950000	0.22876500
H	0.95785500	1.70928300	0.00143700	C	-3.07425100	-1.76799000	1.58246600
1a				O	-1.84695000	-1.81756000	2.35712900
C	-2.36382900	-0.43821400	1.18350300	H	1.66461800	-1.16209000	5.54668700
C	-2.82719300	-0.18089400	-0.28655700	H	3.69262700	-0.37040000	4.32625900
C	-1.69625500	-0.34803300	-1.33356100	H	-0.47550100	-1.48089300	4.31058400
C	-1.33851400	0.56429400	1.74375700	H	-3.30039300	-0.35911900	-0.06041200
C	0.02512000	0.40890400	1.24322900	H	-3.77898800	-1.11619200	2.11862500
C	1.15892600	0.26384900	0.83054600	H	-3.47718100	-2.78514100	1.53168900
C	-3.90248600	-1.14938100	-0.58957300	Ni	-0.51949900	0.77117600	-0.43995900
N	-4.71053800	-1.94630100	-0.81669700	C	-2.56642000	-2.18282100	-0.95449400
C	-3.38629700	1.18409600	-0.38696200	C	-1.65325500	-3.37162200	-0.62476900
N	-3.77004200	2.27487800	-0.43994700	H	-2.00258200	-3.93456600	0.25453100
C	2.48674200	0.09691400	0.32392200	H	-1.62608800	-4.07432200	-1.47075800
C	3.08146500	1.10040800	-0.46813100	H	-0.62129500	-3.04753000	-0.43761900
C	4.37292100	0.93262800	-0.96560700	C	-3.99675900	-2.67081000	-1.23979600
C	5.09121600	-0.23364700	-0.68373400	H	-4.00239200	-3.33148400	-2.11965200
C	4.51051300	-1.23474400	0.10127400	H	-4.41804800	-3.24570900	-0.40052000
C	3.21979400	-1.07454500	0.60310900	H	-4.67210200	-1.82599600	-1.44893400
H	-3.26005200	-0.41122400	1.82079200	C	-2.03944600	-1.44941100	-2.19673000
H	-1.96146200	-1.46136500	1.22841700	H	-1.94749900	-2.14450600	-3.04451700
H	-1.24585100	-1.34453800	-1.22814400	H	-2.71252400	-0.63336200	-2.49439700
H	-2.10213100	-0.24178100	-2.34884300	H	-1.04182600	-1.02299600	-2.01491800
H	-1.69057200	1.59457900	1.56227800	C	2.87873700	0.88698700	-0.48412300
H	-1.32697400	0.44273200	2.84063500	C	3.94921900	0.37161800	-1.23313300
H	2.51832000	2.00999600	-0.68528900	C	2.91863700	2.21443700	-0.01227100
H	4.82281400	1.71776900	-1.57779300	C	5.05413700	1.18065100	-1.50783000
H	6.10300000	-0.36210700	-1.07517300	H	3.92673600	-0.65672100	-1.59568700
H	5.06825200	-2.14727500	0.32458300	C	4.02922200	3.01103000	-0.29566600
H	2.76388400	-1.85351800	1.21706100	H	2.07854400	2.62320200	0.55846800
H	-0.91789900	0.40688200	-1.17330400	C	5.09525100	2.49777600	-1.04212700
INT1				H	5.88659700	0.77779700	-2.08855700
C	1.61717400	-0.95562900	4.47584000	H	4.05862800	4.04104000	0.06616900
C	2.75016700	-0.51266400	3.79338700	H	5.96018000	3.12709000	-1.26288600
C	2.68641900	-0.25055900	2.41987200	C	1.68522200	-1.74736900	-0.86471800
				C	1.49656200	-1.85036500	-2.25380000
				C	2.04701200	-2.88057400	-0.12189400

C	1.66794400	-3.07882300	-2.89074800	H	-3.25512500	-0.66226800	-0.05507500
H	1.21860500	-0.96977300	-2.83807900	H	-3.61877400	-1.51764100	2.11810600
C	2.21155300	-4.10940700	-0.76604400	H	-3.18939200	-3.13041700	1.45805800
H	2.19724200	-2.80887200	0.95639400	Ni	-0.56352500	0.79015800	-0.36741700
C	2.02024200	-4.21026400	-2.14649200	C	-2.30985100	-2.36743100	-0.99253300
H	1.52253800	-3.15538100	-3.97031800	C	-1.27710900	-3.46078900	-0.68154800
H	2.49098100	-4.99103400	-0.18548000	H	-1.56769500	-4.07753300	0.18270000
H	2.14795800	-5.17301000	-2.64598400	H	-1.17216300	-4.13647900	-1.54339500
H	3.57876900	0.08851200	1.89207400	H	-0.28473500	-3.03476200	-0.48238500
O	0.07982100	2.24206600	-1.39213900	C	-3.67533700	-2.99968100	-1.31033300
H	1.02691400	2.44592300	-1.43395000	H	-3.59889400	-3.63386500	-2.20628800
B	-0.68809300	3.26607200	-0.42886000	H	-4.04201300	-3.63837700	-0.49175100
O	-0.78221800	4.54411500	-1.01620300	H	-4.43537600	-2.22714600	-1.50825700
H	-1.44951800	4.60930200	-1.70661400	C	-1.84867400	-1.55377000	-2.21031100
O	0.05008500	3.30757400	0.80687900	H	-1.67313200	-2.21748600	-3.07005800
H	0.15286500	4.22745000	1.08045500	H	-2.60178500	-0.80879800	-2.50106800
C	-2.11610400	2.42692200	-0.27850500	H	-0.90575900	-1.02663600	-2.00441000
C	-2.76946900	2.36161500	0.97565800	C	2.80556900	1.17749900	-0.39981300
C	-2.85159100	2.02109500	-1.41771200	C	3.90937300	0.87567000	-1.21159100
C	-4.10140900	1.96923600	1.08055300	C	2.68718500	2.45918400	0.17658000
H	-2.20361700	2.65714800	1.86266100	C	4.88824700	1.84569900	-1.44323600
C	-4.19458000	1.63475200	-1.32264000	H	4.00907900	-0.11456700	-1.65848300
H	-2.37208400	2.05775400	-2.40045800	C	3.67194100	3.41976400	-0.06215500
C	-4.82145500	1.62022600	-0.07440700	H	1.83258900	2.70946400	0.81156800
H	-4.59759200	1.95440800	2.05432700	C	4.77101400	3.11570300	-0.87240200
H	-4.75278100	1.35414700	-2.21897700	H	5.74721300	1.60550800	-2.07340600
H	-5.87286100	1.33288900	0.00485800	H	3.57778800	4.41116900	0.38609400
TS1				H	5.53731900	3.87105700	-1.05915500
C	1.76281600	-1.03414800	4.43529500	C	1.93205200	-1.55948900	-0.94800100
C	2.86591700	-0.51028000	3.76080900	C	1.73291100	-1.61826400	-2.33829300
C	2.77407600	-0.20110100	2.39916400	C	2.43307700	-2.67842200	-0.26698400
C	1.57898600	-0.40011600	1.70165400	C	2.03604200	-2.78592800	-3.03786200
C	0.45912700	-0.92767400	2.38799500	H	1.33971500	-0.75105200	-2.87461000
C	0.56618300	-1.24854000	3.74958600	C	2.72676400	-3.84796200	-0.97263100
C	-0.81785900	-1.19737200	1.70789800	H	2.58850800	-2.64289000	0.81242900
P	1.47554700	-0.02541800	-0.08768500	C	2.52776100	-3.90359600	-2.35458300
N	-1.24608700	-0.70531400	0.58827100	H	1.88230800	-2.82680800	-4.11825500
C	-2.50222300	-1.40894100	0.21635100	H	3.11287100	-4.71901700	-0.43905300
C	-2.87104800	-2.08635000	1.54671800	H	2.75677100	-4.82021700	-2.90239400
O	-1.63173700	-2.06486700	2.30263000	H	3.64299000	0.20196100	1.87675100
H	1.83097900	-1.27827200	5.49710600	O	-0.06338900	2.32606900	-1.31524500
H	3.80573700	-0.34176500	4.29080200	H	0.86097000	2.61351500	-1.22377200
H	-0.29951900	-1.66441500	4.26513300	B	-0.98887400	3.17596600	-0.53074300
				O	-1.60263800	4.13824500	-1.31878800

H	-2.37057200	4.55372700	-0.91171100	C	-1.96941200	-0.60950700	-2.52529800
O	-0.43309900	3.48508400	0.72959900	H	-1.83709400	-0.93405500	-3.56853600
H	-0.70886600	4.34819900	1.05854100	H	-2.62156300	0.27612800	-2.52194300
C	-2.35356500	1.78165300	-0.23624600	H	-0.97983200	-0.31133600	-2.14766400
C	-2.94364700	1.81093400	1.04454800	C	2.75299000	0.89002600	0.30670300
C	-3.20601200	1.60352000	-1.34682500	C	3.93378000	0.64764500	-0.40896200
C	-4.32066700	1.65636400	1.21530900	C	2.65102900	2.03968500	1.10898400
H	-2.30453100	1.97370200	1.91696300	C	4.99744700	1.55153400	-0.32851100
C	-4.58523300	1.44989200	-1.18912500	H	4.02192100	-0.24492400	-1.03092100
H	-2.78051000	1.61744800	-2.35372000	C	3.71514400	2.93894700	1.18615600
C	-5.14212900	1.46726300	0.09578300	H	1.73462100	2.23570200	1.67069900
H	-4.76083100	1.69270100	2.21511800	C	4.88896700	2.69847800	0.46359100
H	-5.22910800	1.32190200	-2.06260000	H	5.91767900	1.35476000	-0.88342700
H	-6.22077800	1.34824800	0.22436700	H	3.62750700	3.83088100	1.81017800
INT2				H	5.72197400	3.40237500	0.52420300
C	0.99334100	-2.34165400	4.27068300	C	1.72736300	-1.52287400	-0.99247500
C	2.18654700	-1.73590900	3.87745100	C	1.65476400	-1.26023500	-2.37209400
C	2.26733000	-1.07958200	2.64415700	C	2.07427400	-2.80745500	-0.54830000
C	1.15788900	-1.00385000	1.79625400	C	1.93116800	-2.27218500	-3.29147200
C	-0.05469300	-1.61377100	2.20206400	H	1.37861100	-0.26288800	-2.71792600
C	-0.12030400	-2.28718700	3.43148400	C	2.34068800	-3.81903500	-1.47482700
C	-1.26227300	-1.60311300	1.35904600	H	2.12929700	-3.02546100	0.51928800
P	1.28100800	-0.17823100	0.15699300	C	2.26864100	-3.55425800	-2.84472400
N	-1.57308100	-0.76882200	0.41857500	H	1.87290800	-2.06339400	-4.36204200
C	-2.81914400	-1.23837600	-0.24042200	H	2.60483700	-4.81862800	-1.12296400
C	-3.31426600	-2.29450500	0.76371200	H	2.47430700	-4.34812200	-3.56608500
O	-2.14955000	-2.56948100	1.58489400	H	3.20916200	-0.62107000	2.33949300
H	0.92627800	-2.85890700	5.22966500	O	-0.00971400	2.62331800	-0.56381100
H	3.06383600	-1.77577500	4.52668700	H	-0.53782400	3.34245600	-0.18126700
H	-1.05615200	-2.76346700	3.72419000	B	1.01743800	3.04499100	-1.40922500
H	-3.51482700	-0.39216700	-0.28961100	O	1.51344800	2.09060500	-2.23708100
H	-4.10479700	-1.91395900	1.42690600	H	2.33594600	2.30429200	-2.69244600
H	-3.63601300	-3.24004900	0.31418100	O	1.36157400	4.34890600	-1.31210400
Ni	-0.74049800	0.87289900	-0.02642900	H	2.01680100	4.68717400	-1.93267900
C	-2.57171600	-1.74781500	-1.68741300	C	-2.39642200	1.78202500	0.29628100
C	-1.62562800	-2.95744900	-1.70052800	C	-3.00491900	1.71189200	1.56100600
H	-2.03780800	-3.81551400	-1.14774600	C	-2.99742500	2.58553900	-0.68736500
H	-1.45178400	-3.29021300	-2.73468600	C	-4.17880500	2.42304900	1.83460000
H	-0.64557700	-2.71011900	-1.27150600	H	-2.56638900	1.09327000	2.35024400
C	-3.93513800	-2.13297700	-2.28553500	C	-4.17943800	3.28964700	-0.42015700
H	-3.81153300	-2.46583500	-3.32707700	H	-2.55354300	2.66357700	-1.68514200
H	-4.41411400	-2.95835100	-1.73587300	C	-4.77176600	3.20995900	0.84219800
H	-4.62764800	-1.27618200	-2.28571100	H	-4.63286300	2.36230700	2.82727500
				H	-4.63726800	3.90037400	-1.20278700

H	-5.69199200	3.75930200	1.05333600	C	1.78577700	-1.19126300	-2.87298300
INT3				C	1.42191000	-2.52348700	-3.15057900
				C	0.14015800	-2.81865800	-3.61365700
C	-2.77641200	-4.23997700	-1.47872100	C	-0.79661500	-1.79858900	-3.80307400
C	-3.77457100	-3.26675100	-1.43092000	C	-0.44384900	-0.47504500	-3.52627200
C	-3.48823800	-1.99883000	-0.91798300	C	0.83379800	-0.16731300	-3.06149600
C	-2.20295600	-1.67190300	-0.46566800	H	4.87663500	2.15891700	-2.17542400
C	-1.19497500	-2.66360100	-0.50831200	H	6.32175300	2.05729800	-1.14964900
C	-1.49943000	-3.93974800	-1.01033900	H	3.88012600	3.77095900	1.07419400
C	0.16772300	-2.45303200	0.00812500	H	5.50753800	3.86189100	0.33629000
P	-1.89301200	-0.01373700	0.26244900	H	6.20330100	0.01411700	-2.43309400
N	0.72950900	-1.35406300	0.39174400	H	5.86763300	-0.40168600	-0.75638700
C	2.00261400	-1.70664600	1.07150200	H	2.15642000	-3.31917500	-3.01441400
C	2.22143600	-3.14688400	0.58135200	H	-0.12986700	-3.85346500	-3.83224600
O	0.90596800	-3.55905900	0.14335500	H	-1.79866500	-2.03677300	-4.16558900
H	-2.99219700	-5.23526800	-1.87210900	H	-1.16131500	0.33058200	-3.69129200
H	-4.78403100	-3.49208900	-1.78155100	H	1.11205600	0.86793000	-2.86228900
H	-4.28303100	-1.25528500	-0.86398000	C	1.90411500	-1.53340800	2.61726800
H	-0.71498800	-4.69451200	-1.03122400	C	0.76111700	-2.38398000	3.19327500
H	2.80208900	-1.05678700	0.69832000	H	-0.21659000	-2.05553500	2.81382900
H	2.89613500	-3.19594600	-0.28633100	H	0.88004400	-3.45413200	2.96376400
H	2.55551000	-3.85057200	1.35104600	H	0.73498800	-2.28510200	4.28871300
Ni	0.18343500	0.56975300	0.02830800	C	3.24711000	-1.95372700	3.23850200
C	-0.35121300	2.39602400	-0.18897000	H	3.46475300	-3.02186200	3.08421200
C	-0.19825200	3.28037900	0.89177900	H	4.08372800	-1.36538700	2.83163500
C	-0.82887800	2.91011700	-1.40207100	H	3.22375100	-1.78483700	4.32569800
C	-0.56045300	4.62838400	0.77700200	C	1.65019500	-0.05570800	2.95214500
H	0.21672900	2.92664000	1.84096800	H	0.71657600	0.30435700	2.49795000
C	-1.18284500	4.25755500	-1.52466300	H	1.55756000	0.07437500	4.04076900
H	-0.95583200	2.25490200	-2.26597300	H	2.47743100	0.58227800	2.60907400
C	-1.06062600	5.11958200	-0.43138400	H	4.04625700	4.02309700	-0.68760400
H	-0.44691200	5.29591700	1.63542400	C	-3.18228400	1.07278700	-0.43293200
H	-1.56414100	4.63211500	-2.47794800	C	-3.45006700	1.04714800	-1.81156500
H	-1.34799600	6.16949200	-0.52252700	C	-3.78666300	2.05187800	0.36689600
C	5.32206000	1.63048400	-1.31924700	C	-4.31327900	1.98383000	-2.37857600
C	4.48046800	1.98423800	-0.05664700	H	-2.98043200	0.29485400	-2.44556000
C	4.47559600	3.51582600	0.18747500	C	-4.64042000	2.99580100	-0.20732800
C	5.45475000	0.13033600	-1.63097000	H	-3.58765600	2.09052700	1.43786500
C	4.19030100	-0.46651400	-2.05243100	C	-4.90447700	2.96591200	-1.57830800
C	3.09999200	-0.84917000	-2.42835800	H	-4.51972700	1.95154200	-3.45068700
C	3.07965400	1.52554700	-0.16032800	H	-5.10105200	3.75879500	0.42348200
N	1.98020500	1.18048800	-0.11902600	H	-5.57325000	3.70560000	-2.02363300
C	5.03456400	1.27607000	1.11697400	C	-2.28973700	-0.23943000	2.03618000
N	5.46318500	0.68919200	2.01766800	C	-2.93069700	-1.39303200	2.51239000

C	-1.89672000	0.75762800	2.94521600
C	-3.17262300	-1.54530500	3.87979600
H	-3.23618400	-2.18025700	1.82259600
C	-2.14903400	0.60392000	4.30888300
H	-1.39471600	1.65580000	2.58497900
C	-2.78264700	-0.55002000	4.77941000
H	-3.66818000	-2.44840700	4.24254700
H	-1.84314400	1.38609000	5.00706900
H	-2.97240400	-0.67343900	5.84785500

TS3

C	-3.89294400	2.43165400	-2.79365100
C	-3.61229000	3.20018600	-1.66352000
C	-2.82108800	2.67545500	-0.63682900
C	-2.27915900	1.38868200	-0.72966300
C	-2.56961700	0.61072800	-1.87498900
C	-3.38229700	1.13745100	-2.89179900
C	-2.06444000	-0.75963000	-2.04482300
P	-1.27513800	0.70352100	0.65021800
N	-1.09153900	-1.33180300	-1.41629900
C	-1.06024900	-2.76284800	-1.81199900
C	-1.95835700	-2.75548600	-3.06226000
O	-2.68888600	-1.50776600	-2.95562200
H	-4.51357300	2.83426100	-3.59643800
H	-4.01562300	4.21084000	-1.57059500
H	-2.62298800	3.28105600	0.24731900
H	-3.60249900	0.52112600	-3.76315400
H	-0.02617000	-3.02131500	-2.06936800
H	-1.38675100	-2.72742600	-4.00199500
H	-2.69037300	-3.56909600	-3.10570700
Ni	0.25249200	-0.63080300	-0.19083500
C	1.56724600	-0.17492100	1.21548600
C	1.52077300	-0.92303300	2.41158800
C	2.19956800	1.08146800	1.23751200
C	2.00985100	-0.38985500	3.60663400
H	1.10328900	-1.93228900	2.41099300
C	2.68970900	1.61565400	2.43142100
H	2.29168700	1.65663500	0.31625500
C	2.58163200	0.88882300	3.61977900
H	1.95277800	-0.97553000	4.52713800
H	3.15004200	2.60554800	2.43387300
H	2.95912200	1.30853100	4.55483200
C	4.60849800	-2.25549700	-1.13530200
C	3.82517600	-1.88355000	0.16642800

C	4.62638700	-0.91223200	1.04507200
C	5.19909300	-1.04174500	-1.88148700
C	4.25344600	0.04947000	-2.09905300
C	3.42717900	0.93258100	-2.21435000
C	2.44914100	-1.42341800	-0.27949400
N	1.62375100	-1.63651600	-1.11288900
C	3.53809900	-3.11464500	0.92911500
N	3.27751000	-4.07127900	1.52722600
C	2.41038400	1.92813100	-2.34730000
C	2.68542100	3.28324400	-2.06995200
C	1.69267400	4.25057000	-2.22472000
C	0.41361300	3.88409600	-2.65667200
C	0.12726800	2.54131300	-2.92199100
C	1.11105000	1.56495100	-2.76339000
H	5.43180800	-2.92447600	-0.84452100
H	3.93822400	-2.82339400	-1.79454500
H	4.16245800	-0.78651900	2.02750600
H	5.63471700	-1.32584800	1.18782200
H	6.07395200	-0.65470600	-1.33416900
H	5.58822000	-1.39915600	-2.84991000
H	3.68879400	3.56710700	-1.74759800
H	1.92172200	5.29862800	-2.01887500
H	-0.36047900	4.64319400	-2.78697900
H	-0.86834000	2.25779000	-3.26340900
H	0.89801400	0.51694200	-2.97888200
C	-1.52865300	-3.70540800	-0.66445900
C	-2.97015200	-3.38756000	-0.23847500
H	-3.05585200	-2.36857000	0.16329200
H	-3.68598700	-3.49303600	-1.06810700
H	-3.28916000	-4.07761800	0.55683500
C	-1.42815800	-5.15322500	-1.17299200
H	-2.10733500	-5.35015600	-2.01699900
H	-0.40239600	-5.39259900	-1.49590100
H	-1.69766400	-5.85525700	-0.36976300
C	-0.59707700	-3.54550400	0.54604300
H	-0.63938200	-2.52049500	0.94345400
H	-0.90941100	-4.22023600	1.35713400
H	0.44702100	-3.78260800	0.29552800
H	4.70160400	0.06650500	0.55920600
C	-0.71106400	2.16824200	1.57169400
C	-0.86605900	2.28007900	2.95852800
C	-0.01414800	3.16410200	0.86522000
C	-0.32787700	3.38078200	3.63219300
H	-1.40493900	1.51453200	3.51798100

C	0.50373000	4.26722300	1.53954300	C	-0.50637600	-3.26776900	2.77440700
H	0.12389000	3.08022700	-0.21289600	H	0.75981700	-2.70100000	1.14287700
C	0.35297900	4.37516400	2.92649400	C	-1.63570500	-2.96313700	3.54147000
H	-0.45009900	3.46264300	4.71431700	H	-3.28813300	-1.59217200	3.80284900
H	1.03591800	5.03897900	0.97912500	H	0.09720300	-4.14721400	3.01192900
H	0.76498000	5.23662500	3.45681000	H	-1.91844000	-3.59943900	4.38299900
C	-2.50358700	-0.15142400	1.69960500	C	1.66519800	-2.29635800	-1.47913300
C	-3.88302100	-0.04982000	1.46375700	C	3.08089200	-2.47051900	-2.10349700
C	-2.03943600	-0.97449200	2.74021600	C	3.62163500	-1.16013600	-2.72673700
C	-4.78303200	-0.76839900	2.25454100	C	0.56187600	-1.90811800	-2.46861100
H	-4.26065600	0.58213300	0.65929900	C	-0.73584300	-1.77692900	-1.79325000
C	-2.94325300	-1.68381800	3.53145800	C	-1.89291100	-1.90514100	-1.40201600
H	-0.96993100	-1.05866100	2.93278700	C	3.97674200	-2.87329300	-0.99918300
C	-4.31648600	-1.58675500	3.28625900	N	4.63478800	-3.10735900	-0.07648600
H	-5.85487400	-0.68751900	2.06134800	C	3.03832400	-3.53255800	-3.12782900
H	-2.57319000	-2.31967000	4.33863500	N	2.94379800	-4.32762300	-3.96331300
H	-5.02307900	-2.14887500	3.90066100	C	-3.23900500	-2.15206600	-0.99151500
INT4				C	-3.49663100	-2.97388000	0.12408000
C	4.16737700	2.54935500	-1.87886800	C	-4.81148300	-3.21359000	0.51813100
C	4.47854900	2.18671700	-0.56835400	C	-5.87606000	-2.64551800	-0.18812600
C	3.48352200	1.68135000	0.27518300	C	-5.62756500	-1.83855100	-1.30443100
C	2.16859200	1.50719000	-0.17582600	C	-4.31762600	-1.59160800	-1.70752100
C	1.85706400	1.88310900	-1.50685400	H	1.38637500	-3.23210200	-0.97565500
C	2.85907600	2.40737100	-2.34011700	H	1.73842500	-1.52464200	-0.70144800
C	0.49589800	1.79491500	-2.05579800	H	2.98969800	-0.84903900	-3.56887300
P	0.87590400	0.91075700	1.00043400	H	3.62705600	-0.36859200	-1.96627600
N	-0.49934700	1.11986000	-1.58611500	H	0.80936800	-0.95956600	-2.96946000
C	-1.71145700	1.48570200	-2.35757700	H	0.46892100	-2.67396900	-3.25738600
C	-1.09673700	2.17697500	-3.58902800	H	-2.66377900	-3.41378500	0.67129500
O	0.25113400	2.49950000	-3.16317400	H	-5.00488700	-3.84895100	1.38466600
H	4.93809400	2.94920300	-2.54053700	H	-6.90422500	-2.83800000	0.12607800
H	5.49641900	2.30283500	-0.19027300	H	-6.45926400	-1.40652000	-1.86480200
H	3.73858500	1.42376200	1.30280900	H	-4.11937400	-0.97527100	-2.58634400
H	2.59760900	2.70237500	-3.35616700	C	-2.68888500	2.35917200	-1.51885500
H	-2.23322500	0.56312400	-2.64462000	C	-2.03182400	3.68402200	-1.10261100
H	-1.02209000	1.51309900	-4.46340000	H	-2.74182500	4.28647700	-0.51687800
H	-1.58919100	3.11032300	-3.88283600	H	-1.15175500	3.51557000	-0.46628800
Ni	-0.58933400	-0.20149600	-0.13272600	H	-1.72445000	4.29203900	-1.96703100
C	-0.88978400	-1.31123400	1.36960000	C	-3.94035400	2.62506100	-2.37058200
C	-2.02817100	-1.02301500	2.14225700	H	-3.71299800	3.20025100	-3.28164700
C	-0.13801900	-2.44543600	1.70535500	H	-4.42609600	1.68351000	-2.67276400
C	-2.39632900	-1.83783900	3.22063200	H	-4.67389000	3.20778600	-1.79361900
H	-2.66769600	-0.17074200	1.90150400	C	-3.09467200	1.58063600	-0.26055700
				H	-3.79574400	2.17023800	0.34879100

H	-3.58207700	0.62706300	-0.50663700	H	-0.41123400	-4.77930500	1.08133100
H	-2.21737800	1.37783200	0.37200600	H	1.32966900	-5.10778600	0.79811600
H	4.64474100	-1.30432800	-3.09806500	Ni	-0.30625400	-0.40974600	-0.33461600
C	1.79482600	0.02375500	2.29817800	C	-1.79696400	-1.45906300	-0.90875600
C	1.44820200	0.16196000	3.64884100	C	-2.14942600	-1.61031600	-2.25635300
C	2.75670100	-0.93079500	1.92762300	C	-2.58722900	-2.08332200	0.06740600
C	2.05299700	-0.65249000	4.60925500	C	-3.25186500	-2.39223200	-2.62448700
H	0.70409600	0.89587600	3.95858700	H	-1.58283700	-1.10042400	-3.03936200
C	3.36452100	-1.73646100	2.88822100	C	-3.70685400	-2.84244300	-0.29391400
H	3.04674300	-1.05455600	0.88526300	H	-2.35665600	-1.96916300	1.13055700
C	3.00630500	-1.60232900	4.23336700	C	-4.03635700	-3.00678700	-1.64311200
H	1.77514000	-0.54114000	5.65940200	H	-3.50666700	-2.50733200	-3.68119300
H	4.10992000	-2.46867500	2.57100700	H	-4.32578900	-3.29321700	0.48511200
H	3.47397100	-2.23644600	4.98961300	H	-4.90374200	-3.60637200	-1.92844400
C	0.22033400	2.44891900	1.73876500	C	-4.14398100	0.91637000	-0.73598400
C	-0.93809000	2.37387900	2.53147800	C	-5.44257700	0.94843600	0.12081200
C	0.81170100	3.69833500	1.49585000	C	-6.66620900	0.55852900	-0.74274000
C	-1.49179600	3.53330300	3.07514300	C	-2.89436700	1.29850900	0.06817500
H	-1.40582000	1.40822700	2.72473400	C	-1.63886100	1.13133800	-0.67933600
C	0.24710900	4.85612100	2.03637200	C	-0.73348800	1.28714900	-1.51212400
H	1.70960200	3.77679900	0.88227900	C	-5.29989600	-0.00664200	1.24129800
C	-0.90394100	4.77691500	2.82423300	N	-5.14384900	-0.78517900	2.08328500
H	-2.38887100	3.46487300	3.69430200	C	-5.61869100	2.30514300	0.68012900
H	0.71177200	5.82482700	1.84048800	N	-5.70661700	3.38917100	1.07620500
H	-1.34235300	5.68448400	3.24474900	C	0.25604900	1.75726700	-2.43799600
INT4'				C	0.73748700	0.93401000	-3.47552200
C	0.92527200	-0.81394200	5.15573600	C	1.73002000	1.39920000	-4.33511300
C	1.23046500	0.52386200	4.90794100	C	2.25286100	2.68733000	-4.17166900
C	1.36585300	0.98151600	3.59238100	C	1.76804400	3.51611700	-3.15464200
C	1.18483400	0.11721800	2.50774000	C	0.77307800	3.06104000	-2.29129400
C	0.87860100	-1.24184300	2.76307000	H	-4.04036700	-0.09585300	-1.14381000
C	0.76067900	-1.69488300	4.08624400	H	-4.27647700	1.60720300	-1.58159800
C	0.72757100	-2.23243100	1.68398500	H	-6.77391500	1.27359300	-1.57013700
P	1.36900200	0.72630300	0.78117500	H	-6.51103400	-0.44891500	-1.15346600
N	0.44390200	-2.02545000	0.43660600	H	-2.95536000	2.35679300	0.37429200
C	0.53902000	-3.32399800	-0.28380100	H	-2.85588800	0.70237700	0.99241300
C	0.57006600	-4.32343600	0.88426000	H	0.33303600	-0.06991500	-3.59684900
O	0.90878400	-3.50382300	2.03191500	H	2.09760300	0.75547100	-5.13678600
H	0.81851600	-1.17636500	6.17985400	H	3.03346900	3.04870000	-4.84465300
H	1.36853800	1.22001200	5.73799500	H	2.16740900	4.52479500	-3.03146400
H	1.61493900	2.02755800	3.41154200	H	0.39198000	3.70308800	-1.49826700
H	0.53564900	-2.74584700	4.26715700	C	1.75165900	-3.38424500	-1.25166900
H	-0.37383500	-3.45303900	-0.87593600	C	3.08186600	-3.23901800	-0.49960300
				H	3.92316500	-3.27392800	-1.20776700

H	3.14344500	-2.27951000	0.02986000	C	-1.93641600	2.72823400	-0.14005100	
H	3.23765300	-4.04750300	0.23111300	C	-2.22004300	3.56738800	1.11713800	
C	1.69990500	-4.73446700	-1.98581200	O	-2.20090300	2.58949500	2.18753000	
H	1.81590100	-5.58766400	-1.29939600	H	-1.53285000	-0.05596000	6.06034000	
H	0.74837400	-4.85939400	-2.52703200	H	-1.18925500	-2.42599600	5.34430200	
H	2.51621000	-4.79713600	-2.72114900	H	-0.98575200	-2.97773600	2.94518600	
C	1.61042700	-2.25463100	-2.27979400	H	-1.71428400	1.73192500	4.33601900	
H	2.43846500	-2.28385600	-3.00409800	H	-1.19806200	3.22672000	-0.77931300	
H	0.66451900	-2.34438200	-2.83448600	H	-1.43280800	4.30546300	1.32163300	
H	1.63675200	-1.26952700	-1.79526900	H	-3.20080000	4.05371000	1.13070800	
H	-7.58667300	0.56551300	-0.14393900	Ni	-0.06345500	0.33174700	-0.51022900	
C	1.26375400	2.53990600	0.94208500	C	0.53688300	-0.64487000	-2.07055300	
C	2.34300800	3.38088900	0.63700700	C	0.13431500	0.07176400	-3.20855500	
C	0.03461900	3.10475400	1.32570300	C	0.92509300	-1.98309100	-2.21220900	
C	2.18829800	4.76879500	0.69923400	C	-0.00545300	-0.57446500	-4.44114200	
H	3.30297600	2.95606400	0.34178400	H	-0.06471300	1.14176300	-3.14237900	
C	-0.11601000	4.48953900	1.38830700	C	0.80508800	-2.62229300	-3.44950900	
H	-0.80360400	2.45925200	1.59259900	H	1.30849100	-2.54734600	-1.36548800	
C	0.96031300	5.32503500	1.06560600	C	0.32009100	-1.92794400	-4.56256300	
H	3.03401000	5.41726300	0.46026300	H	-0.34375600	-0.00808200	-5.31201400	
H	-1.07361300	4.91940300	1.69043500	H	1.09019300	-3.67320800	-3.53750900	
H	0.84141700	6.40978100	1.10993700	H	0.22600100	-2.43171600	-5.52695400	
C	3.10540400	0.37532800	0.34716200	C	4.24732800	0.62203100	-0.24395600	
C	3.49368400	0.53995400	-0.99351200	C	5.49388100	-0.25174700	0.09696300	
C	4.04262700	-0.06687700	1.29210700	C	6.17020100	-0.84252400	-1.16468600	
C	4.80452300	0.26208700	-1.38076300	C	3.13872000	-0.15277600	-0.96827900	
H	2.77450600	0.88705600	-1.73608500	C	1.87578900	0.62185800	-0.93519800	
C	5.35202100	-0.35183400	0.89619600	C	1.31423400	1.73570400	-0.69977200	
H	3.75331200	-0.19589700	2.33625500	C	6.45934900	0.59543900	0.82512900	
C	5.73391300	-0.19029600	-0.43830700	N	7.20948800	1.29327300	1.36282000	
H	5.09871700	0.39450500	-2.42415000	C	5.05797500	-1.34785500	0.98928500	
H	6.07650000	-0.70106800	1.63502100	N	4.64325100	-2.20799900	1.64272600	
H	6.75785000	-0.41555100	-0.74435600	C	1.31718400	3.14080300	-0.37744100	
TS4				C	1.32117000	3.55414100	0.96995800	
				C	1.31707100	4.91212900	1.28806700	
	C	-1.44823200	-0.30683200	5.00129000	C	1.28916300	5.87410300	0.27262100
	C	-1.25465400	-1.62854900	4.60106300	C	1.27929200	5.47100200	-1.06712600
	C	-1.14024100	-1.94043600	3.24252300	C	1.29520800	4.11516700	-1.39458400
	C	-1.21156100	-0.94346700	2.26154900	H	3.85332200	1.03694300	0.69513600
	C	-1.42513000	0.39478100	2.67233100	H	4.58588800	1.47418800	-0.85196000
	C	-1.54242200	0.69766400	4.03872500	H	5.48095300	-1.52276600	-1.68271600
	C	-1.61440600	1.49168100	1.71181000	H	6.45102200	-0.02441500	-1.84293500
	P	-1.02679900	-1.40615000	0.48562800	H	3.41252100	-0.37138300	-2.01136300
	N	-1.32025800	1.50889400	0.45177600	H	2.97372100	-1.12692800	-0.48357900

H	1.33811200	2.80021600	1.75966300	C	-3.46262000	1.58142100	-3.81482400
H	1.33778900	5.22268000	2.33519800	C	-2.63967500	1.82598900	-2.71007500
H	1.28374600	6.93657600	0.52461000	C	-2.30482600	0.80171000	-1.81690400
H	1.26635600	6.21922800	-1.86265100	C	-2.83771500	-0.49122100	-2.04214300
H	1.29236700	3.79839000	-2.43953500	C	-3.67487800	-0.72430600	-3.14429000
C	-3.19361100	2.40653900	-1.00023400	C	-2.58672500	-1.61000200	-1.12160500
C	-4.26100200	1.66886500	-0.17815900	P	-1.27511800	1.17589200	-0.32754900
H	-5.15314500	1.48755600	-0.79599500	N	-1.62273500	-1.72128100	-0.27014300
H	-3.89908900	0.68905300	0.16201200	C	-1.86573500	-2.92946800	0.55452200
H	-4.58374800	2.24424500	0.70297800	C	-2.94469800	-3.65315400	-0.27237400
C	-3.75611800	3.73565600	-1.53366600	O	-3.45497200	-2.62207200	-1.15595700
H	-4.14800200	4.38128400	-0.73309600	H	-4.62501200	0.10970900	-4.89336100
H	-2.98836900	4.30305600	-2.08436800	H	-3.70217700	2.39830600	-4.49897800
H	-4.58823600	3.53985700	-2.22650200	H	-2.25697300	2.83275900	-2.54283400
C	-2.77758100	1.53883600	-2.19201200	H	-4.08460300	-1.72348300	-3.29282800
H	-3.65363200	1.27899200	-2.80505400	H	-0.94505900	-3.52359700	0.58904900
H	-2.06208800	2.07063800	-2.83692500	H	-2.53042000	-4.45537800	-0.90053500
H	-2.31643800	0.59924900	-1.86400500	H	-3.78659500	-4.04181100	0.31073800
H	7.07493500	-1.40218900	-0.89248500	Ni	0.01139600	-0.64459500	-0.13962100
C	-0.10545900	-2.97464700	0.58835400	C	1.08009600	-2.27401100	-0.42847000
C	-0.62553000	-4.17764400	0.09481300	C	1.65835700	-2.84133200	0.71539300
C	1.19650500	-2.94433900	1.12084600	C	0.79341300	-3.09373300	-1.53458000
C	0.15327800	-5.33917800	0.13015100	C	1.89140300	-4.22226200	0.77871800
H	-1.63307700	-4.21123900	-0.32193900	H	1.95038900	-2.20674500	1.55290000
C	1.96828300	-4.10460400	1.15762700	C	1.04359600	-4.46477000	-1.47812000
H	1.61526500	-2.01288000	1.51100600	H	0.35467800	-2.66084100	-2.43779300
C	1.44635600	-5.30412100	0.65660400	C	1.58462100	-5.03455100	-0.31522200
H	-0.25672400	-6.27508800	-0.25577100	H	2.33079300	-4.65498400	1.68060300
H	2.97818100	-4.05634700	1.56783800	H	0.81324000	-5.09664400	-2.33952100
H	2.05132200	-6.21318600	0.68096400	H	1.77848000	-6.10865400	-0.27308600
C	-2.69652100	-1.83327500	-0.10218600	C	4.19301000	-1.64460400	-1.36363900
C	-2.88264800	-1.97636000	-1.48870500	C	5.12571900	-0.95794400	-0.31624300
C	-3.78511100	-1.98983100	0.76769500	C	6.45449600	-1.74881600	-0.19320400
C	-4.14791700	-2.27737700	-1.99340800	C	2.99050300	-0.81888000	-1.83812200
H	-2.03959800	-1.85198700	-2.17165300	C	1.97609800	-0.48170200	-0.79957700
C	-5.05120700	-2.28179400	0.25402000	C	1.62928700	0.36689000	0.09459300
H	-3.64953600	-1.87774200	1.84469800	C	5.40698900	0.42650800	-0.74702800
C	-5.23402300	-2.42484100	-1.12404200	N	5.59583300	1.49883700	-1.13936400
H	-4.28768600	-2.39059200	-3.07062300	C	4.49056300	-0.91249600	1.01784400
H	-5.89774200	-2.39783700	0.93419500	N	4.02543900	-0.93538500	2.07698200
H	-6.22522500	-2.65242200	-1.52233500	C	1.95909200	1.51838400	0.90708800
TS4'	C	-3.97972100	0.30513600	C	1.51108300	1.57787700	2.23928200
					1.82703900	2.67029500	3.04506500
					2.59754700	3.71716200	2.52984900

C	3.06781800	3.65445700	1.21437700	H	-4.22913500	1.62885900	-0.38271200
C	2.75869400	2.56174800	0.40740500	C	-4.36620100	2.14934600	2.98109100
H	4.81870500	-1.86720800	-2.24104600	H	-2.66393400	2.13609400	4.31743400
H	3.86445200	-2.60550600	-0.94237500	H	-5.85700900	2.11148000	1.41511500
H	6.23358700	-2.78559800	0.09687500	H	-5.08840600	2.35942000	3.77298700
H	6.97461000	-1.74750800	-1.16112000				
H	3.34656200	0.13824700	-2.25369700	INT5			
H	2.51329200	-1.36324100	-2.66484600	C	1.94542900	-1.88165400	4.45059900
H	0.94300300	0.73856000	2.64350400	C	2.45279900	-0.58263000	4.44087600
H	1.48182500	2.70139100	4.08084500	C	2.44109400	0.16828000	3.25962500
H	2.84386000	4.57565800	3.15858100	C	1.91290500	-0.36125800	2.07841200
H	3.68232300	4.46199800	0.81133100	C	1.39396500	-1.67970700	2.09341900
H	3.13148900	2.51901200	-0.61425300	C	1.42426000	-2.43032800	3.27773800
C	-2.26557900	-2.57621400	2.01550000	C	0.83392700	-2.31463500	0.89093200
C	-3.57606800	-1.77687500	2.05833500	P	1.91184000	0.63080300	0.52797400
H	-3.83962600	-1.53940500	3.09972800	N	0.35256900	-1.72854100	-0.15662900
H	-3.48565700	-0.82310300	1.52244100	C	0.00137700	-2.75652700	-1.16342700
H	-4.42085400	-2.33597700	1.62784600	C	0.07434600	-4.04369100	-0.32097700
C	-2.42135000	-3.89432200	2.79194300	O	0.80625300	-3.64341300	0.86845600
H	-3.23933300	-4.51698200	2.39707100	H	1.95375100	-2.47084500	5.36957400
H	-1.49381200	-4.48809800	2.75953600	H	2.86323300	-0.14550400	5.35364300
H	-2.65185200	-3.68780900	3.84792500	H	2.84589000	1.18120300	3.26135800
C	-1.13965500	-1.75409400	2.66085800	H	1.02701900	-3.44544300	3.26896100
H	-1.41073100	-1.47779300	3.69087900	H	-1.02994200	-2.57924700	-1.48787900
H	-0.19917300	-2.32115400	2.69632100	H	-0.91858000	-4.38712000	0.00371200
H	-0.95698600	-0.82013200	2.10754200	H	0.62362500	-4.86870900	-0.78752800
H	7.10890500	-1.29864700	0.56501600	Ni	-0.09146000	0.10285700	-0.37926100
C	-0.43465000	2.72805700	-0.78129900	C	-1.69906400	1.49802900	-2.10848100
C	-0.54188900	3.89057700	-0.00867500	C	-0.58939800	1.94117000	-1.34528100
C	0.39405600	2.72090300	-1.91747000	C	-1.80572800	1.93759100	-3.43799600
C	0.17201400	5.03633800	-0.37084700	C	0.39843100	2.77011700	-1.90055400
H	-1.17749500	3.90621600	0.87737800	H	-0.67810100	1.86931000	-0.23414000
C	1.09034300	3.87121600	-2.28280500	C	-0.81877800	2.75630000	-3.98838800
H	0.49269600	1.81310600	-2.51707000	H	-2.64371000	1.60932300	-4.05614400
C	0.98295400	5.03089100	-1.50709600	C	0.28803300	3.16942800	-3.22965100
H	0.08956400	5.93773000	0.23984800	H	1.22175900	3.12538700	-1.27907600
H	1.72723900	3.86245200	-3.17008900	H	-0.90785700	3.07872800	-5.02860000
H	1.53606700	5.92938300	-1.78902200	H	1.04220200	3.82243800	-3.67317900
C	-2.51466800	1.59818500	0.94756200	C	-4.71243500	1.85578200	-1.01281300
C	-2.08639800	1.74208300	2.27773000	C	-4.69587000	1.87298300	0.54885700
C	-3.87778500	1.73796400	0.64377100	C	-5.56496200	3.04853600	1.07235200
C	-3.00774200	2.02213000	3.28706700	C	-4.08790700	0.62031700	-1.67877400
H	-1.02938400	1.64318200	2.52243100	C	-2.59655700	0.52158200	-1.46099300
C	-4.79752300	2.00922500	1.65960600	C	-1.96060300	-0.30424400	-0.59451800

C	-5.23354600	0.60117200	1.07364800	H	0.39854500	4.86318400	2.54940900
N	-5.69775200	-0.38600300	1.45944100	H	2.57204900	6.04763100	2.21957900
C	-3.32620800	2.05731300	1.07767800	C	3.43346400	0.14150100	-0.34752100
N	-2.27676800	2.27153200	1.51554500	C	4.41497800	-0.66946700	0.23973000
C	-2.56144800	-1.37499000	0.20740400	C	3.58998000	0.57073900	-1.67698000
C	-2.30704900	-1.42702900	1.59321300	C	5.53811500	-1.05200100	-0.49886300
C	-2.82900600	-2.45186400	2.37916000	H	4.30265700	-1.00944000	1.27055300
C	-3.60232300	-3.46132200	1.79572100	C	4.71769900	0.19458200	-2.40593300
C	-3.85244200	-3.43347400	0.42082200	H	2.82492000	1.19462500	-2.14480200
C	-3.33763400	-2.40120400	-0.36536800	C	5.69053300	-0.62239300	-1.81953800
H	-5.77065600	1.92868100	-1.30701100	H	6.29724200	-1.68813000	-0.03863500
H	-4.21702700	2.77816000	-1.35521100	H	4.83455000	0.53203200	-3.43805500
H	-5.18012100	3.99603300	0.66972400	H	6.56872700	-0.92446200	-2.39428100
H	-6.60238000	2.91006300	0.73842400				
H	-4.59062600	-0.28195800	-1.30770600	INT5'			
H	-4.31186400	0.68008900	-2.75671400	C	5.02923800	-0.32416300	2.84416000
H	-1.70744900	-0.63733100	2.05142900	C	4.42446600	0.91104100	3.07515500
H	-2.63769300	-2.46219000	3.45462900	C	3.29352500	1.28732600	2.34283500
H	-4.01457000	-4.26312900	2.41189300	C	2.74156800	0.43550500	1.37936900
H	-4.45953900	-4.21582000	-0.04042000	C	3.35511000	-0.82129600	1.15277100
H	-3.53008500	-2.38911300	-1.44084200	C	4.49849700	-1.18337000	1.88205400
C	0.90755800	-2.69771600	-2.42181200	C	2.84611400	-1.77515500	0.15804700
C	2.37659200	-2.96776300	-2.06765100	P	1.30038300	1.00847200	0.38490800
H	3.00301300	-2.90564400	-2.97001600	N	1.67632600	-1.78259200	-0.38607700
H	2.76201300	-2.22908000	-1.35277400	C	1.62661200	-2.86161200	-1.39664700
H	2.52158700	-3.97122700	-1.63857900	C	2.93852600	-3.62604700	-1.11410900
C	0.39718800	-3.75532000	-3.41428200	O	3.67266400	-2.74988000	-0.22457200
H	0.47892100	-4.77732400	-3.01226700	H	5.91415100	-0.62124900	3.41017900
H	-0.65715300	-3.57783700	-3.68102200	H	4.83308700	1.59315000	3.82376200
H	0.98826300	-3.72271400	-4.34191400	H	2.83880300	2.26158300	2.52371700
C	0.77050000	-1.30745400	-3.06198100	H	4.96334400	-2.14997200	1.68806700
H	-0.27832600	-1.07485100	-3.30147600	H	0.75263100	-3.49832600	-1.18622400
H	1.14803400	-0.52003800	-2.39379800	H	2.78022300	-4.58024100	-0.59117400
H	1.35470800	-1.25377100	-3.99302700	H	3.55825000	-3.80002000	-2.00137500
H	-5.54714100	3.09190400	2.16952100	Ni	0.09107400	-0.71130200	-0.02060100
C	2.17569200	2.34622500	1.08334600	C	-1.62520700	-1.40155900	2.00751900
C	3.39788200	3.01091700	0.90066600	C	-0.87205900	-2.34926800	1.27401100
C	1.09415600	3.02057700	1.67906700	C	-1.62471900	-1.49545100	3.41112500
C	3.53578900	4.34034700	1.30986600	C	-0.10090900	-3.32205500	1.92516000
H	4.24070900	2.49348900	0.43943100	H	-1.06229400	-2.43261400	0.18875000

H	-0.85629000	-2.51731500	5.14603000	C	0.71146000	3.70994000	0.95265100
H	0.50254700	-4.13828800	3.83225900	C	-0.05926100	2.05482400	2.55619700
C	-4.73106400	-0.99199500	1.34233900	C	0.13272800	4.72051500	1.72670900
C	-4.99688600	-1.31604800	-0.16116200	H	1.22587000	3.96198400	0.02439500
C	-6.20115700	-2.28733500	-0.28853200	C	-0.62802600	3.06701100	3.32652400
C	-3.68563100	0.09749900	1.61965400	H	-0.14403300	1.01337700	2.87322300
C	-2.27780200	-0.30864000	1.25456200	C	-0.53833900	4.40142100	2.90896200
C	-1.55659700	0.18843700	0.22026400	H	0.20446400	5.75996800	1.39981800
C	-5.29877000	-0.06917200	-0.89314000	H	-1.14926500	2.81748000	4.25333100
N	-5.57356400	0.91800600	-1.43058100	H	-0.99269500	5.19237100	3.50970600
C	-3.82525100	-1.96290700	-0.79247700	C	2.03747700	1.73738300	-1.11523600
N	-2.94572100	-2.52996700	-1.28694800	C	1.17285900	2.12341000	-2.15485200
C	-2.00118600	1.25679300	-0.69047100	C	3.42500700	1.86734600	-1.27804200
C	-2.20358500	0.97682100	-2.05672300	C	1.69683700	2.63510100	-3.34161100
C	-2.59490900	1.97939300	-2.94288500	H	0.09340400	2.02326800	-2.04153700
C	-2.77964200	3.28786900	-2.48663600	C	3.94165900	2.37393600	-2.47343700
C	-2.59287800	3.57864000	-1.13259600	H	4.10584100	1.57202000	-0.47858900
C	-2.21324400	2.57426100	-0.24128400	C	3.08078400	2.75610200	-3.50566800
H	-5.69999700	-0.68153600	1.76232600	H	1.01764500	2.93541900	-4.14232900
H	-4.45137200	-1.93593300	1.83639900	H	5.02250200	2.47065900	-2.59672400
H	-5.98733200	-3.21065300	0.26795200	H	3.48882200	3.15047400	-4.43890100
H	-7.09764000	-1.81201000	0.13262600				
H	-3.96336500	1.01860000	1.08976900	TS-rot1			
H	-3.73629800	0.33223000	2.69650400	C	2.34603400	-3.26704700	-3.03954200
H	-2.07949100	-0.04436600	-2.41519300	C	2.23359400	-3.87028100	-1.78860800
H	-2.76839500	1.73612900	-3.99347200	C	1.95291900	-3.09384100	-0.65995800
H	-3.08592500	4.07384600	-3.18017100	C	1.75642900	-1.71239300	-0.75506600
H	-2.75023400	4.59482900	-0.76399900	C	1.80362300	-1.11156600	-2.04187200
H	-2.07709300	2.80742000	0.81427700	C	2.12537100	-1.89716100	-3.16185600
C	1.45929500	-2.30075000	-2.83486100	C	1.52907600	0.31234600	-2.29608800
C	2.63918300	-1.39438200	-3.21441200	P	1.62605200	-0.70948300	0.79245700
H	2.49876300	-1.00057200	-4.23197900	N	0.87383500	1.15375000	-1.56454900
H	2.71657800	-0.53117900	-2.53901900	C	1.04899600	2.50031800	-2.13776100
H	3.60081000	-1.93056000	-3.20357800	C	1.52646900	2.17354500	-3.56174600
C	1.35488900	-3.48856100	-3.80384000	O	2.00787700	0.81284200	-3.44499000
H	2.27085200	-4.10031300	-3.81338400	H	2.58759900	-3.86120300	-3.92284500
H	0.50764200	-4.14335800	-3.54425400	H	2.37984600	-4.94701500	-1.67933100
H	1.19545500	-3.12700600	-4.83072400	H	1.90527300	-3.57328000	0.31825300
C	0.15639400	-1.49223000	-2.88373500	H	2.18144600	-1.41849500	-4.13904400
H	-0.03256300	-1.11574900	-3.90035500	H	0.07858100	3.01859100	-2.14578600
H	-0.71373300	-2.09435100	-2.58017000	H	0.70740500	2.18168600	-4.29677300
H	0.22055200	-0.60147300	-2.23432600	H	2.35038700	2.79613500	-3.92874600
H	-6.39284700	-2.53952300	-1.34003300	Ni	0.29363100	1.07223500	0.31377800
C	0.61241400	2.37536200	1.36386700	C	-2.27253800	-0.52104800	-0.06166300

C	-1.45553400	0.45825100	0.32424200	H	6.95735100	1.19819100	1.67443600
C	-1.55138700	1.65452400	1.12827700	H	-1.11940100	4.98528000	3.11671900
C	-0.80549600	1.67434000	2.34478000	H	-0.07733900	2.90416700	3.97650300
C	-0.63939700	2.88948400	3.04041000	C	-1.87869900	-1.61599700	-0.98516300
C	-1.23143800	4.05049500	2.56269100	C	-1.46158200	-1.33407100	-2.29383000
C	-2.00989100	4.03093200	1.38265300	C	-1.97948000	-2.95773400	-0.58004600
C	-2.15698300	2.85990500	0.66390000	C	-1.14088900	-2.36799900	-3.17475700
H	-0.49191700	0.73524000	2.80213100	H	-1.40122100	-0.29283800	-2.61506600
H	-2.50268700	4.94341200	1.04143700	C	-1.64102000	-3.99037000	-1.45497400
H	-2.75153100	2.83552400	-0.25031100	H	-2.31343300	-3.19630400	0.43190600
C	2.03739600	3.32435400	-1.25712500	C	-1.22126900	-3.69772700	-2.75579900
C	3.46909400	2.77117300	-1.33560400	H	-0.82357100	-2.13498700	-4.19341600
H	3.52117400	1.71993200	-1.01896000	H	-1.70995900	-5.02831500	-1.12176900
H	3.89289600	2.85030000	-2.34708700	H	-0.96300200	-4.50582400	-3.44347800
H	4.12686000	3.34003200	-0.66164900	C	-3.70504500	-0.53417900	0.44239600
C	2.00148200	4.78549700	-1.72784500	H	-3.88568300	-1.44078100	1.04356600
H	2.30452600	4.87742600	-2.78274100	H	-3.85030400	0.32101200	1.11760900
H	0.99218400	5.21503000	-1.62555600	C	-4.72404400	-0.47858300	-0.70723900
H	2.69373900	5.40125500	-1.13418500	H	-4.91730100	-1.48315400	-1.11125000
C	1.56017500	3.25207300	0.20073900	H	-4.33452500	0.13149700	-1.53663700
H	2.17786700	3.88812500	0.85242400	C	-6.08607200	0.15004400	-0.28936700
H	0.51817900	3.57604000	0.31996200	C	-7.11467500	0.07199100	-1.44268900
H	1.73522000	2.23562400	0.64283800	H	-6.71431900	0.58673500	-2.32749500
C	1.29054500	-1.91547100	2.11812400	H	-7.30288300	-0.98120300	-1.69343900
C	2.31401200	-2.54999500	2.84040300	H	-8.06384500	0.54371800	-1.15497500
C	-0.05213500	-2.19062300	2.43021800	C	-5.83024800	1.56578600	0.05666100
C	1.99475000	-3.45657000	3.85394600	C	-6.60899700	-0.55439600	0.89904800
H	3.35941100	-2.33416400	2.61156600	N	-5.54816600	2.66972700	0.26199100
C	-0.36503700	-3.10187900	3.44040000	N	-6.99144100	-1.15469200	1.81152700
H	-0.84775800	-1.68734600	1.87930600				
C	0.65758800	-3.73586900	4.15300900	TS5			
H	2.79445000	-3.94694200	4.41350000	C	-4.02964200	0.35268300	3.74157300
H	-1.41030900	-3.31191500	3.67842700	C	-4.39583500	-0.65699500	2.85348500
H	0.41221500	-4.44416600	4.94739700	C	-3.68272500	-0.83250600	1.66453200
C	3.36639600	-0.19293100	1.05847500	C	-2.58981700	-0.01955000	1.34813800
C	3.60489600	0.73564000	2.08810900	C	-2.23445600	1.02444200	2.23905000
C	4.43651700	-0.61651000	0.25711400	C	-2.96498500	1.19538600	3.42662000
C	4.89006800	1.22684600	2.31400800	C	-1.16106300	2.00052700	1.97236800
H	2.77648800	1.07398200	2.71676300	P	-1.64036300	-0.32407800	-0.19268900
C	5.72232200	-0.11315400	0.47933800	N	-0.16053800	1.92318400	1.15233300
H	4.27233700	-1.33727000	-0.54475800	C	0.49745800	3.24721300	1.10623200
C	5.95179300	0.80760300	1.50397900	C	-0.07747700	3.92942700	2.36143000
H	5.06533300	1.94201200	3.12087400	O	-1.25159000	3.14436400	2.66114600
H	6.54903400	-0.44681500	-0.15177400	H	-4.57500900	0.49273600	4.67676100

H	-5.23759700	-1.31447200	3.08115200	H	4.18030600	-1.18010300	-1.61862400
H	-3.97762000	-1.62634200	0.97791600	C	0.22825800	3.99403100	-0.23526000
H	-2.68605800	2.00072200	4.10505500	C	-1.27578900	4.23812500	-0.43367900
H	1.58064900	3.10447600	1.20845700	H	-1.44664200	4.78963100	-1.37019900
H	0.59839900	3.87172100	3.22814600	H	-1.82791600	3.29161800	-0.51044400
H	-0.39439300	4.96812700	2.21700900	H	-1.71714300	4.83178000	0.38116500
Ni	0.51304600	0.29123900	0.15501500	C	0.98614200	5.33136500	-0.19616400
C	1.35283400	-1.54045500	-1.97998000	H	0.61905700	5.99987000	0.59779500
C	1.54445900	-0.61556200	-3.02945500	H	2.06593500	5.17558700	-0.03786800
C	0.85141700	-2.81182100	-2.30724700	H	0.86334700	5.86431000	-1.15098300
C	1.25435800	-0.95447600	-4.34895800	C	0.75782700	3.16051000	-1.41149900
H	1.92096100	0.38494400	-2.80846100	H	0.54774600	3.67308000	-2.36230400
C	0.55819600	-3.14838300	-3.63103600	H	1.84409100	3.00522900	-1.34455200
H	0.65829000	-3.54649300	-1.52617600	H	0.27171100	2.17639900	-1.45496100
C	0.75710500	-2.22606600	-4.65864500	H	1.54965700	-4.57084200	3.87904800
H	1.41702700	-0.22157400	-5.14273900	C	-2.02750700	-2.04698100	-0.66219800
H	0.16184500	-4.14116700	-3.85357400	C	-2.47348300	-2.37615400	-1.94872900
H	0.52796500	-2.49189000	-5.69266600	C	-1.77718800	-3.07549300	0.26544800
C	2.47403800	-1.88984800	1.76365300	C	-2.65889700	-3.71446400	-2.30680400
C	1.89491600	-2.57554100	3.03691700	H	-2.67297500	-1.59251900	-2.67993800
C	1.94123600	-4.12016900	2.95725000	C	-1.96538600	-4.40909100	-0.09745100
C	1.76326200	-2.29574400	0.46023800	H	-1.46759000	-2.82871300	1.28172000
C	1.62848300	-1.15924900	-0.56340100	C	-2.40064700	-4.73292100	-1.38786800
C	2.24767800	0.08527700	-0.25966500	H	-3.00684700	-3.95832700	-3.31283700
C	2.67046700	-2.11100600	4.20449000	H	-1.78151100	-5.19991400	0.63367300
N	3.31492600	-1.74525500	5.09324500	H	-2.54852900	-5.77760600	-1.67022600
C	0.49922900	-2.11466100	3.19934900	C	-2.44089800	0.72631400	-1.45566000
N	-0.59557500	-1.74162300	3.25144800	C	-1.77397600	0.90813700	-2.67936300
C	3.55576200	0.58270300	-0.51726100	C	-3.66173800	1.37714400	-1.22769200
C	3.97267100	1.84425800	-0.02229700	C	-2.32650000	1.72981500	-3.66224300
C	5.26630900	2.30062400	-0.23926600	H	-0.82495900	0.40200000	-2.86696500
C	6.16979300	1.50957600	-0.96255500	C	-4.20509400	2.20681600	-2.21211600
C	5.78382700	0.25573700	-1.45896600	H	-4.18690000	1.24439800	-0.28054000
C	4.49467300	-0.20815400	-1.23477100	C	-3.53955700	2.38546800	-3.42787900
H	2.40327100	-0.80540300	1.92806300	H	-1.80469900	1.86205800	-4.61267900
H	3.54681900	-2.12771100	1.71541300	H	-5.15387200	2.71523600	-2.02718400
H	1.33973400	-4.47176000	2.10828000	H	-3.96745700	3.03503500	-4.19465200
H	2.98245800	-4.44387900	2.81945700				
H	2.32068700	-3.11839700	-0.01649600	TS5'			
H	0.76288700	-2.70298100	0.67166000	C	2.22478300	0.72086800	4.60100200
H	3.26376300	2.44088700	0.54919000	C	2.26374500	1.95165400	3.94892600
H	5.58185500	3.26916000	0.15339700	C	2.15590900	2.01275600	2.55462100
H	7.18626700	1.87059600	-1.13624500	C	1.99106800	0.85428400	1.78982900
H	6.49775900	-0.35380500	-2.01646400	C	1.87865200	-0.39405000	2.46554100

C	2.02693300	-0.44526200	3.85974500	H	-5.85879700	0.16452300	3.38418300
C	1.50301700	-1.64706300	1.78087100	H	-4.57134500	1.02235400	4.28860100
P	1.85606000	0.91695500	-0.04574800	H	-1.41177300	-0.00753500	1.99521000
N	0.86754600	-1.74855800	0.66160500	H	-1.70702900	-1.72696600	1.83023600
C	0.58342700	-3.17057200	0.39197100	H	-3.99040500	0.81510900	-1.92403700
C	1.10388500	-3.85985500	1.67739800	H	-4.90881500	2.87299400	-2.93639200
O	1.74449600	-2.79241400	2.42308600	H	-3.70907400	5.04233500	-2.67337300
H	2.32968800	0.66496200	5.68614100	H	-1.57460700	5.14407700	-1.38275900
H	2.38609900	2.87466400	4.51949100	H	-0.62700700	3.06456600	-0.40740900
H	2.19975200	2.98374700	2.06257600	C	1.18862600	-3.67177400	-0.94522900
H	1.96100400	-1.41212200	4.35915700	C	2.72213800	-3.67504800	-0.89599100
H	-0.50902600	-3.27766800	0.30754600	H	3.13170500	-3.93318900	-1.88365700
H	0.30103300	-4.27005800	2.30623100	H	3.11720400	-2.68903100	-0.62273400
H	1.85350500	-4.63954000	1.49895400	H	3.11581900	-4.41437700	-0.18184100
Ni	-0.08881400	-0.17619400	-0.21276000	C	0.65723000	-5.09271400	-1.19317200
C	-2.69201100	-1.66196300	-0.81086800	H	0.95160400	-5.78842800	-0.39056200
C	-2.72590100	-1.55205700	-2.21767200	H	-0.44218900	-5.09888000	-1.26717400
C	-3.19980300	-2.84461600	-0.23909200	H	1.06126200	-5.49287100	-2.13538300
C	-3.25997200	-2.56387300	-3.01011100	C	0.70533700	-2.75032700	-2.07541300
H	-2.30050500	-0.67064700	-2.70034100	H	1.07637600	-3.11071000	-3.04683700
C	-3.72698600	-3.86474100	-1.03582900	H	-0.39221900	-2.71822700	-2.12449900
H	-3.18522300	-2.98734900	0.84112800	H	1.08081100	-1.72468300	-1.94107200
C	-3.76533600	-3.73032100	-2.42421600	H	-5.69837800	1.93898600	3.24414700
H	-3.27212200	-2.44774700	-4.09615200	C	2.29846500	2.58847800	-0.63420200
H	-4.11576000	-4.76920200	-0.56234500	C	3.42671500	3.28088900	-0.15942200
H	-4.18182800	-4.52538900	-3.04577400	C	1.59296000	3.09699200	-1.73457800
C	-3.45389900	-0.59067800	2.27613200	C	3.79802300	4.49343700	-0.73933000
C	-4.17251700	0.79055200	2.15675200	H	4.03024500	2.86515600	0.64944100
C	-5.14286800	0.99769300	3.35035900	C	1.97406200	4.30720300	-2.32034000
C	-2.10557500	-0.73804800	1.55472900	H	0.75003500	2.53760800	-2.14178800
C	-2.06200500	-0.60524300	0.01997000	C	3.06788700	5.01249300	-1.81509700
C	-1.63707700	0.63473500	-0.52102500	H	4.66990300	5.03080100	-0.35995800
C	-3.16820800	1.87295500	2.14526800	H	1.41507100	4.69471600	-3.17486300
N	-2.33060500	2.67122200	2.17379800	H	3.36490500	5.96068200	-2.26860400
C	-4.96477700	0.82342700	0.91327100	C	3.32458800	-0.01549000	-0.63732800
N	-5.65140900	0.78377900	-0.01707500	C	3.41963200	-0.24426500	-2.01951100
C	-2.20957000	1.78613100	-1.13625800	C	4.36058000	-0.43976100	0.20525700
C	-3.44912600	1.75332800	-1.82629100	C	4.53347500	-0.89445600	-2.55025200
C	-3.96330000	2.91278600	-2.39237300	H	2.62309900	0.09514200	-2.68651500
C	-3.28781500	4.13149100	-2.24154400	C	5.47349400	-1.09521700	-0.33048700
C	-2.08505900	4.18971000	-1.52644400	H	4.30941000	-0.26080500	1.28020300
C	-1.54000200	3.02762800	-0.99676600	C	5.56194100	-1.32439100	-1.70552100
H	-3.26411500	-0.75680100	3.34806600	H	4.59867000	-1.06809500	-3.62656000
H	-4.17434400	-1.35510300	1.95389700	H	6.27680900	-1.42405800	0.33250800

H	6.43314800	-1.83583700	-2.12025500	C	1.58126400	1.89312000	0.73673500
INT6				C	0.85967500	2.50195500	-0.33610500
				C	0.15814800	3.71028700	-0.13564600
C	-2.96971300	-3.35166800	-2.87749800	C	0.18717300	4.32693500	1.10362200
C	-3.51159700	-2.12480500	-3.26069800	C	0.92150500	3.75073000	2.16738100
C	-3.21882200	-0.97010600	-2.52755400	C	1.58951400	2.55320300	2.00056500
C	-2.37839600	-1.02215000	-1.41092900	H	4.37920700	-2.88638600	-1.20279000
C	-1.83596900	-2.27112000	-1.01807400	H	4.47343100	-1.17164300	-1.62330700
C	-2.14311100	-3.42558300	-1.75616800	H	2.50429300	-2.74527300	-4.40533900
C	-0.98618200	-2.44478000	0.17441400	H	3.92478600	-1.73199700	-4.00921300
P	-1.98303100	0.50295600	-0.47324300	H	2.34820500	-2.07613500	0.36849000
N	-0.22562700	-1.57620700	0.77195700	H	4.02067000	-2.00326300	0.90655200
C	0.28359800	-2.19927700	2.02510700	H	0.94027000	2.07835200	-1.33982000
C	0.01524000	-3.68749600	1.74405500	H	-0.38841600	4.15577300	-0.96874400
O	-1.00592400	-3.65657500	0.71980700	H	-0.34284400	5.26884500	1.26067700
H	-3.19019100	-4.25540800	-3.44887800	H	0.95708300	4.26014800	3.13328500
H	-4.16504000	-2.05943000	-4.13338600	H	2.14263200	2.10098400	2.82489800
H	-3.64512100	-0.01385200	-2.83402700	C	-0.39361400	-1.63913200	3.30947900
H	-1.70925600	-4.37606900	-1.44780300	C	-1.91036700	-1.87765100	3.29376800
H	1.35817400	-1.99463000	2.10373600	H	-2.38887700	-1.36940300	2.44652400
H	0.88401100	-4.21075700	1.31924900	H	-2.16504200	-2.94709900	3.24347600
H	-0.38023500	-4.25225800	2.59434800	H	-2.36489800	-1.47476200	4.21109500
Ni	0.11581300	0.23883700	0.24434200	C	0.24203800	-2.34538300	4.51951100
C	4.44771700	0.69459300	0.35969300	H	0.04233600	-3.42786500	4.52857500
C	4.52843100	1.90113000	-0.35833100	H	1.33422900	-2.19938500	4.54059800
C	5.59964700	0.23979900	1.02739900	H	-0.16781600	-1.93315900	5.45377800
C	5.71404100	2.63604800	-0.39456500	C	-0.10780000	-0.13641900	3.41827800
H	3.65601100	2.25680400	-0.90704200	H	-0.53910200	0.27011300	4.34546600
C	6.78357500	0.97905400	0.99829200	H	0.97389600	0.06090600	3.42565900
H	5.56963300	-0.69108200	1.59753700	H	-0.54743800	0.41933500	2.57886000
C	6.84580800	2.18041100	0.28726100	H	3.90405600	-3.46184000	-3.55304400
H	5.75596600	3.56743400	-0.96401500	C	-2.35836800	1.88008200	-1.60915200
H	7.66192800	0.61510100	1.53633400	C	-3.34846600	2.82895600	-1.31950500
H	7.77361000	2.75601400	0.26060100	C	-1.56712500	2.02585400	-2.76307200
C	3.80200500	-1.95018600	-1.23121900	C	-3.54033100	3.92041400	-2.17265500
C	2.67792700	-2.18661400	-2.28510900	H	-3.96918200	2.72280900	-0.42884000
C	3.28921200	-2.55760400	-3.66036400	C	-1.77011800	3.11290700	-3.61258500
C	3.30853400	-1.58229000	0.18051200	H	-0.78848000	1.29498800	-2.98886900
C	3.17689600	-0.08996700	0.40191300	C	-2.75258300	4.06574200	-3.31657400
C	1.98867900	0.50921200	0.55817500	H	-4.31257600	4.65728100	-1.94106400
C	1.80818300	-3.28430200	-1.81217900	H	-1.15479500	3.22060300	-4.50864100
N	1.15357500	-4.14985500	-1.41020200	H	-2.90481000	4.91922800	-3.98094400
C	1.81002100	-1.00210700	-2.45372000	C	-3.22087400	0.60601900	0.85959000
N	1.11050300	-0.09557300	-2.61607400	C	-2.97613000	1.52170800	1.89797400

C	-4.36084200	-0.20786500	0.90259000
C	-3.86748700	1.62088400	2.96589800
H	-2.08620400	2.15631100	1.86895300
C	-5.24492600	-0.11162300	1.98082200
H	-4.55564900	-0.92303500	0.10142700
C	-4.99953400	0.79944200	3.01145400
H	-3.67545700	2.33495300	3.76972200
H	-6.12906300	-0.75185700	2.01485800
H	-5.69184100	0.87073000	3.85318500

INT6'

C	-4.30667500	2.86005900	-2.68759600
C	-3.41517400	3.73872600	-2.07352600
C	-2.42799400	3.24839500	-1.21132800
C	-2.30359600	1.87750100	-0.96331400
C	-3.20390800	0.98482400	-1.60019100
C	-4.20322900	1.48961300	-2.44610800
C	-3.13778400	-0.47411400	-1.41617500
P	-1.06949400	1.27721800	0.26698600
N	-2.13202000	-1.15743900	-0.98141600
C	-2.51483500	-2.58323600	-0.90000800
C	-3.89595700	-2.58380800	-1.59492100
O	-4.21920800	-1.17900300	-1.74795500
H	-5.08346600	3.23731000	-3.35541200
H	-3.48797600	4.81330700	-2.25425000
H	-1.75077700	3.94755400	-0.71968400
H	-4.89456300	0.79214900	-2.91924300
H	-1.78718000	-3.16252200	-1.48815800
H	-3.87306500	-3.03285500	-2.59785800
H	-4.69687300	-3.04881600	-1.00834900
Ni	-0.33457200	-0.55171900	-0.56762900
C	3.91200100	0.26132800	-0.63692700
C	4.39619100	-0.81243100	-1.40314800
C	4.72802200	1.39788600	-0.48213200
C	5.65202900	-0.74528500	-2.00919400
H	3.79329100	-1.71492700	-1.50149300
C	5.98043000	1.46621900	-1.09502100
H	4.37149100	2.24607900	0.10622100
C	6.44715600	0.39455300	-1.86175200
H	6.01461400	-1.59331200	-2.59474900
H	6.59506900	2.36140500	-0.97401800
H	7.42938300	0.44560600	-2.33671600
C	3.43464900	-0.15454900	2.35658200
C	3.02726600	-1.62497700	2.67756600

C	4.12985600	-2.30299000	3.53406400
C	2.48871500	0.64573200	1.44930500
C	2.56230500	0.22363500	-0.00159000
C	1.49035000	-0.19494400	-0.68672600
C	1.75746700	-1.62891100	3.43298300
N	0.77361700	-1.61398700	4.04227500
C	2.80302100	-2.44796400	1.46882500
N	2.62486300	-3.15116200	0.56752300
C	1.33445400	-0.72870900	-2.03983900
C	0.94177100	-2.09126300	-2.14910800
C	0.50129700	-2.60787900	-3.37986700
C	0.45786800	-1.79041100	-4.50290700
C	0.86582500	-0.44429700	-4.41237300
C	1.28569100	0.08523700	-3.20296300
H	3.52802000	0.34920200	3.33061000
H	4.44121200	-0.18600200	1.91399200
H	3.84738000	-3.33034900	3.79997100
H	5.06724300	-2.32643000	2.96141500
H	1.45546100	0.56290100	1.81102100
H	2.76105300	1.70867500	1.54946100
H	1.09049400	-2.75185400	-1.29149300
H	0.22337900	-3.66179000	-3.45508300
H	0.12748500	-2.19282600	-5.46301800
H	0.85040300	0.18543100	-5.30493900
H	1.59807300	1.12869500	-3.13092300
C	-2.47985600	-3.11656500	0.55824100
C	-3.47422600	-2.35242900	1.44419900
H	-3.25695900	-1.27648900	1.45975300
H	-4.51525200	-2.49040500	1.11366000
H	-3.41167200	-2.71320900	2.48131200
C	-2.83151700	-4.61256700	0.52916800
H	-3.85132500	-4.79209800	0.15371700
H	-2.12928400	-5.17774000	-0.10465400
H	-2.77969900	-5.03421900	1.54412700
C	-1.05506500	-2.95256100	1.11115700
H	-0.99098500	-3.32123100	2.14525800
H	-0.31687000	-3.50588100	0.51203200
H	-0.75297100	-1.88980600	1.14958300
H	4.28526000	-1.72404700	4.45493700
C	0.04444200	2.68963800	0.55038400
C	0.07341000	3.37114800	1.77506200
C	0.93555800	3.05655800	-0.47209600
C	0.99609700	4.40197200	1.97781600
H	-0.61613800	3.09411400	2.57383600

C	1.84888800	4.08907700	-0.26788500	C	-5.70012700	1.08202700	-1.39696100
H	0.91874700	2.52668800	-1.42468900	H	-4.02924200	-0.19309900	-1.87903500
C	1.88565700	4.75868200	0.96152600	C	-6.25838100	1.96743000	-0.47122000
H	1.01716400	4.92759600	2.93488300	H	-5.98499500	2.96647000	1.42793800
H	2.54048500	4.36696800	-1.06601100	H	-6.24712400	0.82513300	-2.30700600
H	2.60689700	5.56277000	1.12375500	H	-7.23914300	2.41093800	-0.65619100
C	-2.04619700	1.08019300	1.79407400	C	-3.17892900	-1.41230700	2.02235700
C	-1.47120800	0.35210700	2.84636900	C	-3.01226400	-2.80972300	1.35377000
C	-3.34403600	1.59514300	1.93490800	C	-4.19768600	-3.73100800	1.74632900
C	-2.17636400	0.14301200	4.03039100	C	-2.13986600	-0.34893000	1.64202500
H	-0.47471400	-0.07420300	2.74673000	C	-2.37438200	0.24890700	0.27110700
C	-4.05184400	1.37634700	3.11975400	C	-1.42388700	0.30013600	-0.66458700
H	-3.80672000	2.16101900	1.12511300	C	-2.93647000	-2.74249800	-0.12180600
C	-3.47155800	0.65249000	4.16625000	N	-2.88116300	-2.76098100	-1.27707200
H	-1.70718100	-0.43435100	4.82911300	C	-1.74923200	-3.42672400	1.80797000
H	-5.06352000	1.77434900	3.22477200	N	-0.77147700	-3.91826500	2.18374800
H	-4.03292500	0.48241900	5.08767200	C	-1.34065000	0.69419300	-2.06631100
TS-rot2				C	-0.88237300	1.98174600	-2.45576400
C	1.23353100	-0.98132600	4.60000200	C	-0.65886800	2.26916200	-3.79703600
C	1.16430900	0.40855600	4.51612800	C	-0.87115700	1.28234500	-4.77311400
C	1.19535900	1.03632000	3.26694600	C	-1.31663000	0.00928300	-4.40920500
C	1.27667400	0.29706300	2.08069900	C	-1.55385100	-0.29129800	-3.06597900
C	1.33200400	-1.12069700	2.17039400	H	-4.19210800	-1.05534400	1.78617700
C	1.32579800	-1.73828500	3.43237800	H	-3.14660900	-1.59313900	3.10733000
C	1.38145000	-2.02873100	1.00660000	H	-4.07938200	-4.73365600	1.31427400
P	1.35409200	1.19087800	0.46557900	H	-4.24701100	-3.81600100	2.84072700
N	0.86126300	-1.85352500	-0.16457200	H	-2.18138600	0.44248800	2.40952900
C	1.29663100	-2.96912100	-1.02612400	H	-1.12956700	-0.76840600	1.70080200
C	1.76040600	-4.00154300	0.01571400	H	-0.72213600	2.74080100	-1.68902700
O	2.01483900	-3.18917300	1.18934200	H	-1.48851300	-0.75085100	-5.17416800
H	1.21615600	-1.48024700	5.57090200	H	-1.92795400	-1.27193800	-2.76634200
H	1.09506100	1.01401300	5.42259100	C	2.38645300	-2.47726600	-2.02916400
H	1.15914900	2.12495200	3.21671800	C	3.71751500	-2.17095500	-1.32415700
H	1.36363100	-2.82583100	3.47918500	H	3.59871000	-1.42119000	-0.53019000
H	0.43099700	-3.33441300	-1.59802600	H	4.17299500	-3.06970700	-0.88480400
H	0.97075300	-4.71824500	0.28133800	H	4.43831900	-1.76025300	-2.04690700
H	2.68338400	-4.53590100	-0.23456300	C	2.58762000	-3.56803300	-3.09133200
Ni	0.31150200	-0.14808700	-1.00718400	H	2.90867100	-4.51751100	-2.63476900
C	-3.72699800	0.82306200	0.00315100	H	1.65836900	-3.75926300	-3.65122700
C	-4.30475800	1.70566100	0.93518700	H	3.36459500	-3.27151000	-3.81212000
C	-4.44646300	0.51356700	-1.16246500	C	1.89120100	-1.19420700	-2.71462500
C	-5.55636200	2.27629700	0.69749800	H	2.59549700	-0.87015000	-3.49555500
H	-3.76604000	1.96086500	1.85084300	H	0.90870900	-1.31615100	-3.18787400
				H	1.90188600	-0.31718500	-2.01674500

H	-5.13416600	-3.29040700	1.37749700	H	0.44478300	-4.75535300	-0.93936000
C	0.89650000	2.91185000	0.87329200	Ni	0.03932200	0.25531400	-0.33223900
C	1.85876700	3.91922200	1.04610300	C	-4.33668500	-0.09823600	-0.37174200
C	-0.46837100	3.23303800	0.99366900	C	-5.24304500	-0.74306400	-1.23303000
C	1.46001100	5.22693400	1.33643300	C	-4.78429500	0.27568100	0.90711900
H	2.92042600	3.68391800	0.95572200	C	-6.54860400	-1.02190400	-0.82315700
C	-0.85956700	4.53923400	1.28881900	H	-4.92106100	-1.05419000	-2.22998100
H	-1.22471000	2.46191800	0.84626200	C	-6.09071100	0.00558600	1.31395500
C	0.10357800	5.53942500	1.45936500	H	-4.10568500	0.79691100	1.58134900
H	2.21536000	6.00476900	1.46876800	C	-6.97728600	-0.64777000	0.45309900
H	-1.92206600	4.77691200	1.37744500	H	-7.23287400	-1.53459100	-1.50331900
H	-0.20372500	6.56286800	1.68529300	H	-6.41972400	0.31426600	2.30874300
C	3.14933600	1.25058200	0.10944600	H	-7.99988600	-0.85969800	0.77322400
C	3.54171100	1.71776000	-1.15802000	C	-3.31239700	2.32897800	-2.20858500
C	4.12632700	0.80125200	1.00957200	C	-2.60930900	3.36519200	-1.24151100
C	4.88915200	1.73688900	-1.51626000	C	-2.53797100	4.77262000	-1.86944800
H	2.78576800	2.06913500	-1.86575300	C	-2.80942100	0.87261900	-2.15734400
C	5.47535800	0.81197800	0.64242900	C	-2.93447600	0.17847300	-0.81300800
H	3.83820900	0.43752600	1.99684500	C	-1.86123800	-0.14565700	-0.05634100
C	5.85871100	1.27683300	-0.61776500	C	-3.31582200	3.42755100	0.05448000
H	5.18529900	2.10694300	-2.50037500	N	-3.86540400	3.50222400	1.07011800
H	6.22983900	0.45643200	1.34762000	C	-1.28617100	2.79638800	-0.91472100
H	6.91343600	1.28299200	-0.90114400	N	-0.51390100	1.98663900	-0.62966100
H	-0.69186800	1.51532200	-5.82536600	C	-1.92459800	-0.86076900	1.23472700
H	-0.31677900	3.26346000	-4.09151800	C	-1.29458600	-0.32016000	2.37326900
INT7				C	-1.22563600	-1.03622300	3.56857700
C	2.87893400	-1.91345700	3.95284200	C	-1.78146300	-2.31607000	3.65290000
C	3.44579300	-0.64345800	3.84952500	C	-2.42405800	-2.86200300	2.53618700
C	3.25128500	0.12120200	2.69336200	C	-2.49892500	-2.14211000	1.34312400
C	2.47922900	-0.36561700	1.63419000	H	-4.38777700	2.37067000	-1.98178100
C	1.90299800	-1.65468800	1.74402600	H	-3.17513600	2.71171900	-3.23088100
C	2.11602500	-2.41921800	2.89948400	H	-2.08796700	5.49538600	-1.17527100
C	1.08384100	-2.24283600	0.67282700	H	-1.94226900	4.73696300	-2.79241100
P	2.22178300	0.64817500	0.12030400	H	-3.40080500	0.32818200	-2.91101300
N	0.44419900	-1.62161900	-0.26425100	H	-1.76964900	0.83095400	-2.50559600
C	-0.17361400	-2.62195700	-1.16479000	H	-0.86070500	0.68130700	2.31723000
C	0.01858900	-3.92607900	-0.36408900	H	-0.73399600	-0.59379800	4.43796700
O	0.97583000	-3.56797500	0.66491200	H	-1.72571700	-2.88082900	4.58602800
H	3.02764800	-2.51286300	4.85301100	H	-2.87926100	-3.85350100	2.59975200
H	4.04548300	-0.24004900	4.66828200	H	-3.01731600	-2.56506600	0.48017900
H	1.66302600	-3.40796200	2.96773600	C	0.45220500	-2.61523100	-2.58665800
H	-1.23964500	-2.37404200	-1.25880300	C	1.94831800	-2.95759100	-2.53783400
H	-0.89859300	-4.25563400	0.14170300	H	2.13318800	-3.95987600	-2.12207000
				H	2.37339200	-2.94348000	-3.55249300

H	2.50917300	-2.22863400	-1.93877500	C	0.44010800	-1.98914600	1.97367500
C	-0.30240700	-3.64847200	-3.43953200	C	0.27763100	-3.51262500	1.80236200
H	0.07828800	-3.64005000	-4.47202000	O	-0.75477200	-3.64299400	0.79196100
H	-0.18042000	-4.67381000	-3.05712600	H	-3.10591000	-4.51141600	-3.27474800
H	-1.38092800	-3.42538700	-3.47685100	H	-4.22784300	-2.39871000	-3.99142700
C	0.26108400	-1.22558400	-3.21026500	H	-1.58433800	-4.48956600	-1.29991500
H	0.75964300	-0.44673100	-2.61409100	H	1.49515700	-1.69629200	1.88952300
H	0.69257700	-1.19619400	-4.22222700	H	1.18257400	-3.99616400	1.41056000
H	-0.80592900	-0.97089900	-3.28764700	H	-0.06740900	-4.03854900	2.69923000
H	-3.55520300	5.10663100	-2.11550500	Ni	0.04393800	0.26608700	0.03124300
C	2.69702300	2.33570800	0.61364000	C	4.41214900	0.17542300	-0.04699000
C	3.91170000	2.91693000	0.22157000	C	5.41410400	-0.10535400	0.89823600
C	1.80613700	3.06417400	1.42168300	C	4.74825300	0.12065400	-1.41076100
C	4.23036400	4.21361900	0.63552200	C	6.70478900	-0.45145800	0.49292200
H	4.61022700	2.35850000	-0.40383700	H	5.17876000	-0.07488000	1.96518400
C	2.13398400	4.35318700	1.84018300	C	6.04006000	-0.21572000	-1.81757600
H	0.85755300	2.61928700	1.73038500	H	3.98147800	0.33961200	-2.15595300
C	3.34582900	4.93096700	1.44450500	C	7.02248000	-0.50731000	-0.86707100
H	5.17718300	4.66204900	0.32681900	H	7.46595400	-0.67959400	1.24270800
H	1.44150200	4.91089300	2.47455600	H	6.28137000	-0.25069000	-2.88252600
H	3.59970800	5.94259000	1.76867700	H	8.03303500	-0.77382500	-1.18441200
C	3.49323000	0.08342200	-1.05433000	C	3.31928500	3.06772000	0.65076700
C	4.51219600	-0.80962800	-0.69407100	C	2.08338000	3.94512300	0.23532200
C	3.40513600	0.54098100	-2.38030500	C	2.45825700	5.01460600	-0.81003700
C	5.42932400	-1.24514900	-1.65457700	C	2.96540700	1.72184500	1.33480700
H	4.58844000	-1.17133400	0.33264800	C	3.02373000	0.53619900	0.38189900
C	4.32844900	0.11087200	-3.33262000	C	1.94858100	-0.11550500	-0.11279400
H	2.61022900	1.23407200	-2.66726100	C	1.06924500	2.98838900	-0.24891700
C	5.33836800	-0.78796400	-2.97166500	N	0.47834000	2.00359200	-0.36517500
H	6.21869000	-1.94451400	-1.37085300	C	1.49397300	4.57010200	1.43834800
H	4.25707600	0.47118600	-4.36114600	N	1.04400000	5.04419400	2.39349400
H	6.05591300	-1.13170200	-3.71982500	C	2.02133000	-1.29774200	-0.99818100
H	3.70423700	1.11077200	2.62018100	C	1.30396200	-1.32135500	-2.21142600
INT8				C	1.23920500	-2.47643200	-2.99105800
C	-2.93299600	-3.58236600	-2.72820300	C	1.89034700	-3.64148200	-2.57496100
C	-3.55824700	-2.40174400	-3.12866100	C	2.62155100	-3.63135000	-1.38212800
C	-3.33256700	-1.21351300	-2.42432700	C	2.68907700	-2.47395900	-0.60523500
C	-2.47297300	-1.18672800	-1.32185300	H	3.90990000	2.88082900	-0.25816200
C	-1.83750700	-2.38685000	-0.91951000	H	3.93055800	3.70306100	1.30816200
C	-2.08126500	-3.57501100	-1.62275100	H	3.25049000	5.65472400	-0.39833100
C	-0.92865400	-2.44727500	0.23650100	H	2.83431500	4.52572800	-1.71957600
P	-2.16983900	0.37990700	-0.40890800	H	3.69234000	1.56021200	2.14404300
N	-0.26849700	-1.47551600	0.77819500	H	1.98477500	1.78758700	1.82531700
				H	0.79183400	-0.41553100	-2.54606200

H	0.67576700	-2.46806900	-3.92695700	C	3.00924700	-0.67371300	-3.93902600
H	1.83817600	-4.54866000	-3.18080500	C	2.99960000	-0.91286400	-2.56011800
H	3.14984200	-4.53172900	-1.05879300	C	2.20994800	-0.14002600	-1.70403500
H	3.27130000	-2.46905100	0.31843100	C	1.42204000	0.90007100	-2.25459300
C	-0.11997400	-1.40326700	3.29927800	C	1.45296400	1.14337100	-3.63515200
C	-1.59909200	-1.76973100	3.48813400	C	0.57623100	1.76791400	-1.42177300
H	-2.22028300	-1.36822000	2.67723300	P	2.21804800	-0.45024100	0.11101000
H	-1.75636800	-2.85821900	3.53575500	N	0.11262200	1.52520000	-0.23801700
H	-1.97688000	-1.34510700	4.43008600	C	-0.57369200	2.73941900	0.26298800
C	0.71942700	-1.96823900	4.45723900	C	-0.70164800	3.57052400	-1.02871000
H	0.62404600	-3.06149700	4.54775600	O	0.24176000	2.95000400	-1.93721100
H	1.78763200	-1.72860900	4.33108800	H	2.24546900	0.54847300	-5.55138300
H	0.38895900	-1.53361300	5.41265000	H	3.62735800	-1.29604000	-4.58975400
C	0.03575900	0.12359100	3.27658500	H	0.84327200	1.94968800	-4.04156700
H	-0.51461300	0.57114700	2.43598200	H	-1.56438300	2.44323400	0.63135500
H	-0.35924000	0.56520900	4.20370400	H	-1.69946700	3.50286200	-1.48586500
H	1.09335600	0.41051300	3.18775500	H	-0.42075900	4.62383800	-0.92304600
H	1.59380200	5.64260100	-1.06525700	Ni	0.02893800	-0.19542400	0.61489700
C	-2.74583000	1.69001100	-1.53489300	C	-4.33471600	0.28855700	0.15771500
C	-3.97176200	2.34662600	-1.35323700	C	-5.14078700	1.40754200	0.44155700
C	-1.92455700	2.03823900	-2.62144400	C	-4.81597700	-0.66514100	-0.75693100
C	-4.37143600	3.33938600	-2.25253300	C	-6.37933200	1.57730700	-0.17957700
H	-4.61485800	2.08370100	-0.51168500	H	-4.78939500	2.16948300	1.14164100
C	-2.33308900	3.02187200	-3.52136400	C	-6.05891200	-0.50027700	-1.36816400
H	-0.96595300	1.53458200	-2.76554100	H	-4.22493400	-1.55289400	-0.97419600
C	-3.55645700	3.67599000	-3.33602900	C	-6.84379200	0.62179600	-1.08710500
H	-5.32609900	3.84911800	-2.10568300	H	-6.98402200	2.45825300	0.04794600
H	-1.69488500	3.28306500	-4.36842300	H	-6.41922900	-1.25973900	-2.06569200
H	-3.87321900	4.45040400	-4.03806700	H	-7.81612000	0.74808300	-1.56841400
C	-3.33610600	0.36286200	0.98797700	C	-3.24960200	-0.90790700	3.06724100
C	-3.17803000	1.34668400	1.97943500	C	-2.44916900	-2.16288800	2.58585500
C	-4.34152200	-0.60501600	1.12186300	C	-2.92855300	0.38403700	2.29961100
C	-4.01968600	1.36071300	3.09112200	C	-2.99633500	0.16382500	0.80437600
H	-2.39400700	2.10213800	1.88306600	C	-1.88193200	-0.23242500	0.15677400
C	-5.17652000	-0.59134800	2.24252500	C	-1.10275600	-1.79502500	2.08871200
H	-4.47072100	-1.37321800	0.35752400	N	0.05166900	-1.72685900	1.89695100
C	-5.01628400	0.38770400	3.22641400	C	-1.74296100	-0.61423400	-1.25702400
H	-3.89387600	2.12828400	3.85773700	C	-1.17506900	-1.85683400	-1.60150500
H	-5.95578400	-1.34948800	2.34588800	C	-0.90536800	-2.17890700	-2.93416500
H	-5.66954200	0.39414800	4.10162600	C	-1.20550500	-1.27017800	-3.94999200
H	-3.83022000	-0.29623500	-2.74198800	C	-1.79318200	-0.04095400	-3.62522100
				C	-2.05187400	0.28698300	-2.29711900
				H	-4.31705300	-1.15812400	2.98240000
				H	-3.02784700	-0.76588300	4.13548600
TS7							
C	2.23884100	0.35648000	-4.47680500				

H	-3.62726600	1.16080900	2.64073100	H	-1.74064500	-4.07944900	3.40904500
H	-1.91734100	0.71154100	2.57573300	H	-1.67975400	-2.70514600	4.55798500
H	-0.97397600	-2.58841600	-0.81692000	H	-3.25020900	-3.45302300	4.13434300
H	-0.46555300	-3.14857700	-3.17772600	C	-3.12621000	-2.85017800	1.46946500
H	-0.99289700	-1.51936600	-4.99154100	N	-3.64367400	-3.45120800	0.62687400
H	-2.04951900	0.66725100	-4.41678200	TS8			
H	-2.51479200	1.24326500	-2.04800000				
C	0.20044100	3.43289800	1.41981100	C	-2.01502400	-3.02820700	3.58923300
C	1.58985600	3.89666800	0.95792900	C	-2.89720600	-3.31427800	2.54777300
H	2.21125500	3.05119800	0.63693100	C	-2.92939400	-2.49878800	1.41125900
H	1.53521000	4.61865700	0.12909400	C	-2.07520100	-1.39809200	1.29375800
H	2.11716200	4.39201100	1.78658500	C	-1.17646000	-1.11245200	2.34987900
C	-0.63066900	4.63793300	1.89060700	C	-1.16377500	-1.92779600	3.49188600
H	-0.73704700	5.40441200	1.10730000	C	-0.25786800	0.03672800	2.31977500
H	-1.64120000	4.32969700	2.20457500	P	-2.12055600	-0.34058300	-0.20767100
H	-0.14478100	5.12056100	2.75196800	N	0.13876900	0.72761700	1.29777100
C	0.35241500	2.44902300	2.58908400	C	0.93546200	1.87930000	1.79318700
H	0.85557100	1.52424400	2.27330400	C	1.21829800	1.45204300	3.24470600
H	0.95516300	2.89814500	3.39243200	O	0.23460800	0.42021300	3.49753000
H	-0.62646100	2.18434000	3.01532400	H	-1.98754100	-3.65965000	4.47931300
C	2.94936100	-2.10813300	0.28658800	H	-3.56886100	-4.17282100	2.61489100
C	4.25387900	-2.30514900	0.76182100	H	-0.47224600	-1.69258400	4.30037300
C	2.16484400	-3.21828200	-0.07051600	H	1.86759900	1.92518500	1.21772000
C	4.76699900	-3.60061900	0.87503700	H	2.21499700	1.00457300	3.37623300
H	4.87209400	-1.45046800	1.04066300	H	1.07369700	2.24223800	3.98887800
C	2.68482000	-4.50723900	0.03538000	Ni	0.03343700	0.14852600	-0.54975300
H	1.15084100	-3.06956500	-0.44424400	C	4.41934700	-0.13879700	-0.19873700
C	3.98634500	-4.70053300	0.51210000	C	5.28633800	0.58080600	0.64304600
H	5.78364900	-3.74837000	1.24576100	C	4.80279900	-1.42351000	-0.62008700
H	2.07222300	-5.36535200	-0.24986700	C	6.49216400	0.02236800	1.07046900
H	4.39110800	-5.71111700	0.60057000	H	5.00869900	1.58269600	0.98071900
C	3.45554900	0.71162900	0.77396400	C	6.01517400	-1.97457100	-0.20532500
C	3.53548300	0.85108600	2.17009200	H	4.14770600	-1.98947800	-1.28333200
C	4.29409800	1.47656000	-0.04913500	C	6.86080200	-1.25721900	0.64617000
C	4.44350300	1.74716200	2.73364400	H	7.14852700	0.59050700	1.73346200
H	2.88614900	0.25509700	2.81618700	H	6.30321800	-2.96980100	-0.55118700
C	5.19633500	2.37930500	0.52028300	H	7.80816500	-1.69154700	0.97269300
H	4.24107500	1.37439500	-1.13421000	C	3.11219800	1.65393400	-2.77209300
C	5.27082000	2.51715500	1.90864900	C	1.68611600	1.33938800	-3.26942200
H	4.50359100	1.84960300	3.81936300	C	1.70381400	0.77593300	-4.70862400
H	5.84435500	2.97628700	-0.12504200	C	3.18529700	1.83514100	-1.25044500
H	5.97630400	3.22430700	2.35030600	C	3.12325200	0.46592700	-0.61594800
H	3.61429800	-1.71411400	-2.14829900	C	1.96710600	-0.22600900	-0.57039000
C	-2.25906300	-3.17383100	3.75076200	C	0.88731100	0.37498000	-2.40852500

N	-0.13202200	-0.26148800	-2.45983000	H	-4.89643500	-3.52346700	-4.04894100
C	0.88113600	2.57947400	-3.22752700	C	-3.20491400	1.06023000	0.20720000
N	0.24177000	3.54323000	-3.17345000	C	-3.20342100	2.16399700	-0.66246900
C	1.76470000	-1.59732500	-0.05688100	C	-4.02031000	1.06993700	1.34779800
C	1.22091800	-2.62927300	-0.84835000	C	-4.00995800	3.26839700	-0.38779200
C	0.95998800	-3.88754600	-0.29891000	H	-2.56983400	2.16391400	-1.55292700
C	1.23694300	-4.14392000	1.04499400	C	-4.82147500	2.18175600	1.62026400
C	1.79755200	-3.13508500	1.83750400	H	-4.02748400	0.21515100	2.02642100
C	2.05156900	-1.87851100	1.29671800	C	-4.81553600	3.28013100	0.75602200
H	3.78101800	0.83541300	-3.07886900	H	-4.00431900	4.12451200	-1.06574200
H	3.44807800	2.56152500	-3.29465300	H	-5.45263400	2.18908400	2.51149900
H	2.21952100	1.48356900	-5.37289500	H	-5.44154700	4.14837600	0.97316200
H	2.24516300	-0.18048300	-4.71744000	H	-3.62673400	-2.72599600	0.60418600
H	4.12408400	2.34083000	-0.99210400				
H	2.35883900	2.47944200	-0.91930700	Pro-S			
H	1.00865300	-2.44575300	-1.90133300	C	3.44315700	0.00401100	-4.38196200
H	0.54062500	-4.67408400	-0.93044700	C	3.01418600	-1.30626400	-4.17557000
H	1.02684200	-5.12628500	1.47281000	C	2.41031500	-1.66628700	-2.96599200
H	2.03508000	-3.33088500	2.88549600	C	2.21282600	-0.72606700	-1.94827600
H	2.49352000	-1.09687300	1.91624500	C	2.66515300	0.59879800	-2.15723000
C	0.19039600	3.23602600	1.64133500	C	3.27686800	0.94973800	-3.37063800
C	-1.13552500	3.22631800	2.41622600	C	2.56210700	1.63265400	-1.11893300
H	-1.82605800	2.47000800	2.02213600	P	1.45322100	-1.22923400	-0.34233000
H	-0.99216100	3.03666000	3.49122900	N	1.82906800	1.61698200	-0.05500900
H	-1.63332600	4.20246100	2.32063600	C	2.11773500	2.83078200	0.74413700
C	1.10822100	4.34761000	2.17776700	C	2.96747200	3.65804700	-0.23933800
H	1.28541200	4.26359900	3.26126900	O	3.32286900	2.71280100	-1.28069700
H	2.08610100	4.34066500	1.66915400	H	3.91160700	0.29166200	-5.32501500
H	0.64890400	5.33161000	2.00043000	H	3.14952300	-2.05973200	-4.95443500
C	-0.07983000	3.49611200	0.15447800	H	3.61970600	1.97463200	-3.51048600
H	-0.59330000	2.64908800	-0.31804700	H	1.15425700	3.32188100	0.93152300
H	-0.71687600	4.38214200	0.02050100	H	2.40362100	4.47442500	-0.71317200
H	0.85062400	3.68180700	-0.39884800	H	3.89866900	4.05317600	0.18170300
H	0.68277700	0.61267500	-5.07756200	Ni	0.20582600	0.59430400	0.28293600
C	-3.02592100	-1.32211300	-1.44176800	C	-5.01814200	-0.11031800	0.30282200
C	-4.33124100	-0.99131900	-1.83323500	C	-5.90061800	-0.63686500	-0.65674100
C	-2.39426200	-2.44669900	-1.99879200	C	-5.02258500	-0.65793400	1.59778300
C	-4.99900600	-1.78367200	-2.77168600	C	-6.73738800	-1.70810300	-0.33925700
H	-4.82997400	-0.11961500	-1.40734000	H	-5.91917800	-0.21661200	-1.66481900
C	-3.06941500	-3.23832700	-2.92556400	C	-5.87042900	-1.71815900	1.91776300

H	-7.38586100	-3.08476800	1.19841300	H	1.82657700	-4.01513200	0.65850000
C	-4.07242800	3.53008600	-0.35470400	C	-0.96212500	-4.05127100	-2.05389700
C	-2.58530700	3.44924200	-0.74719000	H	-0.61131100	-1.93385600	-2.24191000
C	-1.83803300	4.74157000	-0.38690000	C	-0.61226800	-5.23404300	-1.39012200
C	-4.81194400	2.23347300	-0.65780200	H	0.66719600	-6.13663900	0.10055200
C	-4.13437000	1.03024100	-0.04400200	H	-1.73868100	-4.06222300	-2.82186700
C	-2.79259100	1.03174400	0.19213300	H	-1.11595800	-6.17035800	-1.63995500
C	-1.92786000	2.20329200	-0.08609900	C	2.90208600	-1.61794000	0.70536000
N	-0.67083300	2.22199500	0.10743300	C	2.70812700	-1.79750500	2.08453200
C	-2.47470200	3.19736900	-2.19723800	C	4.19817900	-1.70970100	0.17564500
N	-2.38884400	2.95996300	-3.32836900	C	3.79218400	-2.06692800	2.92047700
C	-2.07778400	-0.13191700	0.79556000	H	1.70505500	-1.72477100	2.50336400
C	-1.29474300	0.05655200	1.96710800	C	5.28228000	-1.97022300	1.01739100
C	-0.79517500	-1.05785500	2.67348100	H	4.36812400	-1.57209800	-0.89274500
C	-1.06499200	-2.34657400	2.23045900	C	5.08277700	-2.14776400	2.38887500
C	-1.81541800	-2.54076300	1.05951600	H	3.63018800	-2.20584700	3.99161100
C	-2.29897300	-1.45560200	0.34522200	H	6.28833500	-2.03424200	0.59732900
H	-1.88773500	4.90224600	0.70007400	H	5.93309100	-2.34891100	3.04402500
H	-0.78356900	4.67196900	-0.67914200	H	2.09319100	-2.69804700	-2.81847800
H	-5.84667700	2.29029400	-0.28968600	H	-4.11876700	3.74053800	0.72639500
H	-4.88513500	2.08916500	-1.75173600	H	-4.54516900	4.37675800	-0.87426400
H	-1.23329300	1.04717000	2.41808300				
H	-0.23516400	-0.89291000	3.59623100	Pro-R			
H	-0.69470500	-3.20950000	2.78755200	C	3.64125400	0.59353700	4.32450500
H	-2.00836000	-3.55256700	0.70095800	C	3.24556300	1.86837000	3.92196200
H	-2.89081200	-1.61395700	-0.55553400	C	2.60073900	2.04929000	2.69368700
C	2.79260000	2.50392300	2.10305800	C	2.32744400	0.96416500	1.85269300
C	4.12006000	1.75819200	1.90320300	C	2.74368900	-0.32556100	2.26041800
H	4.84344500	2.34831500	1.31930400	C	3.39857800	-0.49721500	3.49015100
H	4.58664300	1.54241000	2.87611500	C	2.56437100	-1.51081700	1.41024700
H	3.96805000	0.79837700	1.39159300	P	1.52796500	1.22872200	0.20832400
C	3.03054000	3.82827800	2.84720000	N	1.77802000	-1.64879500	0.39422600
H	3.44912400	3.63271200	3.84609100	C	2.01448700	-2.98191500	-0.21405300
H	3.74288000	4.48183200	2.32021500	C	2.88421600	-3.66321200	0.85758700
H	2.09004300	4.38685700	2.97984200	O	3.31078000	-2.57071000	1.71289700
C	1.83385400	1.63709100	2.93108500	H	4.14499700	0.44603800	5.28166500
H	2.27349200	1.40489700	3.91310300	H	3.44160500	2.73337600	4.55919700
H	0.87714200	2.15567600	3.09842300	H	3.71727400	-1.49776200	3.78162500
H	1.62781300	0.68489200	2.42490300	H	1.03393800	-3.46736600	-0.29175600
H	-2.29972200	5.60012300	-0.89513700	H	2.32142600	-4.37121700	1.48319000
C	0.68482500	-2.83326300	-0.75140200	H	3.78476600	-4.15328600	0.47150300
C	1.03982500	-4.01919900	-0.09727000	Ni	0.19795100	-0.62274300	-0.09522000
C	-0.32427000	-2.85571500	-1.73007700	C	-4.93462900	0.39030400	0.13592000
C	0.38612100	-5.21505100	-0.41375400	C	-5.59931300	1.18395800	1.08558700

C	-5.11867200	0.66899900	-1.22970300	C	1.23162100	3.95910300	-0.47724100
C	-6.40092500	2.25284700	0.68016100	C	-0.12457000	3.14858100	1.36118800
H	-5.47202400	0.97780700	2.15110400	C	0.64670500	5.22294300	-0.34226200
C	-5.93161300	1.72770600	-1.63380400	H	1.98862600	3.79186000	-1.24466400
H	-4.62750700	0.03935700	-1.97422400	C	-0.69394500	4.41210600	1.50314500
C	-6.56824800	2.52794500	-0.68020900	H	-0.43564500	2.33780800	2.02437100
H	-6.90204400	2.86997300	1.42932500	C	-0.31356600	5.45203800	0.64537500
H	-6.07415000	1.92591600	-2.69846400	H	0.95153600	6.03285100	-1.00854000
H	-7.20331300	3.35823300	-0.99692200	H	-1.44134100	4.58788400	2.27997100
C	-3.80604600	-2.87698600	1.91744500	H	-0.76381500	6.44126400	0.75249200
C	-2.80038800	-3.35534400	0.84634600	C	2.95562200	1.38091900	-0.92689300
C	-4.74935500	-1.81108500	1.37566600	C	2.72273900	1.33378600	-2.31086000
C	-4.07238400	-0.74468500	0.55241200	C	4.27026700	1.51525700	-0.45502800
C	-2.77821200	-0.87541700	0.14991200	C	3.78688200	1.42121300	-3.20891000
C	-1.99401500	-2.11069500	0.39707000	H	1.70517600	1.22690000	-2.68479300
N	-0.74061800	-2.20392300	0.21560800	C	5.33393400	1.59302100	-1.35730300
C	-1.89275600	-4.46890100	1.38294300	H	4.47104200	1.55309300	0.61615500
C	-2.05597100	0.15413300	-0.65104700	C	5.09572900	1.54480200	-2.73328700
C	-1.32978700	-0.24642100	-1.80686400	H	3.59450000	1.38372800	-4.28334100
C	-0.82147300	0.72066800	-2.69876300	H	6.35448400	1.69133500	-0.98112600
C	-1.02585200	2.07302000	-2.45769400	H	5.93016400	1.60303300	-3.43544800
C	-1.72141000	2.47908500	-1.30688900	H	2.31378900	3.05515700	2.38925100
C	-2.21145000	1.54186000	-0.41162300	H	-4.37740000	-3.73527000	2.30093100
H	-5.52512800	-2.27216300	0.73769600	H	-3.21418400	-2.47613100	2.75686200
H	-5.30510200	-1.33434000	2.19963300	H	-1.18085300	-4.79794700	0.61604900
H	-1.32711300	-1.29542600	-2.10334200	H	-1.32130800	-4.09289000	2.24354700
H	-0.30992000	0.38801000	-3.60430200	H	-2.49884400	-5.32920700	1.70106000
H	-0.64899300	2.82142900	-3.15766800	C	-3.52022500	-3.82786600	-0.34991700
H	-1.86259600	3.54181600	-1.10607900	N	-4.07825400	-4.16534700	-1.30795900
H	-2.75370200	1.86845000	0.47415100				
C	2.64444300	-2.89089800	-1.62965900	Ni-OH			
C	3.99963600	-2.16975400	-1.59571200	C	-0.61136600	-4.42921000	1.02324200
H	4.73250900	-2.69331200	-0.96228700	C	-1.85781000	-3.80326500	0.96857100
H	4.42711200	-2.11338200	-2.60806300	C	-1.94715100	-2.45935400	0.59637000
H	3.89875400	-1.14095000	-1.22506400	C	-0.79814900	-1.72642100	0.27446800
C	2.81491000	-4.32276700	-2.16401300	C	0.46420400	-2.36644900	0.30811700
H	3.20392400	-4.29967400	-3.19322600	C	0.54061900	-3.71669800	0.69343200
H	3.52503000	-4.91171000	-1.56288900	C	1.71550300	-1.69936900	-0.08272000
H	1.85340800	-4.86035900	-2.17989000	P	-0.97159500	0.04918600	-0.09689100
C	1.67714100	-2.13377800	-2.55022600	N	1.86849300	-0.54568300	-0.65470700
H	2.08149800	-2.07829400	-3.57242500	C	3.31250700	-0.33277000	-0.92654300
H	0.69905200	-2.63638900	-2.59453800	C	3.96181500	-1.56644300	-0.26794600
H	1.52295500	-1.10501600	-2.19841500	O	2.83758200	-2.37945500	0.14342500
C	0.84567400	2.91447400	0.37131900	H	-0.53397100	-5.47836300	1.31474700

H	-2.76508900	-4.35816900	1.21613200				
H	1.51429200	-4.20484400	0.71924600	H₂O			
H	3.44930900	-0.37016000	-2.02066600	O	0.00000000	0.00000000	0.12021100
H	4.57783200	-2.16013100	-0.95432200	H	0.00000000	0.75701000	-0.48084200
H	4.54686600	-1.32916100	0.63107000	H	0.00000000	-0.75701000	-0.48084200
Ni	0.67757600	0.82308000	-1.15313600				
C	3.80455600	1.05293800	-0.44774300	3a			
C	3.58347000	1.23694600	1.06081700	C	1.21033300	-1.41382700	-0.03122900
H	4.17452000	0.52795100	1.66015500	C	1.84920300	-2.31032000	-0.90453300
H	3.88723900	2.24940400	1.36589900	C	1.92325700	-0.94069200	1.08432600
H	2.52229700	1.11174600	1.32738300	C	3.17151700	-2.70166900	-0.68532000
C	5.29557300	1.17757700	-0.79828500	H	1.31553000	-2.68757200	-1.78007200
H	5.67849800	2.16303300	-0.49415700	C	3.23881800	-1.34262000	1.31131400
H	5.90319000	0.41781000	-0.28189700	H	1.43402500	-0.25490500	1.77713700
H	5.46417200	1.07144600	-1.88189800	C	3.87057600	-2.21967600	0.42416200
C	3.01022300	2.12432700	-1.21106100	H	3.65707900	-3.38665900	-1.38451300
H	3.44907500	3.12398500	-1.07340100	H	3.77458300	-0.96856200	2.18689100
H	2.97250100	1.93221700	-2.29491800	H	4.90345600	-2.52952700	0.59959500
H	1.98046000	2.24319200	-0.81129400	C	-2.57295300	-1.66055800	-0.87513100
C	-2.58018500	0.23943000	-0.91125700	C	-3.03998200	-0.39061000	-0.12934500
C	-3.70565200	0.70678800	-0.21685200	C	-1.19657100	-2.11521700	-0.40891900
C	-2.68184000	-0.10966500	-2.26932100	C	-0.19697100	-0.99390300	-0.26280300
C	-4.93062000	0.81428500	-0.88079500	C	-0.57020900	0.31540500	-0.28470900
H	-3.62471100	0.99079600	0.83395300	C	-2.00011000	0.71209800	-0.40833400
C	-3.90834500	0.00031000	-2.92357600	N	-2.42524400	1.87372300	-0.71534900
H	-1.79992100	-0.45935100	-2.81240200	C	-4.45101000	0.02825000	-0.56325900
C	-5.03277600	0.46128100	-2.22905100	C	0.42062500	1.42709600	-0.21258300
H	-5.80730200	1.17992800	-0.34209100	C	0.32769900	2.39694100	0.80089500
H	-3.98759700	-0.26886400	-3.97887500	C	1.26756500	3.42541400	0.89003600
H	-5.99135300	0.55115400	-2.74454900	C	2.30959200	3.50637400	-0.03827300
C	-1.04582800	0.91726700	1.49671100	C	2.40299700	2.55528000	-1.05829800
C	-0.98150800	2.32312300	1.46679100	C	1.46507600	1.52568300	-1.14523600
C	-1.16462800	0.23864900	2.71883400	H	-1.27220100	-2.62042600	0.57138500
C	-1.05859600	3.03936300	2.66073900	H	-0.79511200	-2.87827300	-1.09484200
H	-0.86684800	2.83474300	0.50700900	H	-0.48135800	2.33157300	1.53236100
C	-1.23078200	0.96788400	3.90889400	H	1.18762100	4.16463400	1.69062500
H	-1.20738000	-0.85119300	2.74781000	H	3.04523500	4.31114800	0.03128900
C	-1.18150500	2.36420400	3.88066000	H	3.21144200	2.61510400	-1.79083500
H	-1.01519500	4.13042400	2.64002500	H	1.54291800	0.77931900	-1.93777400
H	-1.32313000	0.44139700	4.86119900	H	-3.31190500	-2.46486600	-0.74085400
H	-1.23519600	2.92958000	4.81362100	H	-2.55008900	-1.41035100	-1.94858300
H	-2.92373000	-1.97369000	0.55777500	H	-4.75703600	0.95024800	-0.05509800
O	-0.23839500	2.22579400	-1.70693100	H	-4.45653700	0.22576500	-1.64433000
H	-1.14034700	2.09178200	-2.02834500	H	-5.16918000	-0.77333600	-0.33635900

C	-3.02872900	-0.64516300	1.32431600
N	-3.00931500	-0.85478300	2.46395200
H	-1.64091800	2.51438700	-0.87871300

INT4'-2

C	-2.72987700	-1.37954700	4.35993800
C	-1.38640900	-1.18864900	4.68050000
C	-0.43181700	-1.06530800	3.66400600
C	-0.80547300	-1.10767100	2.31744900
C	-2.17289000	-1.30258600	1.99498400
C	-3.11820300	-1.44874100	3.02072700
C	-2.65057100	-1.39795600	0.60277600
P	0.44698900	-0.96686800	0.97484100
N	-2.10075300	-0.89804400	-0.45545300
C	-2.88342000	-1.32005600	-1.64411600
C	-4.15226100	-1.89961000	-0.98976700
O	-3.78630400	-2.06216900	0.40757000
H	-3.47734000	-1.48294900	5.14880000
H	-1.07051600	-1.14425900	5.72499500
H	0.61846300	-0.93770600	3.92777100
H	-4.16269100	-1.61502300	2.75625900
H	-3.12610500	-0.42049100	-2.22166200
H	-5.00583300	-1.20768700	-1.02761000
H	-4.45707800	-2.88042200	-1.37045900
Ni	-0.70536800	0.44034300	-0.47920200
C	-1.89360400	1.57938700	-1.44838300
C	-1.56169900	2.04069000	-2.72665500
C	-3.12287200	1.95024600	-0.88845900
C	-2.46114100	2.83344000	-3.45200200
H	-0.59585100	1.79376500	-3.17616700
C	-4.01546900	2.75551900	-1.60418500
H	-3.39534200	1.62176000	0.11841300
C	-3.68947100	3.19268300	-2.89191100
H	-2.19327900	3.17797000	-4.45413700
H	-4.96828900	3.04410600	-1.15263700
H	-4.38700500	3.81851800	-3.45295100
C	3.42694400	1.70338500	-0.87701100
C	4.69276200	1.12743800	-1.57647900
C	5.97646700	1.68907300	-0.91908000
C	2.11823100	1.14653300	-1.45112200
C	0.93796700	1.61691900	-0.71775400
C	0.17592300	2.25753400	0.02404700
C	4.67339400	-0.34667800	-1.45759300
N	4.61062300	-1.49429000	-1.32078100

C	4.65665600	1.47768000	-3.01148600
N	4.58820400	1.79251100	-4.12305000
C	-0.53545000	3.21393000	0.82130400
C	-1.28187200	2.80297500	1.94359400
C	-1.97892500	3.74195300	2.70009300
C	-1.94448400	5.09446300	2.34390800
C	-1.21095600	5.50694900	1.22675800
C	-0.51023700	4.57468900	0.46349600
H	3.49778200	1.46591000	0.19219400
H	3.45378800	2.79837400	-0.97900500
H	5.98662500	2.78365800	-1.01478200
H	5.98531700	1.41927300	0.14607400
H	2.01355100	1.41744300	-2.51588500
H	2.14321100	0.04633000	-1.42314100
H	-1.32398100	1.74472800	2.20826400
H	-2.55655100	3.41841700	3.56851800
H	-2.49501000	5.82870200	2.93596900
H	-1.19133100	6.56155500	0.94426900
H	0.04848000	4.88571900	-0.42038900
C	-2.09539300	-2.28459800	-2.57075300
C	-1.78727600	-3.61408600	-1.86819300
H	-1.18552900	-4.25931200	-2.52512600
H	-1.21186800	-3.46300400	-0.94643600
H	-2.70192100	-4.17217800	-1.61610800
C	-2.95593700	-2.53452500	-3.82041500
H	-3.91242800	-3.02209300	-3.57370700
H	-3.17896000	-1.59320200	-4.34734600
H	-2.42521800	-3.19628800	-4.52137100
C	-0.78742800	-1.60011000	-2.99794100
H	-0.21895900	-2.25060800	-3.67935200
H	-0.98660200	-0.65077100	-3.51564200
H	-0.14369800	-1.39312600	-2.13004100
H	6.87452400	1.28189800	-1.40235200
C	1.96414000	-0.34640000	1.78636200
C	3.18110700	-1.03826300	1.69365000
C	1.93269800	0.90444200	2.43257600
C	4.34689000	-0.48612700	2.23419700
H	3.23382500	-2.00341200	1.19095800
C	3.09519100	1.44420700	2.98178800
H	0.99881300	1.45939100	2.51771900
C	4.30790300	0.75198700	2.87931800
H	5.28672400	-1.03564900	2.14959300
H	3.05425400	2.41102300	3.48806700
H	5.21841300	1.17695700	3.30785100

C	0.80688900	-2.69701300	0.52150200	C	-2.69423500	3.54946400	-1.08147200
C	1.59102800	-2.93676500	-0.61895900	C	-2.79998500	4.96326800	-1.69829600
C	0.31892600	-3.78308700	1.26423900	C	-2.29023000	1.08133700	-1.99220300
C	1.89068100	-4.24227400	-1.00668700	C	-2.49021400	0.40400400	-0.64919900
H	1.99369000	-2.10817300	-1.20224100	C	-1.46284000	0.25263000	0.21955100
C	0.60480200	-5.08955000	0.86090500	C	-3.60265100	3.44867200	0.07828700
H	-0.28754200	-3.61480100	2.15522500	N	-4.32389700	3.41392900	0.98228500
C	1.38963800	-5.32120400	-0.27222200	C	-1.34878900	3.26337700	-0.55571500
H	2.51850700	-4.41200700	-1.88344800	N	-0.39126300	2.73886400	-0.17554200
H	0.21657000	-5.93044300	1.43961300	C	-1.58455900	-0.40212100	1.53955900
H	1.61514400	-6.34428900	-0.58073600	C	-1.25116700	0.30525200	2.71092800
INT7'				C	-1.29243900	-0.31341900	3.96142000
C	3.82248300	-0.99882900	-4.24957300	C	-1.65870600	-1.65921500	4.06564300
C	2.95585200	-2.07145900	-4.04266700	C	-2.01142000	-2.36841900	2.91255900
C	2.11557900	-2.08972900	-2.92430700	C	-1.98328400	-1.74713800	1.66415200
C	2.11686200	-1.03529800	-2.00419500	H	-4.10225900	2.28413600	-2.12700300
C	2.99555700	0.05493100	-2.21955200	H	-2.75895500	2.85737800	-3.13525800
C	3.84489600	0.05631900	-3.33746600	H	-3.80989000	5.09520200	-2.11009200
C	3.07471100	1.19869500	-1.29794100	H	-2.62378600	5.74074200	-0.94259200
P	1.05632100	-1.12544400	-0.50271400	H	-2.66630200	0.44342800	-2.80843800
N	2.22345000	1.54116100	-0.38795000	H	-1.21452600	1.21045300	-2.18496500
C	2.77057800	2.70556200	0.34968800	H	-0.97707200	1.35854700	2.63672200
C	3.96637600	3.11336500	-0.53635800	H	-1.04031700	0.25781600	4.85788500
O	4.14718100	1.98287100	-1.42131500	H	-1.68535400	-2.14811700	5.04195500
H	4.48384000	-0.98134000	-5.11792000	H	-2.31888300	-3.41411600	2.98645900
H	2.93336600	-2.90575500	-4.74703200	H	-2.28561300	-2.29692100	0.77469900
H	4.52223200	0.89746500	-3.48355200	C	3.12058300	2.37050400	1.82619900
H	2.00426200	3.49332000	0.35836300	C	4.18021700	1.26241800	1.90601600
H	3.76243700	3.99722100	-1.15857400	H	5.12450600	1.55085700	1.41868500
H	4.90436500	3.26523000	0.00934300	H	4.41284500	1.03747700	2.95744100
Ni	0.34349200	0.88236000	-0.09499100	H	3.82381900	0.33241400	1.44446600
C	-3.88040600	-0.06490000	-0.36789400	C	3.63709700	3.65370900	2.49728300
C	-4.59901700	-0.76991300	-1.35178900	H	3.84502900	3.46579600	3.56134300
C	-4.50817600	0.16733600	0.86858700	H	4.57252800	4.01696000	2.04373100
C	-5.88788000	-1.24577900	-1.10245600	H	2.89254700	4.46417100	2.44007700
H	-4.14153000	-0.97084100	-2.32262500	C	1.84345900	1.91313800	2.54096600
C	-5.79784000	-0.30080400	1.11638900	H	2.04759800	1.69103500	3.59909600
H	-3.98823500	0.73693000	1.63675600	H	1.06364100	2.68898700	2.50151300
C	-6.49250700	-1.01408500	0.13522300	H	1.44147000	0.99451200	2.09193600
H	-6.42121900	-1.79944800	-1.87889300	H	-2.06714300	5.07100800	-2.51024200
H	-6.26677600	-0.09798000	2.08175300	C	-0.07885400	-2.50602800	-0.83927600
H	-7.50290900	-1.37976200	0.33122100	C	0.01088400	-3.71633200	-0.13869300
C	-3.01285600	2.43257800	-2.15267400	C	-1.08624200	-2.33202600	-1.80246900
				C	-0.91140300	-4.73652400	-0.38758400

H	0.78761900	-3.86020100	0.61258700	H	4.39159900	0.89249900	2.03961600
C	-2.00204200	-3.35286200	-2.04875900	C	5.79117900	1.10037800	-1.57385100
H	-1.15431900	-1.39628000	-2.35695300	H	3.73220000	1.21903800	-2.20965400
C	-1.92148900	-4.55408400	-1.33434600	C	6.66796900	0.99014700	-0.49059000
H	-0.84195000	-5.67448500	0.16725100	H	6.83231200	0.83378300	1.66000300
H	-2.78809900	-3.21115900	-2.79277100	H	6.18371400	1.16309200	-2.59141200
H	-2.64741200	-5.34855300	-1.52022400	H	7.74712000	0.96268000	-0.65676900
C	2.18208300	-1.72463300	0.80627200	C	1.88657500	3.51644300	0.72713500
C	1.72933500	-1.70027600	2.13645000	C	0.59020100	3.94985700	-0.02145100
C	3.47152800	-2.19620400	0.51773300	C	0.73280100	5.37469400	-0.61102500
C	2.56387300	-2.14051100	3.16389000	C	1.90472900	2.05427700	1.20504900
H	0.72767600	-1.34343700	2.37295700	C	2.40588800	1.07300800	0.15849200
C	4.30317000	-2.63003100	1.55322900	C	1.55856700	0.30926700	-0.56422800
H	3.83267600	-2.22493700	-0.51116900	C	0.26503700	2.99975800	-1.10475800
C	3.85264400	-2.60063400	2.87584300	N	-0.02976000	2.26424500	-1.95583100
H	2.20206700	-2.11983100	4.19400600	C	-0.57137700	3.88540700	0.89441700
H	5.30725200	-2.99315900	1.32368200	N	-1.49192300	3.80598600	1.59158000
H	4.50610600	-2.93945200	3.68277900	C	1.93206600	-0.76108600	-1.50465100
H	1.45537900	-2.94222600	-2.76488000	C	1.40150700	-0.79139700	-2.81071200
INT8'				C	1.66599600	-1.86253500	-3.66560700
C	-3.05951600	0.54869800	4.45992100	C	2.45516300	-2.93177500	-3.22951800
C	-2.06993600	-0.41355400	4.65841400	C	2.99608400	-2.90911900	-1.93956900
C	-1.32196200	-0.88321000	3.57415300	C	2.74279100	-1.83521300	-1.08685200
C	-1.54579000	-0.39663300	2.28069800	H	2.73982800	3.70639100	0.05852400
C	-2.56468900	0.56712500	2.07871400	H	1.97936000	4.20718400	1.57877200
C	-3.30953200	1.02922200	3.17492600	H	1.56290500	5.39077400	-1.33057200
C	-2.91593300	1.09606600	0.75072200	H	-0.18955400	5.69302900	-1.11546100
P	-0.55001400	-1.02825600	0.87589200	H	2.55759000	2.01066400	2.08937700
N	-2.22128900	1.04928900	-0.34150700	H	0.89797800	1.77087100	1.55444700
C	-3.05474300	1.59952500	-1.44237200	H	0.79036500	0.04183400	-3.15942600
C	-4.20257000	2.26816100	-0.66101900	H	1.25429100	-1.86223700	-4.67761500
O	-4.10458800	1.68868000	0.65982600	H	2.65646300	-3.77401400	-3.89519700
H	-3.64156000	0.92529500	5.30316700	H	3.62261100	-3.73497700	-1.59462000
H	-1.87414900	-0.80571500	5.65867800	H	3.17111700	-1.81806100	-0.08502400
H	-4.08318500	1.77695700	3.00571400	C	-3.47992100	0.51262400	-2.46843300
H	-2.46791100	2.35211400	-1.98383900	C	-4.29652700	-0.59661900	-1.79119400
H	-4.07258200	3.35514700	-0.55499100	H	-5.21553700	-0.21160900	-1.32258900
H	-5.20489000	2.05504700	-1.04849000	H	-4.59928800	-1.35039500	-2.53315200
Ni	-0.30336400	0.60283700	-0.50441000	H	-3.70832000	-1.11377200	-1.02237100
C	3.88079000	1.05721300	-0.06165500	C	-4.31359200	1.19266500	-3.56709500
C	4.77535300	0.96146300	1.01939500	H	-4.57601900	0.46251100	-4.34739600
C	4.41287800	1.13374500	-1.36121100	H	-5.25779800	1.60777000	-3.18147100
C	6.15473200	0.92118200	0.80740400	H	-3.75211900	2.00925900	-4.04912100
				C	-2.21792000	-0.08690600	-3.10403200

H	-2.48711600	-0.87088100	-3.82766000	H	2.46306000	3.18044500	-0.65951900
H	-1.63107600	0.68073500	-3.62897100	H	4.15608100	2.93674000	-2.30798200
H	-1.57271100	-0.55274000	-2.34688400	H	5.27098800	2.44814900	-0.99479200
H	0.95389400	6.07683600	0.20461600	Ni	0.43470700	0.87675400	-0.45126900
C	0.85947100	-1.89812100	1.63804800	C	-3.90213000	-0.07453500	-0.49191400
C	1.07832400	-3.26372300	1.41239300	C	-4.60145500	-1.02310800	-1.26502100
C	1.77115700	-1.17398300	2.42529600	C	-4.54688400	0.45227300	0.64592100
C	2.20349300	-3.89262900	1.95417400	C	-5.87407500	-1.45972700	-0.89793800
H	0.38116400	-3.84080700	0.80576500	H	-4.14030200	-1.44564200	-2.15757100
C	2.88950700	-1.80468900	2.96492400	C	-5.82431600	0.02819600	1.00261300
H	1.60148600	-0.11705400	2.62463900	H	-4.06301600	1.22555700	1.23663900
C	3.11312800	-3.16570600	2.72278100	C	-6.49065300	-0.93716700	0.24093600
H	2.36791000	-4.95582600	1.76735000	H	-6.38768100	-2.20613400	-1.50801800
H	3.59294000	-1.23454300	3.57518200	H	-6.30813500	0.46545800	1.87851800
H	3.99467800	-3.65710400	3.14002500	H	-7.49121200	-1.26932300	0.52640900
C	-1.55594800	-2.34300300	0.10959300	C	-2.72328200	2.04631100	-2.72133600
C	-1.15022600	-2.85122600	-1.13643700	C	-2.19438400	3.08296000	-1.68343000
C	-2.70367000	-2.85266200	0.73327900	C	-1.81143800	4.41608700	-2.36453200
C	-1.89521500	-3.85794800	-1.75092100	C	-2.32810700	0.59142200	-2.38269200
H	-0.25290400	-2.46823400	-1.62542600	C	-2.54551800	0.35851400	-0.90772200
C	-3.44670000	-3.85747200	0.10852700	C	-1.54265400	0.77084500	-0.07429600
H	-3.02289200	-2.46579700	1.70231200	C	-3.19221500	3.35167100	-0.63387500
C	-3.04597300	-4.35840600	-1.13306600	N	-3.95823500	3.60891500	0.19473700
H	-1.57436200	-4.24984000	-2.71841500	C	-0.96851800	2.52993500	-0.98814800
H	-4.34254100	-4.24933400	0.59489600	N	0.19475300	2.77310800	-0.82218500
H	-3.63023200	-5.14272400	-1.61927600	C	-1.56150600	0.75190400	1.40377500
H	-0.55472100	-1.63937600	3.74028300	C	-1.15081900	1.85936700	2.16882800
TS7'				C	-1.12526700	1.79480900	3.56381400
C	3.46856800	-2.69767900	-3.72166800	C	-1.50498200	0.62409500	4.22451600
C	2.49062500	-3.54103000	-3.19537100	C	-1.92367700	-0.48245800	3.47606200
C	1.68936200	-3.10922300	-2.13311200	C	-1.94840300	-0.42290300	2.08537300
C	1.84266200	-1.82857600	-1.59050200	H	-3.81687000	2.13693400	-2.77405300
C	2.84009200	-0.97650800	-2.12210500	H	-2.31774100	2.31430900	-3.70740000
C	3.64652500	-1.42432200	-3.18094600	H	-2.69061400	4.82741200	-2.87990500
C	3.10422300	0.36683000	-1.58076800	H	-1.45772800	5.14648300	-1.62498400
P	0.82119000	-1.27824900	-0.16670700	H	-2.91735000	-0.08399100	-3.01449900
N	2.35566800	1.08824400	-0.80798400	H	-1.26750600	0.43827500	-2.63158400
C	3.11151400	2.32240900	-0.45225100	H	-0.85991100	2.78441200	1.67271200
C	4.28801200	2.26886500	-1.44371900	H	-0.80964700	2.66995400	4.13582300
O	4.26945900	0.90757900	-1.93458800	H	-1.48455900	0.57590200	5.31531200
H	4.09839700	-3.02970500	-4.54918500	H	-2.23244900	-1.40099400	3.98015800
H	2.34945400	-4.54388100	-3.60411700	H	-2.28914000	-1.28369100	1.51442100
H	4.41614600	-0.76103700	-3.57455400	C	3.51503100	2.37702700	1.04695000
				C	4.39298700	1.17788400	1.43126700

H	5.32958900	1.14584700	0.85297900	P	-0.74834300	1.29507000	-0.35444600
H	4.66915800	1.23524200	2.49462500	N	-2.32372700	-1.12199400	-0.58214200
H	3.86448400	0.22794600	1.28151500	C	-3.11063300	-2.26315800	-0.03442100
C	4.27831700	3.69105500	1.28600400	C	-4.24795700	-2.38333800	-1.06436400
H	4.51352700	3.79937800	2.35557300	O	-4.19504700	-1.13109700	-1.79001000
H	5.23361100	3.72946800	0.73987000	H	-3.90461400	2.27519300	-5.05167700
H	3.67683000	4.56393600	0.98540800	H	-2.15363300	3.91448800	-4.35044600
C	2.24035100	2.38987600	1.89886300	H	-4.27946700	0.22203100	-3.69546800
H	2.48981100	2.41110100	2.97046500	H	-2.46901000	-3.15074900	-0.05517400
H	1.62100400	3.26982200	1.67191200	H	-4.08912900	-3.19522100	-1.78938400
H	1.63142900	1.49555800	1.72288800	H	-5.24949700	-2.47433800	-0.63036300
H	-1.01332700	4.23787600	-3.09793800	Ni	-0.41090700	-0.88090300	-0.22455000
C	-0.49182900	-2.53436400	-0.05157600	C	3.95095900	-0.08521700	-0.34660600
C	-0.59905100	-3.37916300	1.06305200	C	4.71755400	0.68850600	-1.24052500
C	-1.42005300	-2.64877400	-1.09935800	C	4.54709900	-0.45015800	0.87956000
C	-1.63200800	-4.31695200	1.13313000	C	6.00730000	1.10834400	-0.91447400
H	0.11655900	-3.30008100	1.88154700	H	4.29696400	0.98773100	-2.19986100
C	-2.43829100	-3.59885500	-1.03209100	C	5.84106400	-0.04650800	1.19808300
H	-1.33396000	-2.00702000	-1.97754400	H	3.99793000	-1.06401500	1.59105700
C	-2.55253700	-4.42771900	0.08843500	C	6.57572600	0.74325800	0.30732300
H	-1.71318500	-4.96664100	2.00713500	H	6.57221900	1.71876700	-1.62238000
H	-3.15027100	-3.69346000	-1.85342800	H	6.28146700	-0.35388200	2.14901500
H	-3.35794200	-5.16309100	0.14332000	H	7.58845100	1.06320100	0.56157700
C	1.88863200	-1.57471200	1.28770600	C	2.74395100	-2.43951400	-2.29092900
C	1.53598800	-0.98516400	2.51259500	C	2.12087300	-3.32790300	-1.16477700
C	3.03795700	-2.37556100	1.20752400	C	3.16130900	-3.73767300	-0.09863100
C	2.32595900	-1.19696800	3.64282400	C	2.37495300	-0.94717200	-2.15694400
H	0.64327800	-0.36705400	2.59074400	C	2.58603000	-0.52322900	-0.72643200
C	3.82889300	-2.57697300	2.34117700	C	1.56194800	-0.80192800	0.13898400
H	3.32259200	-2.84016900	0.26239500	C	0.96030800	-2.61032200	-0.48663000
C	3.47544800	-1.98817800	3.55861300	N	-0.19507600	-2.80724000	-0.20888100
H	2.04180100	-0.73489200	4.59055800	C	1.54813100	-4.54423500	-1.76939600
H	4.72520400	-3.19703100	2.27163300	N	1.12555100	-5.50494900	-2.25731800
H	4.09706900	-2.14666100	4.44256800	C	1.55021600	-0.55382400	1.59792500
H	0.93932300	-3.78386000	-1.72082000	C	1.10243000	-1.51337600	2.52558600
TS8'				C	1.05375600	-1.21927200	3.89064000
C	-3.29851700	2.08992000	-4.16284900	C	1.44637200	0.03656800	4.35921600
C	-2.31929500	3.00275500	-3.77252200	C	1.89717700	0.99918200	3.44783100
C	-1.54777000	2.75812000	-2.63165800	C	1.94317900	0.71210600	2.08658600
C	-1.73322500	1.59688600	-1.87318400	H	3.61156700	-2.84611300	0.35081900
C	-2.73340900	0.67522000	-2.26611500	H	2.69593300	-4.34656800	0.68861200
C	-3.50854200	0.93613000	-3.40767300	H	2.98522800	-0.37747300	-2.86810500
C	-3.03455300	-0.54609600	-1.49964000	H	1.32038700	-0.80664700	-2.43612200
				H	0.79045000	-2.49822200	2.18096200

H	0.70505000	-1.98140000	4.59091000	TS7-Bn			
H	1.40673000	0.26360900	5.42663100	C	2.67355600	-2.01190000	4.15727800
H	2.21117300	1.98425000	3.80024900	C	3.19693200	-0.72710500	4.01771700
H	2.30182700	1.46531800	1.38818300	C	3.06517700	-0.04187100	2.80439400
C	-3.56864100	-2.03142000	1.43206400	C	2.39564400	-0.62275500	1.72386100
C	-4.42535800	-0.76308500	1.55386200	C	1.85757700	-1.92424700	1.87178500
H	-5.33300200	-0.81365200	0.93222200	C	2.01169500	-2.60982300	3.08469400
H	-4.75160400	-0.62408700	2.59538500	C	1.14739900	-2.60640900	0.77971900
H	-3.86144700	0.13333700	1.26518700	P	2.22604200	0.28177400	0.13193500
C	-4.37660400	-3.26203700	1.87871900	N	0.56399900	-2.06953600	-0.24219800
H	-4.64496300	-3.16919400	2.94198200	C	0.08272400	-3.14538700	-1.13915500
H	-5.31683000	-3.37601800	1.31738000	C	0.23493400	-4.38778200	-0.23795900
H	-3.79284700	-4.18885300	1.75985200	O	1.08999800	-3.93556500	0.84125000
C	-2.32589100	-1.91376200	2.32271800	H	2.77622300	-2.55050900	5.10120500
H	-2.61445800	-1.72487200	3.36783800	H	3.71566200	-0.25072600	4.85246000
H	-1.72784100	-2.83599500	2.29061700	H	1.59417200	-3.61155100	3.18053500
H	-1.68230400	-1.08526100	2.00497800	H	-0.97556700	-2.95217800	-1.36110100
H	3.95523500	-4.32802500	-0.57696200	H	-0.71511100	-4.71769000	0.20557200
C	0.60454700	2.51166200	-0.44453600	H	0.72691800	-5.24030700	-0.71862800
C	0.74564600	3.52158300	0.51854500	Ni	0.11331800	-0.21693400	-0.47869100
C	1.53587500	2.41963200	-1.49226100	C	-4.10695100	-1.53002100	-0.30246200
C	1.81384800	4.41882000	0.44057400	C	-4.74213400	-2.56293100	-1.01784800
H	0.02708300	3.60478600	1.33429900	C	-4.68205200	-1.10544000	0.90826600
C	2.58910000	3.32951100	-1.57573200	C	-5.90467300	-3.16395300	-0.53235300
H	1.42316900	1.64966600	-2.25696500	H	-4.31208800	-2.91850500	-1.95759000
C	2.73643900	4.32443600	-0.60390100	C	-5.85080700	-1.69869400	1.38645700
H	1.91981800	5.19930000	1.19703900	H	-4.22460100	-0.29237000	1.46889900
H	3.30060200	3.26484100	-2.40081200	C	-6.46452100	-2.73209900	0.67298300
H	3.56780100	5.02974400	-0.66609900	H	-6.37528000	-3.97115200	-1.09847500
C	-1.82602400	1.87814900	1.00204300	H	-6.28761000	-1.34561000	2.32335900
C	-1.51766100	1.49792600	2.31828700	H	-7.37840600	-3.19541700	1.05145100
C	-2.94537100	2.68802300	0.75745000	C	-3.39942600	0.93789600	-2.40068700
C	-2.32036400	1.92600000	3.37595100	C	-2.69627100	1.97026300	-1.45788600
H	-0.64977200	0.87313900	2.52252400	C	-2.85437300	-0.49544100	-2.27772700
C	-3.74984400	3.10637100	1.82003200	C	-2.84083000	-0.94323700	-0.83278300
H	-3.19672700	2.98994000	-0.26032400	C	-1.75603300	-0.69172000	-0.07089200
C	-3.43989400	2.72600100	3.12883100	C	-1.27984000	1.60456900	-1.25167700
H	-2.07137900	1.62511200	4.39573300	N	-0.10773500	1.60321000	-1.27538000
H	-4.62316200	3.73180400	1.62306200	C	-1.62163900	-0.91765100	1.37890600
H	-4.07249600	3.05325500	3.95684100	C	-1.23692800	0.14074000	2.22455100
H	-0.79541500	3.48635700	-2.32907600	C	-0.97413300	-0.07885000	3.57909900
H	3.83594200	-2.55462500	-2.24916900	C	-1.09808600	-1.36008800	4.11820400
H	2.41083200	-2.80465300	-3.27165200	C	-1.50262600	-2.41903700	3.29535800
				C	-1.75668500	-2.20272100	1.94330600

H	-4.47428100	0.96690900	-2.17093000	H	3.48577600	0.95930700	2.70168700
H	-3.27112800	1.29330000	-3.43393100	C	-2.72581300	3.41127100	-2.09921900
H	-3.47540700	-1.14647900	-2.90878600	H	-2.26735700	3.31943700	-3.09426500
H	-1.83520500	-0.52138600	-2.68707000	H	-3.79101900	3.64568300	-2.24491600
H	-1.17879300	1.15291500	1.82053200	C	-3.33741800	2.01840800	-0.13368800
H	-0.67804500	0.75842100	4.21484500	N	-3.85783200	2.12620400	0.89407400
H	-0.89045500	-1.53452300	5.17588600	C	-2.03395600	4.48110200	-1.29401400
H	-1.62175300	-3.42112500	3.71441200	C	-0.69451400	4.80619900	-1.55775100
H	-2.08212100	-3.02775700	1.30728500	C	-2.70480200	5.15250800	-0.26061800
C	0.86656900	-3.20238900	-2.48071200	C	-0.03614000	5.77734200	-0.80241300
C	2.35578300	-3.49177400	-2.24166500	H	-0.16085900	4.29476400	-2.36219900
H	2.82625400	-2.70837000	-1.63389900	C	-2.04659000	6.12376500	0.49666700
H	2.51907400	-4.45949300	-1.74343800	H	-3.74905500	4.91615000	-0.04584600
H	2.89257200	-3.52585300	-3.20129900	C	-0.71153800	6.43796900	0.22721300
C	0.24259000	-4.30906700	-3.34677200	H	1.00649700	6.01749900	-1.01923100
H	0.34961300	-5.30606100	-2.89175300	H	-2.58255800	6.64277300	1.29427700
H	-0.83079700	-4.12656500	-3.51748800	H	-0.20054900	7.20440400	0.81474100
H	0.73687500	-4.34654900	-4.32922700	TS8-Bn			
C	0.71798200	-1.85939200	-3.20969400	C	-0.58165000	-4.49349000	-3.17728100
H	1.09975900	-1.02687700	-2.60132700	C	-1.77720300	-3.80474200	-3.38051500
H	1.28631300	-1.86950800	-4.15178500	C	-2.14175200	-2.76452200	-2.51903900
H	-0.33460500	-1.65614500	-3.45618600	C	-1.31680000	-2.39296800	-1.45270100
C	2.56577800	2.02109700	0.54758000	C	-0.10443100	-3.09623800	-1.24512500
C	3.76913100	2.65431300	0.20562500	C	0.24551700	-4.14500000	-2.10962600
C	1.56832400	2.74328600	1.22483700	C	0.80309900	-2.80595000	-0.12210800
C	3.97132900	3.99564900	0.54502600	P	-1.78648000	-0.99801700	-0.35851300
H	4.54930300	2.10362400	-0.32241500	N	0.86788100	-1.74089100	0.61228800
C	1.77734400	4.07737800	1.56721000	C	1.81538700	-1.99749900	1.72569700
H	0.62779600	2.25799500	1.48794900	C	2.54592700	-3.25472900	1.21962500
C	2.97969000	4.70623800	1.22562600	O	1.66858000	-3.77132500	0.19021100
H	4.91077600	4.48452100	0.27782200	H	-0.29114700	-5.30516600	-3.84701900
H	0.99380300	4.63198400	2.08614200	H	-2.43378100	-4.07367000	-4.21075600
H	3.14159000	5.75408800	1.48838700	H	1.17761300	-4.68209400	-1.93678000
C	3.62466100	-0.28071800	-0.88866200	H	2.50623500	-1.14749700	1.79431100
C	3.63554000	0.10334900	-2.24084700	H	3.51694300	-3.03172800	0.75259200
C	4.64514200	-1.10297500	-0.39085200	H	2.67715900	-4.03956900	1.97196800
C	4.65837900	-0.33161500	-3.08297700	Ni	0.13767200	-0.01602300	0.13204200
H	2.84137000	0.74423800	-2.63183600	C	4.37157800	1.27356400	-0.04228600
C	5.66303100	-1.54301500	-1.24161300	C	5.46809500	0.77720300	0.68563700
H	4.64436900	-1.40607400	0.65750100	C	4.60265000	1.82698100	-1.31361600
C	5.67020500	-1.16052900	-2.58536500	C	6.75566300	0.81052100	0.14756300
H	4.66467900	-0.02852500	-4.13226100	H	5.31114800	0.34525900	1.67738300
H	6.45410100	-2.18683100	-0.85112200	C	5.89195000	1.87571800	-1.84307700
H	6.46657500	-1.50722400	-3.24751100				

H	3.76554900	2.22870900	-1.88548300	C	0.36997300	-0.85886900	3.44291200
C	6.97161500	1.36157000	-1.11846200	H	-0.28846700	-0.53081300	2.62900200
H	7.59415000	0.40955800	0.72141500	H	-0.25462400	-0.98319300	4.33912300
H	6.05576400	2.32020900	-2.82728400	H	1.08057700	-0.04820500	3.65416400
H	7.97995400	1.39688800	-1.53652000	H	0.81162000	4.77676200	0.07586900
C	2.18212200	3.17177800	1.77016800	C	-3.01226500	-0.03594500	-1.29696000
C	0.68295000	3.09692000	1.41884200	C	-4.33506800	0.10595800	-0.85814400
C	0.16036100	4.48859100	0.91384900	C	-2.59430100	0.61074800	-2.47236100
C	2.82098800	1.78318200	1.92204800	C	-5.23412400	0.88409000	-1.59464800
C	3.00379500	1.20002700	0.54106100	H	-4.66875600	-0.38753700	0.05559700
C	1.93872000	0.77670100	-0.17460700	C	-3.49797900	1.37224500	-3.20869600
C	0.31177500	2.03378000	0.39906700	H	-1.56082400	0.51387700	-2.80816400
N	-0.67372100	1.71156000	-0.21834500	C	-4.81968900	1.51330100	-2.76917000
C	-0.05670900	2.67580700	2.62710000	H	-6.26363400	0.99282900	-1.24693900
N	-0.62389300	2.31420500	3.56963200	H	-3.17000800	1.86713000	-4.12556800
C	1.94899100	0.26740700	-1.56523500	H	-5.52490800	2.11807100	-3.34370800
C	1.17454700	0.84445300	-2.59206300	C	-2.67408200	-1.72114600	1.05331600
C	1.14717100	0.27769100	-3.86952800	C	-2.88438900	-0.90015300	2.17485200
C	1.88626400	-0.87255400	-4.15051000	C	-3.12602500	-3.04818800	1.06159100
C	2.67420000	-1.44653900	-3.14541400	C	-3.54136800	-1.40893600	3.29519000
C	2.70210100	-0.88730400	-1.87162800	H	-2.53272200	0.13471400	2.17662300
H	2.70378500	3.73257000	0.97978200	C	-3.77751500	-3.55290200	2.18985600
H	2.27873900	3.75121600	2.69972000	H	-2.96448800	-3.68970100	0.19330300
H	0.34744900	5.19975000	1.73345500	C	-3.98341200	-2.73637000	3.30546900
H	3.78734000	1.88617300	2.43095300	H	-3.70053900	-0.76829800	4.16514200
H	2.17882400	1.15163300	2.55148000	H	-4.12495300	-4.58826600	2.19694000
H	0.59258500	1.74277900	-2.38897400	H	-4.49090100	-3.13518700	4.18658300
H	0.54418000	0.74457800	-4.65182300	H	-3.07767800	-2.22937300	-2.68463800
H	1.85746700	-1.31621500	-5.14779800	C	-1.28407300	4.51837500	0.48488200
H	3.27083600	-2.33640000	-3.35848200	C	-2.32103100	4.52826500	1.42951500
H	3.32393200	-1.33320800	-1.09411400	C	-1.61258700	4.47551800	-0.87745000
C	1.09391100	-2.16463100	3.09437000	C	-3.65390100	4.46090600	1.01884000
C	0.08119000	-3.31859500	3.04491300	H	-2.08823400	4.58094700	2.49504400
H	-0.72448800	-3.11536400	2.32754600	C	-2.94364000	4.41468000	-1.29027200
H	0.54982700	-4.27801000	2.77636100	H	-0.81366600	4.47550500	-1.62359900
H	-0.38776900	-3.44866700	4.03136400	C	-3.96803800	4.39507800	-0.34150400
C	2.15972700	-2.44036800	4.16832100	H	-4.45093600	4.46528300	1.76580800
H	2.66535300	-3.40786800	4.02493200	H	-3.18151700	4.37399800	-2.35482000
H	2.92864600	-1.65065200	4.18191000	H	-5.01060800	4.33783100	-0.66174200
H	1.69143100	-2.46476700	5.16372300				

8. References

1. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian 16, Revision B.01; Gaussian, Inc.: Wallingford, CT, 2019.
2. (a) Becke, A. D. Density – functional thermochemistry. III. The role of exact exchange. *J. Chem. Phys.* **1993**, 98, 5648; (b) Lee, C.; Yang, W.; Parr, R. G. Development of the Colle-Salvetti correlation-energy formula into a functional of the electron density. *Phys. Rev. B* **1988**, 37, 785.
3. Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, H. A consistent and accurate *ab initio* parametrization of density functional dispersion correction (DFT-D) for the 94 elements H-Pu. *J. Chem. Phys.* **2010**, 132, 154104.
4. Grimme, S.; Ehrlich, S.; Goerigk, L. Effect of the damping function in dispersion corrected density functional theory. *J. Comput. Chem.* **2011**, 32, 1456.
5. Weigend, F.; Ahlrichs, R. Balanced basis sets of split valence, triple zeta valence and quadruple zeta valence quality for H to Rn: Design and assessment of accuracy. *Phys. Chem. Chem. Phys.* **2005**, 7, 3297.
6. Schafer, A.; Huber, C.; Ahlrichs, R. Fully optimized contracted Gaussian basis sets of triple zeta valence quality for atoms Li to Kr. *J. Chem. Phys.* **1994**, 100, 5829.
7. Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. Universal Solvation Model Based on Solute Electron Density and on a Continuum Model of the Solvent Defined by the Bulk Dielectric Constant and Atomic Surface Tensions. *J. Phys. Chem. B* **2009**, 113, 6378.
8. Keith, J. A.; Carter, E. A. Quantum Chemical Benchmarking, Validation, and Prediction of Acidity Constants for Substituted Pyridinium Ions and Pyridinyl Radicals. *J. Chem. Theory Comput.* **2012**, 8, 3187.
9. Lu, T. Molclus program, Version 1.9.9, <http://www.keinsci.com/research/molclus.html>
10. Bannwarth, C.; Caldeweyher, E.; Ehlert, S.; Hansen, A.; Pracht, P.; Seibert, J.; Spicher, S.; Grimme, S. Extended tight-binding quantum chemistry methods. *WIREs Comput Mol Sci.* **2021**, 11, e1493. <https://doi.org/10.1002/wcms.1493>
11. Legault, C. Y. CYLview20. <http://www.cylview.org>, Université de Sherbrooke, Quebec, Canada, 2020.
12. Eliel, E. L.; Wilen, S. H.; Mander, L. N. Stereochemistry of Organic Compounds; Wiley: New York, **1994**; p 696.
13. Zhao, Y.; Truhlar, D. G. A New Local Density Functional for Main-Group Thermochemistry, Transition Metal Bonding, Thermochemical Kinetics, and Noncovalent Interactions. *J. Chem. Phys.* **2006**, 125, 194101.

14. Zhao, Y.; Truhlar, D. G. The M06 Suite of Density Functionals for Main Group Thermochemistry, Thermochemical Kinetics, Noncovalent Interactions, Excited States, and Transition Elements: Two New Functionals and Systematic Testing of Four M06-Class Functionals and 12 Other Functionals. *Theor. Chem. Acc.* **2008**, *120*, 215.
15. (a) Becke, A. D. Density-Functional Exchange-Energy Approximation with Correct Asymptotic Behavior. *Phys. Rev. A* **1988**, *38*, 3098. (b) Perdew, J. P. Density-Functional Approximation for the Correlation Energy of the Inhomogeneous Electron Gas. *Phys. Rev. B* **1986**, *33*, 8822.
16. (a) Perdew, J. P.; Chevary, J. A.; Vosko, S. H.; Jackson, K. A.; Pederson, M. R.; Singh, D. J.; Fiolhais, C. Atoms, Molecules, Solids, and Surfaces: Applications of the Generalized Gradient Approximation for Exchange and Correlation. *Phys. Rev. B* **1992**, *46*, 6671. (b) Perdew, J. P.; Chevary, J. A.; Vosko, S. H.; Jackson, K. A.; Pederson, M. R.; Singh, D. J.; Fiolhais, C. Erratum: Atoms, Molecules, Solids, and Surfaces: Applications of the Generalized Gradient Approximation for Exchange and Correlation. *Phys. Rev. B: Condens. Matter Mater. Phys.* **1993**, *48*, 4978. (c) Perdew, J. P.; Burke, K.; Wang, Y. Generalized Gradient Approximation for the Exchange-correlation Hole of A Many-electron System. *Phys. Rev. B* **1996**, *54*, 16533.
17. Adamo, C.; Barone, V. Toward reliable density functional methods without adjustable parameters: The PBE0 model. *J. Chem. Phys.* **1999**, *110*, 6158.