

- *Electronic Supplementary Information* -

Formation of cyanate in low-valent uranium chemistry: A synergistic  
experimental/theoretical study

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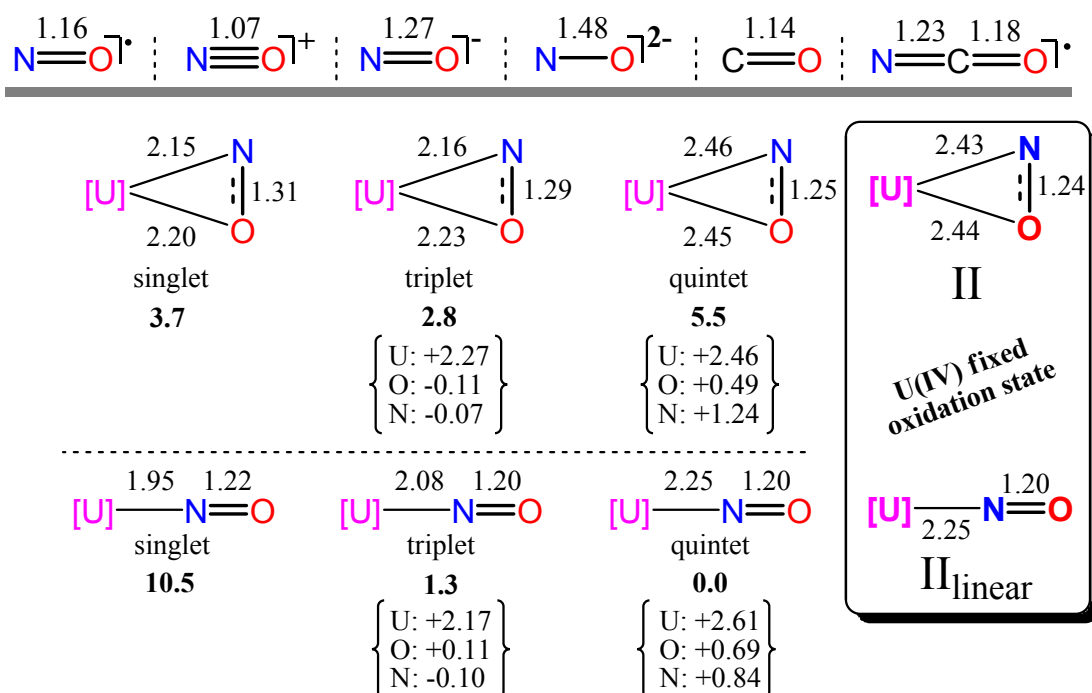
Table S1. Crystal data and structure refinement for [U(1,4-{SiPr<sub>3</sub>}<sub>2</sub>C<sub>8</sub>H<sub>6</sub>)Cp\*]<sub>2</sub>(NCO) **3**.

Empirical formula	C <sub>73</sub> H <sub>126</sub> N O Si <sub>4</sub> U <sub>2</sub>	
Formula weight	1622.16	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P $\bar{1}$ (No.2)	
Unit cell dimensions	a = 13.5419(2) Å	α = 78.856(1)°.
	b = 20.2254(3) Å	β = 87.152(1)°.
	c = 28.0988(4) Å	γ = 89.406(1)°.
Volume	7541.55(19) Å <sup>3</sup>	
Z	2	
Density (calculated)	1.429 Mg/m <sup>3</sup>	
Absorption coefficient	4.392 mm <sup>-1</sup>	
F(000)	3276.4	
Crystal size	0.14 x 0.10 x 0.07 mm <sup>3</sup>	
Theta range for data collection	3.39 to 26.73°.	
Reflections collected	31667	
Independent reflections	21950 [R(int) = 0.0553]	
Completeness to theta = 26.73°	98.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.735 and 0.596	
Refinement method	Full-matrix least-squares on F <sup>2</sup>	
Data / restraints / parameters	31667 / 12 / 1461	
Goodness-of-fit on F <sup>2</sup>	1.013	
Final R indices [I > 2σ(I)]	R1 = 0.0553, wR2 = 0.1056	
R indices (all data)	R1 = 0.098, wR2 = 0.1193	

Due to disorder, the bond lengths and angles associated with the bridging isocyanate group are unreliable.

Data collection KappaCCD , Program package WinGX , Abs correction MULTISCAN  
Refinement using SHELXL-97 , Drawing using ORTEP-3 for Windows

## Theoretical Data and Results



**Scheme S1.** Geometrical features of the  $\text{NO}\cdot$ ,  $\text{NO}^+$ ,  $\text{NO}^-$ ,  $\text{NO}_2^-$ ,  $\text{CO}$ , and  $\text{NCO}\cdot$  free molecules, along with all the spin state combinations for the two different bonding modes of the  $\text{NO}$  substrate on intermediate **II**. Numbers in bold refer to relative enthalpy energies in  $\text{kcal}\cdot\text{mol}^{-1}$ . All given bond lengths are in angstroms. The figures in braces correspond to the Mulliken atomic spin densities.

### Cartesian coordinates and enthalpy energies.

**I** (small core, quartet)

H= -1186.411491 au

U	0.15994600	-2.26845500	5.44798900
C	2.77960000	-2.29745000	5.94260800
C	2.15503500	-2.93267200	7.05734600
C	1.20515200	-3.96672500	7.22766300
C	0.42340800	-4.76323500	6.36092500
C	0.25874200	-4.86677100	4.95939200
C	0.85359600	-4.25654800	3.81471900
C	1.88210600	-3.28051000	3.66770700
C	2.66544800	-2.48403900	4.53352500
C	-1.11584000	-0.03212400	6.20373000
C	-1.68565000	-1.03017100	7.04886700
C	-1.54580200	-0.29485900	4.86445300
C	-2.38328800	-1.45128200	4.89131900
C	-2.46492500	-1.90382400	6.23817600
H	2.05026000	-2.99932300	2.62801400
H	3.26010800	-1.76876200	3.96533500
Si	4.04336000	-0.98545800	6.43258100
H	4.13487200	0.07902700	5.38263700
H	2.43362900	-2.49098200	8.01300600
H	0.94775700	-4.11968000	8.27360000
H	-0.29364000	-5.37724700	6.90168500
H	-0.55670800	-5.54285500	4.70764400
H	1.01935000	-6.04520300	1.65501700

Si	0.19129900	-4.90896000	2.17335500
H	0.20607900	-3.83385500	1.12998000
H	-1.21047700	-5.40885500	2.33736700
C	-3.28465000	-3.05990900	6.73379200
C	-3.11866700	-2.02960700	3.71563300
C	-1.26513200	0.56650700	3.66459100
C	-1.55902800	-1.09813100	8.54435800
C	-0.31577500	1.15848600	6.65378300
H	5.41250800	-1.57166600	6.59769800
H	3.66498000	-0.35223700	7.73602100
H	-3.33289400	-3.09438600	3.84821000
H	-4.08204900	-1.52518300	3.56098600
H	-2.55542900	-1.92529900	2.78196300
H	-3.40873900	-3.83232800	5.96850200
H	-2.83060200	-3.53687100	7.60830500
H	-4.29137600	-2.73695100	7.03062700
H	-1.60906600	-2.12770600	8.91302800
H	-0.61466500	-0.67090800	8.89664600
H	-2.36553500	-0.54041800	9.03918900
H	0.38159800	1.50398700	5.88298500
H	-0.96712000	2.01009700	6.89353700
H	0.27212600	0.94551400	7.55253600
H	-1.31720500	-0.00116600	2.72958600
H	-1.99219000	1.38554600	3.57841800
H	-0.27382900	1.03170000	3.70978100

#### I (large core)

H= -741.196141 au

U	0.08832600	-2.41670200	5.55095500
C	2.84120700	-2.20340400	5.63698300
C	2.46454900	-2.79281200	6.88087900
C	1.65692400	-3.88560000	7.27956000
C	0.85865700	-4.84721000	6.61043500
C	0.53178900	-5.12266100	5.26053900
C	0.87981800	-4.56692600	3.99339600
C	1.72613600	-3.48169800	3.61187900
C	2.52462200	-2.52006400	4.28064700
C	-1.19925800	-0.04383300	6.44642200
C	-1.93050700	-1.09877900	7.06962500
C	-1.45764600	-0.09668700	5.04342400
C	-2.34869900	-1.18512900	4.80013100
C	-2.64072800	-1.80434800	6.05270900
H	1.72343600	-3.30162400	2.53753600
H	2.95785300	-1.81667200	3.57050800
Si	4.05716600	-0.77359300	5.81459300
H	3.88808800	0.20678700	4.69449600
H	2.85713200	-2.25705300	7.74384400
H	1.59271500	-3.97685100	8.36176700
H	0.33036400	-5.49879100	7.30325900
H	-0.19110200	-5.93414300	5.18771700
H	1.02648100	-6.61370400	2.07364400
Si	0.13744100	-5.49767400	2.53159400
H	-0.06443000	-4.57856200	1.36622400
H	-1.18097600	-6.10160000	2.90786800
C	-3.62735600	-2.91665900	6.27545400
C	-2.96631300	-1.54380600	3.47717600
C	-0.97442500	0.89479300	4.02158300
C	-2.04061700	-1.33975700	8.54942600
C	-0.40269000	1.01497400	7.15669900
H	5.47873000	-1.24686400	5.78372600

H	3.84824900	-0.06428000	7.11714300
H	-3.16026300	-2.61805200	3.38682300
H	-3.92957400	-1.03579800	3.33553600
H	-2.33113800	-1.25602400	2.63310000
H	-3.70080300	-3.58395600	5.41044100
H	-3.36868900	-3.53349600	7.14254400
H	-4.63621000	-2.52256000	6.45751700
H	-2.23733800	-2.39106400	8.78364000
H	-1.13030400	-1.05089500	9.08472500
H	-2.86347400	-0.75842400	8.98660000
H	0.40215300	1.41648000	6.53246200
H	-1.03644600	1.86531900	7.44201800
H	0.05634600	0.63945200	8.07708300
H	-0.88972200	0.45351000	3.02289500
H	-1.66452400	1.74449500	3.93326200
H	0.00572800	1.31019600	4.27832800

$\Pi_{\text{linear}}$  (small core, singlet)

H= -1316.274891 au

U	-0.37316500	-0.51431700	-0.33263500
C	-2.68045000	0.76458500	-0.15836300
C	-2.07585200	1.24918300	-1.35295400
C	-1.55357200	0.66400200	-2.52743100
C	-1.25252700	-0.64422900	-2.93699800
C	-1.35167700	-1.92594700	-2.35002800
C	-1.95393200	-2.46149500	-1.17675300
C	-2.66946400	-1.86034000	-0.10823000
C	-2.96328000	-0.54671000	0.30775800
C	1.65700900	1.25015300	-0.46790700
C	1.77250300	0.46158700	-1.65511900
C	1.96450400	0.42636100	0.65116300
C	2.25820800	-0.88584800	0.16236900
C	2.13340100	-0.86281800	-1.25475100
H	-2.93559600	-2.57160000	0.67138400
H	-3.38735100	-0.55417200	1.31016400
Si	-3.26659600	2.13460000	1.00903200
H	-3.28498700	1.64969400	2.42142000
H	-1.97212000	2.33333600	-1.36930900
H	-1.17314400	1.40921100	-3.22177800
H	-0.69473000	-0.66464600	-3.87051600
H	-0.82745200	-2.67522600	-2.94181300
H	-2.89972000	-5.02235400	-1.78042100
Si	-1.79380500	-4.34248600	-1.03333900
H	-1.85719300	-4.76940700	0.39584700
H	-0.50009900	-4.79281700	-1.63806700
C	2.44482500	-2.00107700	-2.18409400
C	2.73195400	-2.03210600	1.00434500
C	2.08936400	0.86206300	2.07956600
C	1.80670200	0.99118600	-3.05720100
C	1.38092100	2.72630500	-0.42282600
H	-4.64914900	2.58093100	0.64536700
H	-2.36414400	3.32398000	0.89651500
H	2.67185600	-2.98247700	0.46634100
H	3.78259200	-1.88944300	1.28897200
H	2.14724100	-2.12747700	1.92434300
H	1.66198200	0.12580300	2.76699800
H	3.14521200	0.99850100	2.34748300
H	1.58673200	1.81716200	2.25659900
H	0.87407400	3.02461200	0.49984800
H	2.31652800	3.29863200	-0.47213300

H	0.75837900	3.05237500	-1.26078700
H	1.47966600	0.24869400	-3.79013600
H	1.17779600	1.87702000	-3.17893300
H	2.82968900	1.28367400	-3.33002200
H	2.19681400	-2.97246100	-1.74558300
H	1.89976200	-1.91638500	-3.12830400
H	3.51506100	-2.02360400	-2.42779000
N	-0.21904500	-1.13167200	1.50715900
O	-0.08979300	-1.51541400	2.65613400

**H<sub>linear</sub>** (small core, triplet)

H= -1316.28944 au

U	-0.38028100	-0.49516300	-0.39404600
C	-2.72179900	0.75222800	-0.12890600
C	-2.15427300	1.27172500	-1.32553700
C	-1.62150200	0.71948000	-2.51067800
C	-1.32459800	-0.57867300	-2.96351000
C	-1.43142700	-1.87870400	-2.42350600
C	-1.98839200	-2.44706200	-1.24400100
C	-2.66087900	-1.87677100	-0.12913900
C	-2.95948200	-0.57366200	0.32469300
C	1.68779400	1.24400000	-0.48338100
C	1.82489800	0.41816400	-1.64278100
C	1.96024500	0.44580400	0.66018600
C	2.25672300	-0.88672400	0.21039300
C	2.16399100	-0.90148900	-1.20740500
H	-2.90767300	-2.61269800	0.63414400
H	-3.36783700	-0.60551900	1.33333300
Si	-3.31161500	2.08702800	1.07390200
H	-3.28487300	1.58022600	2.47963000
H	-2.06779400	2.35754800	-1.32086000
H	-1.25453200	1.48544400	-3.19000600
H	-0.78581000	-0.57082100	-3.90815900
H	-0.92733000	-2.61098700	-3.05302900
H	-2.97411600	-4.99023900	-1.88005800
Si	-1.83551400	-4.33025000	-1.16430900
H	-1.84323900	-4.79982100	0.25444300
H	-0.56988800	-4.77634600	-1.82900100
C	2.50128700	-2.05806400	-2.10529100
C	2.75776100	-2.00414300	1.07516600
C	2.10033100	0.93954000	2.06857400
C	1.85392000	0.90175100	-3.06188700
C	1.44212300	2.72629300	-0.48855800
H	-4.71387300	2.50957100	0.75853900
H	-2.44208000	3.30128600	0.96498800
H	2.63051600	-2.97796400	0.59394900
H	3.83021600	-1.88083700	1.27558900
H	2.24517000	-2.04258500	2.04022600
H	1.76987100	0.19839100	2.80130000
H	3.14946400	1.17708700	2.28855600
H	1.52069600	1.85147900	2.23771200
H	0.94442800	3.06418200	0.42525300
H	2.38662700	3.28127800	-0.56284100
H	0.81989500	3.03493300	-1.33374900
H	1.55640600	0.12336000	-3.76945900
H	1.19950500	1.76325100	-3.21904700
H	2.87037900	1.21495000	-3.33613200
H	2.30125400	-3.02133100	-1.62690500
H	1.93062300	-2.03176100	-3.03851600
H	3.56513700	-2.04900400	-2.37688800

N	-0.18379900	-1.11239100	1.58588900
O	-0.06272600	-1.46886300	2.72571000

**$\Pi_{\text{linear}}$**  (small core, quintet)

H= -1316.291551 au

U	-0.36600800	-0.62241700	-0.35577100
C	-2.61540300	0.73956100	0.02593200
C	-2.02080100	1.31329600	-1.13125000
C	-1.52514800	0.81665800	-2.35353100
C	-1.29012100	-0.45958200	-2.89759100
C	-1.47648400	-1.79075300	-2.46604400
C	-2.09404600	-2.41116300	-1.34545600
C	-2.74178400	-1.87986900	-0.19981800
C	-2.94348400	-0.60190000	0.36242100
C	1.61682500	1.24841200	-0.63567400
C	1.83476100	0.34013900	-1.71262100
C	1.89439800	0.56411000	0.58294200
C	2.29336500	-0.76910000	0.25814300
C	2.23161200	-0.91286100	-1.15674000
H	-3.04001600	-2.65317700	0.50609600
H	-3.34402600	-0.69237100	1.37080800
Si	-3.11287200	2.00322700	1.34008500
H	-3.09576900	1.38449500	2.70098400
H	-1.86705300	2.38809400	-1.04730200
H	-1.11234100	1.60767500	-2.97563400
H	-0.73463600	-0.40844900	-3.83082300
H	-1.00531300	-2.49946500	-3.14611200
H	-3.24622000	-4.82605500	-2.17363800
Si	-2.06948800	-4.30033400	-1.41023500
H	-2.11680000	-4.87607000	-0.03151200
H	-0.83271200	-4.77855500	-2.10611200
C	2.65832400	-2.12452300	-1.93631700
C	2.86069900	-1.78331900	1.20737800
C	1.89365800	1.17397700	1.95543300
C	1.88197400	0.69816300	-3.16766400
C	1.30537400	2.71084300	-0.76743900
H	-4.49342500	2.52715300	1.08725900
H	-2.17723300	3.17232300	1.31557800
H	2.61806800	-2.80849200	0.91121400
H	3.95558200	-1.70560700	1.23283300
H	2.49627500	-1.64580500	2.22708100
H	1.69230800	0.43084600	2.73165300
H	2.86533200	1.63197000	2.18349300
H	1.14059900	1.96236900	2.05363100
H	0.73729200	3.08952200	0.08761500
H	2.22846400	3.30274300	-0.82569300
H	0.72581800	2.92591000	-1.66955200
H	1.66418100	-0.15800900	-3.81211500
H	1.17884000	1.49534000	-3.42311600
H	2.88455000	1.05528300	-3.43880700
H	2.49215800	-3.05132500	-1.37866300
H	2.12151000	-2.21158900	-2.88588300
H	3.72935800	-2.08426800	-2.17561900
N	-0.18727800	-1.58068900	1.66967500
O	0.00106600	-2.07923900	2.74106700

**$\Pi_{\text{linear}}$**  (5f-in-core)

H= -876.702267 au

U	-0.39511200	-0.54239100	-0.32513700
C	-2.75887600	0.77617700	-0.19359300

C	-2.17220500	1.26015000	-1.40905900
C	-1.66012700	0.65871400	-2.57283400
C	-1.36931600	-0.66235000	-2.99246200
C	-1.47066000	-1.94617500	-2.42411700
C	-2.06230300	-2.48257800	-1.23373600
C	-2.76904400	-1.86493800	-0.16528600
C	-3.05216600	-0.54056300	0.25843700
C	1.70110600	1.25525600	-0.42190200
C	1.84655500	0.45917200	-1.60079400
C	1.99749000	0.42905900	0.70244600
C	2.30922200	-0.89325300	0.21275400
C	2.19932800	-0.87157000	-1.20835700
H	-3.06300900	-2.57636900	0.60449800
H	-3.49432800	-0.55093000	1.25330400
Si	-3.38050100	2.14164600	0.95110700
H	-3.40924700	1.66533000	2.36781200
H	-2.08750000	2.34507500	-1.44179000
H	-1.28848300	1.39659100	-3.28023400
H	-0.83200700	-0.67754200	-3.93821000
H	-0.98493000	-2.70171100	-3.03968800
H	-3.07658400	-5.01118500	-1.89343200
Si	-1.96731900	-4.36399900	-1.12115500
H	-2.07138700	-4.80928800	0.30183500
H	-0.67606500	-4.85370400	-1.70153200
C	2.56155200	-1.98848300	-2.14528100
C	2.88354000	-2.01226000	1.02746500
C	2.20118000	0.91179100	2.10625600
C	1.83194300	0.97027800	-3.00878700
C	1.45255900	2.73626600	-0.38713000
H	-4.76639700	2.57335700	0.57936200
H	-2.49552400	3.34552700	0.84951000
H	2.72790200	-2.98235700	0.54793900
H	3.96667100	-1.87669100	1.14513100
H	2.44723500	-2.06626000	2.02791800
H	1.95296400	0.15063800	2.84981600
H	3.25077300	1.19502500	2.25981500
H	1.59127400	1.79305000	2.32222700
H	0.94615000	3.04528800	0.53182900
H	2.39590300	3.29516600	-0.43924900
H	0.83339500	3.06566700	-1.22650000
H	1.49983100	0.20888200	-3.71904600
H	1.18394200	1.84244900	-3.12377900
H	2.84373600	1.27460600	-3.30729300
H	2.42981300	-2.96973000	-1.68092200
H	1.95283600	-1.97297700	-3.05456100
H	3.61183200	-1.91682900	-2.45649800
N	-0.01518400	-1.21740500	1.79235900
O	0.19347300	-1.57649900	2.91513300

## II (small core, singlet)

H= -1316.285647 au

O	0.83786900	-0.63940100	3.41674000
U	0.17596700	-2.13275000	4.89675100
C	2.54200400	-2.40396600	6.12052800
C	1.60455500	-2.94469000	7.03855800
C	0.56458200	-3.89074600	6.97091600
C	-0.06183700	-4.62806000	5.94978000
C	0.12705200	-4.78131500	4.56033800
C	1.08851800	-4.33050000	3.62297800
C	2.21622600	-3.48176800	3.74631800



C	2.79464400	-2.68132100	4.75128500
C	-1.04956300	0.01064000	5.99679500
C	-1.28893500	-1.00894200	6.96606100
C	-1.81006500	-0.29762200	4.83119800
C	-2.47299600	-1.53698400	5.06037800
C	-2.16936500	-1.96553300	6.38659500
H	2.67085800	-3.25839900	2.78341100
H	3.55795300	-2.03240400	4.32596800
Si	3.71405100	-1.12902300	6.88073400
H	4.22038800	-0.18958100	5.83499500
H	1.65049800	-2.48048700	8.02255200
H	0.03954700	-3.98287300	7.91865200
H	-0.95893700	-5.13244400	6.30030600
H	-0.68264900	-5.35527100	4.11023200
H	1.24432200	-6.32644900	1.68194000
Si	0.75173700	-4.92123300	1.85392500
H	1.45422800	-4.05137400	0.86608900
H	-0.71892100	-4.92871900	1.58025100
C	-2.84189200	-3.09476200	7.10804000
C	-3.40751900	-2.21932200	4.10391700
C	-1.98926400	0.59790100	3.64400400
C	-0.85570900	-0.96178000	8.40064400
C	-0.23805100	1.25636900	6.20603200
H	4.89131100	-1.80187400	7.51665000
H	3.01027400	-0.35181600	7.94981800
H	-3.44765300	-3.30003500	4.27174700
H	-4.43190700	-1.83962100	4.21254000
H	-3.10960400	-2.05747500	3.06380600
H	-3.08935000	-3.92507500	6.44049000
H	-2.22855900	-3.49049900	7.92159400
H	-3.78483200	-2.75172900	7.55406800
H	-0.77301100	-1.95882400	8.84163800
H	0.10895400	-0.46121800	8.52373200
H	-1.58491800	-0.40290800	9.00225500
H	0.21985500	1.60038400	5.27436100
H	-0.86375300	2.07537500	6.58469400
H	0.56501700	1.10574700	6.93430700
H	-2.26943600	0.03599500	2.75034300
H	-2.77816000	1.33495500	3.84248100
H	-1.07296800	1.14329400	3.40518100
N	0.01286600	-1.48149400	2.85010300

**H** (small core, triplet)

H= -1316.287162 au

O	0.78967300	-0.66474900	3.35297200
U	0.16598100	-2.14181800	4.90709000
C	2.53117500	-2.40599500	6.13223300
C	1.60494100	-2.96679900	7.04981400
C	0.56551600	-3.91103000	6.97358600
C	-0.06263000	-4.63546300	5.94381600
C	0.13362100	-4.78580100	4.55453000
C	1.09672100	-4.33042000	3.62139600
C	2.21836400	-3.47273900	3.74963300
C	2.78570400	-2.67037900	4.75891300
C	-1.04376600	0.01890800	5.98627600
C	-1.28256000	-0.99981900	6.95837000
C	-1.81358100	-0.28582000	4.82647100
C	-2.48249700	-1.52089800	5.06109900
C	-2.17153100	-1.95141900	6.38542000
H	2.67699300	-3.24708500	2.78897900

H	3.54583600	-2.01358100	4.33936700
Si	3.69950200	-1.13482500	6.90227500
H	4.19160700	-0.17603400	5.86666200
H	1.65488200	-2.51500400	8.03937100
H	0.04087000	-4.01339500	7.92066900
H	-0.96074500	-5.14244200	6.28832000
H	-0.67314500	-5.36044500	4.09979700
H	1.29021600	-6.33311800	1.68954000
Si	0.77847800	-4.93381300	1.85368500
H	1.47575100	-4.06005000	0.86496300
H	-0.69011800	-4.96084200	1.57001600
C	-2.84585000	-3.07975500	7.10689500
C	-3.43403200	-2.20313600	4.12185700
C	-1.98762600	0.60635900	3.63567000
C	-0.84084800	-0.95207900	8.39030200
C	-0.22349400	1.25939600	6.19459400
H	4.88798700	-1.80508800	7.52007600
H	2.99916400	-0.37624900	7.98702300
H	-3.38571600	-3.29363400	4.20962300
H	-4.47192800	-1.91221100	4.33069000
H	-3.22619300	-1.94791000	3.07939900
H	-3.08901400	-3.91126300	6.43903000
H	-2.23439500	-3.47358200	7.92272200
H	-3.79124500	-2.73815600	7.54900400
H	-0.76383400	-1.94880400	8.83287000
H	0.12853100	-0.45901000	8.50668800
H	-1.56242800	-0.38557200	8.99403900
H	0.18962500	1.63320000	5.25365900
H	-0.82923400	2.06574600	6.62888800
H	0.61455300	1.08794200	6.87794500
H	-2.27155100	0.04405900	2.74289600
H	-2.77156500	1.34958600	3.82944900
H	-1.06861500	1.14661900	3.39442000
N	-0.00413000	-1.54121000	2.84371500

## II (small core, quintet)

H= -1316.282725 au

O	0.51086000	-0.95407600	2.84125400
U	0.11552500	-2.22811000	4.89841500
C	2.48691500	-2.33081000	6.11861900
C	1.58851900	-2.92742900	7.04196800
C	0.57727300	-3.90333700	6.97652700
C	-0.02090600	-4.67404900	5.95947100
C	0.21028300	-4.86307600	4.58080500
C	1.16341400	-4.38109200	3.64732200
C	2.22405600	-3.44782200	3.75253500
C	2.74288700	-2.58725600	4.74413600
C	-0.97309900	-0.01654300	6.03918300
C	-1.27468500	-1.03763300	6.98836000
C	-1.75033500	-0.25760500	4.86829300
C	-2.49379800	-1.45513900	5.07667900
C	-2.20545300	-1.93330000	6.38875200
H	2.66460300	-3.21160800	2.78593500
H	3.46008200	-1.89215100	4.30948100
Si	3.61259900	-1.00744600	6.86080200
H	3.91265900	0.05379800	5.85042600
H	1.62096600	-2.46310000	8.02569400
H	0.04517800	-3.99659400	7.92038800
H	-0.90678100	-5.20081100	6.30659900
H	-0.56013500	-5.48778300	4.13002200

H	1.58989200	-6.37045600	1.73804700
Si	0.90080000	-5.04800800	1.89403500
H	1.46726900	-4.10888400	0.88107100
H	-0.55512300	-5.27007400	1.63319800
C	-2.90841200	-3.06376100	7.08024300
C	-3.49242600	-2.04478800	4.12297400
C	-1.89140600	0.67995000	3.70664300
C	-0.85633100	-1.03670800	8.42784600
C	-0.10273600	1.18497400	6.27617500
H	4.91439300	-1.59828700	7.30654500
H	2.96233300	-0.38295000	8.05592700
H	-3.60117800	-3.12554800	4.25871000
H	-4.48609800	-1.60247200	4.27270000
H	-3.20795100	-1.87014600	3.08178000
H	-3.19175400	-3.86037600	6.38600700
H	-2.29284100	-3.51076300	7.86541400
H	-3.83246300	-2.71068400	7.55692200
H	-0.78862600	-2.04569500	8.84383800
H	0.11118500	-0.54912900	8.57530900
H	-1.58801300	-0.48785800	9.03561300
H	0.39621100	1.51740900	5.36009900
H	-0.69398700	2.03477200	6.64234800
H	0.67306400	0.98942400	7.02242900
H	-2.20204500	0.15692900	2.79932600
H	-2.64725000	1.44445400	3.92863100
H	-0.95559600	1.19582200	3.47657600
N	-0.38811600	-1.76380500	2.53664500

## II (5f-in-core)

H= -876.710480 au

O	0.11517100	-1.14482200	2.74175500
U	0.08691700	-2.22562500	4.93325500
C	2.71305300	-1.92562500	5.61768800
C	2.13692300	-2.37006000	6.84327100
C	1.25976300	-3.40902200	7.20884200
C	0.53283700	-4.42555500	6.54577600
C	0.42889200	-4.87982400	5.20902700
C	1.12927400	-4.58921200	3.99847700
C	2.10909700	-3.60835800	3.67725900
C	2.73054800	-2.51007200	4.31346300
C	-1.09687700	-0.22470300	6.44097500
C	-1.63159200	-1.43602800	6.98260100
C	-1.61673600	-0.07031400	5.12176400
C	-2.46998200	-1.18754600	4.84582500
C	-2.47300300	-2.03304900	5.99466600
H	2.35106600	-3.60723600	2.61569800
H	3.28877500	-1.91540900	3.59216400
Si	3.83408200	-0.41550100	5.78410900
H	3.82233300	0.38736300	4.52190500
H	2.34685500	-1.70973600	7.68282300
H	0.98027000	-3.34491400	8.25743000
H	-0.17191600	-4.92545800	7.20637000
H	-0.33222900	-5.65057800	5.09990900
H	1.41077600	-7.01237500	2.63340700
Si	0.65397800	-5.72039900	2.56216400
H	0.96953500	-5.07199400	1.25374600
H	-0.80326700	-6.05735800	2.62304900
C	-3.32513700	-3.25343500	6.19626200
C	-3.35061500	-1.33611500	3.63963300
C	-1.43373100	1.12467000	4.23305800

C	-1.52259500	-1.87536100	8.41190300
C	-0.27084100	0.77736800	7.19495900
H	5.25040100	-0.81868000	6.05771600
H	3.37664100	0.44546300	6.91978200
H	-3.60771400	-2.38081300	3.44568600
H	-4.29097300	-0.78801200	3.78196700
H	-2.88342700	-0.94628000	2.73063300
H	-3.58702400	-3.72924200	5.24710300
H	-2.82585400	-4.00641300	6.81431100
H	-4.26670400	-2.99585400	6.69841800
H	-1.58451800	-2.96202500	8.51541100
H	-0.58801300	-1.54647400	8.87341900
H	-2.34342200	-1.44705700	9.00222700
H	0.30124200	1.42370700	6.52376800
H	-0.90957100	1.43039400	7.80373500
H	0.44151400	0.29761300	7.87283100
H	-1.42434600	0.85336000	3.17383600
H	-2.25078900	1.84306700	4.37844300
H	-0.49884200	1.65252600	4.44261600
N	-0.62680400	-2.12862500	2.61158500

### III<sub>linear</sub> (large core)

H= -1623.608333 au

U	-0.34079100	-0.52469300	-0.18386900
C	-2.69835100	0.82403500	-0.41055300
C	-2.03912500	1.14491300	-1.64000100
C	-1.46174000	0.39700700	-2.67915900
C	-1.12017900	-0.95622200	-2.89763300
C	-1.25716100	-2.15779900	-2.17506700
C	-1.99346600	-2.54546500	-1.01011500
C	-2.78399900	-1.79480800	-0.10034900
C	-3.06136900	-0.42932600	0.15774900
C	1.65745800	1.42367800	-0.38368800
C	1.78573700	0.69243800	-1.60428600
C	2.05836800	0.56756400	0.68230100
C	2.41293500	-0.70264500	0.12264800
C	2.23597800	-0.62759500	-1.28799000
O	0.17170700	-1.62091900	3.10952600
H	-3.17249400	-2.41151800	0.70811200
H	-3.59396600	-0.32109900	1.10057600
Si	-3.40366600	2.32648600	0.47920800
H	-3.64188900	2.02154800	1.92413600
H	-1.94099300	2.21646300	-1.80916100
H	-1.05113700	1.04004700	-3.45327700
H	-0.50120000	-1.08186600	-3.78375200
H	-0.71534700	-2.98004800	-2.64038600
H	-2.98984500	-5.11228200	-1.53158200
Si	-1.97430700	-4.40052400	-0.68781400
H	-2.29240400	-4.69260800	0.74420300
H	-0.63756500	-4.98532400	-1.02690300
C	2.62582700	-1.67663400	-2.28868500
C	3.01385000	-1.85055400	0.87643200
C	2.25203700	0.97973700	2.11009800
C	1.71800400	1.27686200	-2.98165000
C	1.32942500	2.88469000	-0.26723500
H	-4.71128100	2.75444000	-0.11641400
H	-2.46821600	3.49167100	0.37438400
U	0.26146700	-2.28738200	5.25573300
C	2.89967700	-2.05960200	5.85804000
C	2.22735900	-2.22417400	7.11055600

C	1.35922700	-3.19383800	7.65685300
C	0.60432200	-4.27656900	7.16114000
C	0.42599400	-4.88853300	5.89953900
C	1.11558300	-4.81583200	4.64831500
C	2.18418200	-3.99414200	4.21134900
C	2.89895800	-2.86778300	4.69007500
C	-1.09977400	-0.30911200	6.65029800
C	-1.56340600	-1.51276000	7.26830400
C	-1.59603600	-0.28447800	5.31400700
C	-2.34987600	-1.48130600	5.09875000
C	-2.32891200	-2.23959800	6.30626900
H	2.42890200	-4.16627200	3.16503100
H	3.52672600	-2.45689500	3.90257100
Si	4.12884500	-0.62592700	5.84501700
H	4.46812000	-0.24287600	4.44213800
H	2.43764000	-1.42732900	7.82247400
H	1.08266600	-2.95043100	8.67896800
H	-0.10518700	-4.64807100	7.89715000
H	-0.38670100	-5.61277800	5.90933700
H	1.24269400	-7.41576300	3.63670200
Si	0.55010300	-6.10986500	3.39260000
H	0.86617300	-5.66426600	2.00338400
H	-0.92062300	-6.35081300	3.52901000
C	-3.11130400	-3.49054100	6.58264900
C	-3.13265800	-1.80220400	3.86044000
C	-1.46119400	0.84671800	4.33938400
C	-1.48601800	-1.82694700	8.73101400
C	-0.37384900	0.80884400	7.34239600
H	5.39414600	-1.00709700	6.54944500
H	3.55653700	0.55747700	6.56172000
H	2.89022300	-2.79669200	0.34148100
H	4.09215000	-1.70068600	1.02220500
H	2.55222700	-1.96581000	1.85969600
H	2.07037200	0.15057500	2.79744500
H	3.27864900	1.33327000	2.27422300
H	1.58111900	1.79598800	2.39357400
H	0.87046700	3.12503000	0.69633700
H	2.23334600	3.50157700	-0.35650100
H	0.63596500	3.21136400	-1.04762700
H	1.38718700	0.54786600	-3.72634400
H	1.04596500	2.13734500	-3.03248500
H	2.71265200	1.62596800	-3.29082100
H	2.57092800	-2.68451900	-1.86736500
H	1.98330900	-1.65601600	-3.17396800
H	3.65753200	-1.52683800	-2.63329400
H	-3.33362600	-2.87363200	3.76795000
H	-4.10498800	-1.29272300	3.87366400
H	-2.60378600	-1.48383000	2.95848000
H	-3.30283000	-4.06549800	5.67239200
H	-2.59407200	-4.14965300	7.28612900
H	-4.08732500	-3.24917100	7.02301200
H	-1.46262200	-2.90284000	8.92465100
H	-0.60660800	-1.38133600	9.20334100
H	-2.36707000	-1.42673100	9.24999300
H	0.26415300	1.37213400	6.65532200
H	-1.08258900	1.52292000	7.78131200
H	0.26180500	0.44472800	8.15444800
H	-1.27555400	0.48853900	3.32184500
H	-2.37798800	1.44930500	4.32145300
H	-0.64158900	1.51858200	4.61046500

N	-0.08344600	-1.19368800	1.91728400
<b>III (large core)</b>			
H= -1623.620838 au			
U	-0.17205500	-0.81444400	0.24311400
C	-2.36964600	0.52567000	-0.60284900
C	-1.64769600	0.33940500	-1.81525400
C	-0.98038900	-0.73204100	-2.44144400
C	-0.69300200	-2.07773800	-2.14004600
C	-1.15055600	-2.99051700	-1.15660600
C	-2.11657900	-2.91682100	-0.12805700
C	-2.81299100	-1.82951000	0.46551600
C	-2.88167900	-0.42929000	0.33217900
C	1.59640500	1.35532400	0.22390100
C	1.63919700	0.91581000	-1.13363300
C	2.24485800	0.36711000	1.02450600
C	2.62863500	-0.70970400	0.17411800
C	2.24901600	-0.37203200	-1.16136200
O	0.03762000	-0.78259800	2.69190300
H	-3.36902400	-2.14257700	1.34804100
H	-3.46178300	0.02395700	1.13377400
Si	-3.00202500	2.28089200	-0.34012300
H	-3.15950100	2.57766200	1.11776300
H	-1.45542300	1.27387600	-2.33813900
H	-0.42490600	-0.39450000	-3.31307800
H	0.03190400	-2.51870300	-2.81871900
H	-0.69437700	-3.97183400	-1.26601500
H	-3.97916800	-4.79775900	0.68519600
Si	-2.50052700	-4.55466300	0.72476700
H	-2.10432000	-4.58124500	2.16962100
H	-1.81468700	-5.67908200	0.01860600
C	2.65297300	-1.13590500	-2.38730500
C	3.48644700	-1.88437800	0.54540000
C	2.63852600	0.55465700	2.45590600
C	1.34032600	1.77506200	-2.32401900
C	1.16576500	2.71795700	0.68767800
H	-4.33757800	2.47877500	-0.98964700
H	-2.05566900	3.27221000	-0.94302800
U	0.05630000	-2.19206400	4.70838500
C	2.45355700	-2.25478800	5.97164400
C	1.59654500	-2.85967300	6.93265300
C	0.59112400	-3.84688000	6.91205800
C	-0.04281600	-4.64552600	5.93977200
C	0.22874800	-4.95275400	4.58221900
C	1.27232500	-4.61411600	3.69321200
C	2.30688200	-3.64072400	3.74733300
C	2.75977200	-2.63861400	4.62655200
C	-0.96062300	0.00998300	6.11468000
C	-1.28870200	-1.07840100	6.97908000
C	-1.78342100	-0.09115100	4.95282300
C	-2.56448400	-1.27763500	5.06557100
C	-2.25336200	-1.89183000	6.31848800
H	2.83708900	-3.56494100	2.79932500
H	3.52480100	-2.01573500	4.16660000
Si	3.59676400	-0.92411700	6.65955200
H	3.88452900	0.11756400	5.62488300
H	1.63280400	-2.36388700	7.89999200
H	0.07609900	-3.90351500	7.86789300
H	-0.92605900	-5.15332100	6.31747600
H	-0.50094600	-5.64477900	4.16726100

H	2.59292000	-6.12155300	1.78456700
Si	1.24146900	-5.52720100	2.04342600
H	0.93484300	-4.64097100	0.87496500
H	0.23385300	-6.63027300	2.08264600
C	-3.00560200	-3.03951700	6.92342200
C	-3.68920900	-1.70209300	4.16683600
C	-1.93578800	0.98580900	3.92470100
C	-0.89301200	-1.17944600	8.42027900
C	-0.09164300	1.18117300	6.47632400
H	4.90816900	-1.50753400	7.08900700
H	2.97687800	-0.27074200	7.85491800
H	3.08170900	-2.83964500	0.19324500
H	4.48975100	-1.78283200	0.11234400
H	3.60867300	-1.95588800	1.62762400
H	2.68302300	-0.38931500	3.00073800
H	3.62923400	1.02402900	2.51826100
H	1.93730300	1.20157000	2.98888200
H	0.82563700	2.70951800	1.72729900
H	1.99506800	3.43536300	0.62799200
H	0.34920900	3.11877700	0.08031900
H	1.07005400	1.18860000	-3.20547000
H	0.53193200	2.48502300	-2.13091100
H	2.22829200	2.36373500	-2.59074800
H	2.65227600	-2.21639100	-2.21585000
H	1.99285600	-0.93442500	-3.23545200
H	3.66966300	-0.85908100	-2.69699700
H	-3.64065500	-2.76214300	3.89434200
H	-4.65829900	-1.54122600	4.65625700
H	-3.69526500	-1.12255600	3.24210600
H	-3.34954000	-3.74911700	6.16530300
H	-2.40082200	-3.59340200	7.64648600
H	-3.89627700	-2.67974300	7.45577600
H	-0.92773000	-2.20617600	8.79275500
H	0.10992800	-0.78648000	8.60690600
H	-1.58700300	-0.59263400	9.03705000
H	0.34698800	1.65614600	5.59366700
H	-0.66903900	1.95387000	7.00137500
H	0.73171600	0.89082400	7.13527100
H	-2.28584800	0.59719900	2.96760000
H	-2.66255700	1.73452600	4.26659900
H	-0.99375400	1.50759300	3.73679200
N	-0.14584300	-2.09445900	2.29799100

**TS<sub>III-IV</sub> (large core)**

H= -1736.858509 au

U	-0.03270700	-0.79685500	0.07451600
C	-2.39726700	0.51827900	-0.60626200
C	-1.60615700	0.57164600	-1.77850900
C	-0.82505100	-0.33344200	-2.53568500
C	-0.47376000	-1.69409300	-2.45854600
C	-0.90233400	-2.77864700	-1.65190400
C	-1.83592400	-2.91922700	-0.59941800
C	-2.59776800	-1.98664000	0.15754200
C	-2.78592200	-0.59218500	0.20570500
C	1.36265900	1.58336800	0.49094000
C	1.52713200	1.35370100	-0.90892100
C	2.11495100	0.59108900	1.18499800
C	2.71689400	-0.27034000	0.21764500
C	2.34154800	0.19239200	-1.07624000
O	0.10213600	-1.26454400	2.52417100

H	-3.08777700	-2.46420800	1.00283900
H	-3.39798500	-0.30176000	1.05796300
Si	-3.24364800	2.13975800	-0.16206300
H	-3.41778600	2.27294000	1.31797400
H	-1.48284000	1.58472800	-2.15464400
H	-0.26449600	0.18030600	-3.31217600
H	0.28794600	-1.97889900	-3.18002900
H	-0.38402900	-3.70118600	-1.90689500
H	-3.28917400	-5.26911200	-0.89224800
Si	-2.14740900	-4.71424800	-0.09419000
H	-2.52046900	-4.80913100	1.34909700
H	-0.94869000	-5.56027700	-0.37607000
C	2.88631300	-0.30792500	-2.38150900
C	3.73975400	-1.33163400	0.49488700
C	2.40060100	0.59582900	2.65290500
C	1.18360300	2.34104200	-1.98136500
C	0.70629900	2.79167000	1.09445700
H	-4.60494300	2.23261000	-0.78118200
H	-2.44103800	3.30025700	-0.66557000
U	0.12160100	-2.36479200	4.78567500
C	2.87444600	-2.45628200	5.19248000
C	2.29703900	-2.24721600	6.48476400
C	1.35935100	-2.93588000	7.27252600
C	0.43006100	-3.97739200	7.06424700
C	0.05675500	-4.80447800	5.99025600
C	0.60673900	-5.07195300	4.69809800
C	1.72072000	-4.52372100	4.02281500
C	2.62712300	-3.44915300	4.21018200
C	-1.02503700	-0.12087100	6.04632300
C	-1.44597000	-1.19344100	6.88818700
C	-1.70408700	-0.25455900	4.79966600
C	-2.49821800	-1.44038800	4.85047800
C	-2.33307500	-2.02361600	6.14224800
H	1.83260000	-4.92899600	3.02154000
H	3.24415800	-3.31888800	3.32265200
Si	4.44636300	-1.44441000	4.96036700
H	4.88119200	-1.42761400	3.53112000
H	2.69714400	-1.37441100	6.99995600
H	1.21027000	-2.45415200	8.23461300
H	-0.24430900	-4.08784700	7.91012200
H	-0.83197600	-5.39123100	6.21710300
H	0.22632500	-7.81333700	4.35548400
Si	-0.24720800	-6.50066200	3.80697800
H	0.04513100	-6.46989400	2.34543800
H	-1.72711500	-6.44291800	4.03157300
C	-3.12909500	-3.17007600	6.69205300
C	-3.51091600	-1.87455100	3.83444900
C	-1.75147000	0.79623200	3.73623800
C	-1.22808700	-1.26623900	8.36825000
C	-0.18528700	1.04742200	6.47900100
H	5.55725900	-2.04204900	5.76858200
H	4.25832800	-0.03790000	5.43987400
H	3.69977300	-2.14688100	-0.23272200
H	4.75119700	-0.90682700	0.45480800
H	3.61321300	-1.76963400	1.48697400
H	2.54013600	-0.41408800	3.04435400
H	3.31563500	1.16388300	2.86261400
H	1.59123300	1.05836600	3.22376400
H	0.41739500	2.62420600	2.13500700
H	1.38745000	3.65270700	1.08360000



H	-0.19508000	3.08584700	0.54818800
H	1.02228200	1.86952200	-2.95371600
H	0.29568500	2.92890200	-1.73610400
H	2.01350800	3.04988600	-2.10494600
H	3.16269900	-1.36475500	-2.33180100
H	2.16687200	-0.19231500	-3.19753000
H	3.78899300	0.24916300	-2.66479100
H	-3.60087600	-2.96331500	3.77310400
H	-4.50534500	-1.48025600	4.08213100
H	-3.25122800	-1.51151900	2.84012700
H	-3.44144300	-3.86574600	5.90819300
H	-2.56693200	-3.74206500	7.43588300
H	-4.04120700	-2.80779200	7.18448900
H	-1.21289300	-2.29358600	8.74196000
H	-0.30000500	-0.77829300	8.67647700
H	-2.04776500	-0.75076300	8.88676900
H	0.30530000	1.53630600	5.63234100
H	-0.79493200	1.81049000	6.98067000
H	0.59967800	0.74799700	7.18009300
H	-1.93980100	0.37666000	2.74665700
H	-2.55341700	1.51567000	3.94737700
H	-0.81844000	1.36373900	3.68312400
N	-0.16287500	-2.59930200	2.37273200
C	1.05241600	-3.02985400	0.77858700
O	1.49463700	-4.10111800	0.81620100

#### IV (large core)

H= -1736.884702 au

U	-0.20657500	-0.72468200	0.06061300
C	-2.50173800	0.70541900	-0.35204000
C	-1.75611000	0.88497700	-1.55149600
C	-1.11049200	0.04111000	-2.48145500
C	-0.79749200	-1.32600200	-2.57166000
C	-1.13095300	-2.47903500	-1.81884900
C	-2.02535000	-2.73368100	-0.74984800
C	-2.76763600	-1.87115400	0.09980000
C	-2.94535100	-0.48385200	0.29547300
C	1.55032200	1.42664200	0.22155800
C	1.71606200	0.99111900	-1.12874800
C	2.09208300	0.42155600	1.07189900
C	2.55707900	-0.65430200	0.25160500
C	2.31967400	-0.30097700	-1.10875200
O	-0.14231500	-1.21677000	2.45971400
H	-3.26628400	-2.42451600	0.89355800
H	-3.52420500	-0.28373100	1.19455400
Si	-3.26480100	2.30042600	0.30247600
H	-3.62130300	2.17192600	1.74770000
H	-1.59523900	1.93372200	-1.79825700
H	-0.59963500	0.61850300	-3.24577800
H	-0.09683700	-1.54305900	-3.37390400
H	-0.61770800	-3.36722400	-2.18091600
H	-3.66931900	-4.93875600	-0.99369400
Si	-2.33710600	-4.56972300	-0.40889200
H	-2.41064000	-4.84914700	1.05626400
H	-1.29838400	-5.41362300	-1.06656600
C	2.81202500	-1.06573300	-2.30220900
C	3.35409100	-1.84128400	0.70163600
C	2.30477500	0.57076100	2.54362200
C	1.56348800	1.87512600	-2.32792600
C	1.08459600	2.79283100	0.63554700

H	-4.51599900	2.63057000	-0.45162200
H	-2.32215200	3.45032700	0.12555500
U	0.19440900	-2.26173100	4.82439300
C	2.89065700	-2.04208100	5.40903600
C	2.20170900	-2.03419800	6.65834300
C	1.30634100	-2.91256400	7.29913300
C	0.52110600	-4.01914500	6.92224200
C	0.34616900	-4.78671800	5.74921000
C	1.07611500	-4.91133100	4.52963000
C	2.15208300	-4.16158700	4.01061800
C	2.86831100	-2.98431300	4.34833400
C	-1.08188600	-0.16546000	6.21662600
C	-1.48713100	-1.31478200	6.95940500
C	-1.69268400	-0.23954000	4.93175600
C	-2.43597900	-1.45850400	4.86340300
C	-2.30388900	-2.12519700	6.11637500
H	2.42591600	-4.48552900	3.00837900
H	3.55151800	-2.71325800	3.54767600
Si	4.27188900	-0.75865400	5.34403900
H	4.86759300	-0.68476100	3.97661400
H	2.43524400	-1.17108900	7.28075600
H	1.03088000	-2.54939400	8.28413400
H	-0.20436700	-4.27910900	7.68937100
H	-0.47415000	-5.49612700	5.84888200
H	0.35895100	-7.56057800	4.36194800
Si	0.47956600	-6.36370200	3.46486100
H	1.46702000	-6.66429500	2.39112200
H	-0.87424600	-6.13109000	2.87591000
C	-3.05943600	-3.34838700	6.54599800
C	-3.34014600	-1.87627800	3.74583300
C	-1.72242300	0.86752800	3.92584500
C	-1.34082800	-1.47859800	8.44040600
C	-0.32564700	1.00828300	6.76978900
H	5.35505400	-1.13532800	6.30717900
H	3.77605700	0.59627700	5.74653800
H	3.18562100	-2.71763800	0.07043700
H	4.42855900	-1.61605400	0.67849700
H	3.09720600	-2.12648600	1.72189100
H	2.37153900	-0.40108400	3.03650600
H	3.23753600	1.11274600	2.74305800
H	1.49448400	1.12872800	3.02150500
H	0.77659600	2.81955400	1.68446000
H	1.88798300	3.53194500	0.51742500
H	0.23667400	3.13826100	0.03578600
H	1.53935600	1.30743300	-3.26087100
H	0.66450200	2.49667100	-2.28234000
H	2.42106500	2.55820800	-2.39064400
H	2.78449200	-2.14624500	-2.13547000
H	2.22080700	-0.85498300	-3.19715400
H	3.85271400	-0.80040900	-2.52985800
H	-3.54706300	-2.94977900	3.76683700
H	-4.30566500	-1.35706100	3.80603000
H	-2.89000600	-1.64744800	2.78023100
H	-3.26487900	-4.01999500	5.70786300
H	-2.51548500	-3.92218500	7.30143800
H	-4.02772300	-3.07319200	6.98419300
H	-1.28778000	-2.52695500	8.74717800
H	-0.45985900	-0.96241200	8.83078800
H	-2.21446000	-1.04477900	8.94538100
H	0.13277400	1.60705600	5.97781200

H	-0.99218400	1.67572800	7.33159500
H	0.47321500	0.70013600	7.45139300
H	-1.93185400	0.48813600	2.92524100
H	-2.50421700	1.59431000	4.18156300
H	-0.77622500	1.41635900	3.88304900
N	-0.11800400	-2.66514500	2.41799200
C	0.37797300	-3.14794800	1.30464000
O	0.68723600	-4.25676300	0.91096100

**TS<sub>IV-V</sub> (large core)**

H= -1736.875451 au

U	-0.14756800	-0.75233200	0.17385700
C	-2.38726800	0.53718100	-0.68145800
C	-1.57272900	0.50361300	-1.84940200
C	-0.80721800	-0.46009600	-2.53255300
C	-0.45105700	-1.80720200	-2.32075200
C	-0.92939200	-2.83521800	-1.46998500
C	-1.93916800	-2.90455500	-0.48557200
C	-2.73354200	-1.91958000	0.16300900
C	-2.88469600	-0.51978900	0.13991900
C	1.33020000	1.60540500	0.51189500
C	1.50492300	1.30353400	-0.87282400
C	2.02299300	0.61191900	1.26337900
C	2.59180100	-0.32568900	0.34873800
C	2.26930900	0.10076900	-0.97211200
O	-0.00582400	-1.36170200	2.47211100
H	-3.31011000	-2.34740600	0.97933900
H	-3.53058300	-0.17115900	0.94457500
Si	-3.16048400	2.21633300	-0.31518400
H	-3.37840400	2.39361400	1.15448500
H	-1.41619000	1.49187200	-2.27519600
H	-0.22174500	-0.01093900	-3.33087600
H	0.35096300	-2.14217900	-2.97361400
H	-0.38964700	-3.76821500	-1.61725300
H	-3.37095200	-5.26773900	-0.77075300
Si	-2.30729400	-4.66518200	0.09805600
H	-2.82985700	-4.66402200	1.49894200
H	-1.09249400	-5.52431500	-0.00449000
C	2.82866900	-0.48538300	-2.23424600
C	3.54426900	-1.43214400	0.69034300
C	2.29560000	0.67539500	2.73115300
C	1.21478700	2.24798200	-1.99861100
C	0.73603100	2.87391200	1.05391100
H	-4.49056700	2.35580600	-0.99002000
H	-2.28183200	3.31987600	-0.81737400
U	0.16759900	-2.41218000	4.64753100
C	2.89009000	-2.43777200	5.14317800
C	2.23162300	-2.26876200	6.40083100
C	1.30811700	-3.02795000	7.14866600
C	0.42533900	-4.09176100	6.89346100
C	0.11566900	-4.89352800	5.77741300
C	0.77090000	-5.15189300	4.53567100
C	1.90978400	-4.57146700	3.93986900
C	2.74977400	-3.45016300	4.16208900
C	-0.94537900	-0.17911000	5.97087900
C	-1.36137600	-1.25792100	6.80691100
C	-1.64539100	-0.29105600	4.73429000
C	-2.44459500	-1.47235200	4.78320900
C	-2.26391300	-2.07320000	6.06392600
H	2.11489500	-4.98873100	2.95572900

H	3.41272100	-3.30404500	3.31144600
Si	4.41001200	-1.33387100	4.99073300
H	4.89283200	-1.24736800	3.58061800
H	2.55924000	-1.38394700	6.94534600
H	1.11616800	-2.57395600	8.11557400
H	-0.27694700	-4.24018400	7.71039300
H	-0.76999000	-5.50480000	5.94394400
H	0.50953200	-7.90295700	4.16455400
Si	0.02538500	-6.60657100	3.58753900
H	0.40953700	-6.55635400	2.14806600
H	-1.46612100	-6.59936000	3.72071000
C	-3.07009700	-3.21549800	6.60727500
C	-3.46815600	-1.90058100	3.77659600
C	-1.68880200	0.77286600	3.68270300
C	-1.15029400	-1.33363400	8.28758200
C	-0.10267800	0.98664800	6.40295100
H	5.52148000	-1.89314600	5.82470300
H	4.11738400	0.04203200	5.50335900
H	3.41106200	-2.31402800	0.05797300
H	4.58218100	-1.09322600	0.57399900
H	3.42312100	-1.75366000	1.72592600
H	2.29540300	-0.31710300	3.18875900
H	3.27735500	1.12743300	2.91913400
H	1.55577300	1.28396700	3.25756700
H	0.33057100	2.74558700	2.06117400
H	1.49460500	3.66564800	1.11161100
H	-0.07424200	3.24944500	0.42287000
H	1.04320500	1.73220700	-2.94656500
H	0.34816100	2.88207100	-1.79578800
H	2.07379800	2.91544700	-2.14917700
H	2.99017100	-1.56340600	-2.14645500
H	2.17323700	-0.31435400	-3.09260400
H	3.79943400	-0.03087400	-2.47228700
H	-3.49724600	-2.98672300	3.64114200
H	-4.47364400	-1.58603200	4.08504400
H	-3.26578000	-1.45580700	2.80294300
H	-3.39438500	-3.89890800	5.81744100
H	-2.51292700	-3.80148400	7.34343800
H	-3.97596200	-2.84637100	7.10629700
H	-1.13754800	-2.36145900	8.66074400
H	-0.22576400	-0.84323900	8.60289100
H	-1.97449000	-0.81982500	8.80067500
H	0.36606400	1.48757000	5.55111300
H	-0.70739700	1.73950500	6.92578500
H	0.69803200	0.68409500	7.08466900
H	-2.11554600	0.40381400	2.74858000
H	-2.30957000	1.61452000	4.01656000
H	-0.69599700	1.17326200	3.45657100
N	0.03841500	-3.02568700	2.18962500
C	0.83464200	-3.28150900	1.23553300
O	1.45294800	-4.11120200	0.60639800

V (large core)

H= -1569.006234 au

U	4.93141700	21.47059900	7.11706800
U	6.76201000	25.27732800	6.36545200
Si	5.61178600	26.29667600	2.39976900
Si	10.73774100	26.99494200	7.09240500
Si	6.03132500	19.01962000	3.82122600
Si	0.97790200	20.19257700	8.50316200

O	5.85319200	23.44057800	7.08339700
C	6.87948000	25.77442100	3.69390700
C	7.66388900	26.84389700	4.21642700
H	7.30808900	27.81754700	3.88582300
C	8.70719100	26.98910500	5.15248900
H	8.93444600	28.04278400	5.30751700
C	9.40324700	26.15118800	6.06122500
C	9.43109600	24.72868700	6.22304100
H	10.07757000	24.39399200	7.03374000
C	8.86770900	23.64880000	5.51780500
H	9.16856800	22.68945200	5.93033200
C	7.88960400	23.50193600	4.50872900
H	7.63598200	22.45602900	4.35155900
C	7.02783000	24.35566800	3.79997600
H	6.28831000	23.80092200	3.22597300
C	4.78384600	19.99969300	4.83966700
C	3.99537200	19.21270300	5.72933800
H	4.33831700	18.18157600	5.78382600
C	2.96401700	19.44234500	6.66185200
H	2.73056100	18.52673100	7.20287800
C	2.28666700	20.56822400	7.19787500
C	2.26658800	21.94657700	6.81029600
H	1.63756800	22.57023900	7.44497000
C	2.82265300	22.67351400	5.74102900
H	2.53334800	23.72082700	5.76403000
C	3.78798000	22.41823400	4.74094100
H	4.04191400	23.32472600	4.19598200
C	4.64015200	21.35414600	4.40119900
H	5.37462200	21.64581900	3.65323100
C	5.71574800	21.13349100	9.78047900
C	6.92928600	21.34753000	9.06071500
C	7.16197800	20.20625300	8.23860200
C	6.11126800	19.26832700	8.48026900
C	5.21891200	19.84228600	9.43062000
C	7.87198800	22.49131800	9.26214900
H	7.33946400	23.41109600	9.51482000
H	8.46659200	22.69358800	8.36763400
H	8.57062800	22.27790500	10.08168800
C	8.39719100	19.93232500	7.42889800
H	9.13266200	19.36580200	8.01521100
H	8.88806000	20.85534700	7.10978300
H	8.18437200	19.34485900	6.53023000
C	6.10082300	17.84029000	8.02559700
H	6.56247900	17.71331600	7.04293700
H	5.08872000	17.43036200	7.97467600
H	6.66649000	17.21580700	8.73028800
C	4.10234000	19.12409100	10.12555800
H	4.48219600	18.58954600	11.00667400
H	3.62423900	18.38283600	9.48097500
H	3.32583700	19.80856400	10.47831600
C	5.16772000	22.00208000	10.87655700
H	4.07333500	21.99057100	10.91282100
H	5.48332400	23.04254900	10.76716500
C	5.95678300	26.56381000	8.72133700
C	6.49603900	27.62822000	7.94041800
C	5.62828700	27.84506300	6.83124000
C	4.55106100	26.90993000	6.92426800
C	4.74293600	26.13624400	8.10648000
C	6.46024100	26.14001600	10.07132800
H	7.55054300	26.04109000	10.10726900

H	6.02949900	25.18385500	10.37787700
H	6.18331900	26.87555900	10.83818200
C	7.63566000	28.50982900	8.35117900
H	8.13183700	28.96872800	7.49293800
H	8.39405500	27.96536800	8.92097200
H	7.27669800	29.32577100	8.99284200
C	5.68914800	29.01002200	5.88999900
H	5.11758700	29.85566600	6.29557700
H	5.26439300	28.77516800	4.91045600
H	6.71326700	29.35916100	5.73361300
C	3.33012800	26.90849200	6.04845700
H	2.84887900	25.92737100	6.01296100
H	3.56104000	27.19767800	5.01887400
H	2.57996700	27.61905500	6.41996200
C	3.77200400	25.16081600	8.69329400
H	3.02000700	24.85373500	7.96329700
H	3.24076300	25.60423100	9.54506700
H	4.27274300	24.25490500	9.04802900
H	12.09523100	26.64133900	6.56603900
H	10.59730200	28.48211000	7.04805800
H	10.69528500	26.53828700	8.51976000
H	5.09009800	27.67003200	2.68532900
H	6.21758200	26.31962300	1.03018200
H	4.46392600	25.33606100	2.37201900
H	-0.39265300	20.38232000	7.92848800
H	1.08815400	18.78329000	8.98734900
H	1.08634900	21.12316400	9.67390800
H	6.53499100	17.83526600	4.58422700
H	5.41293200	18.51218700	2.55494300
H	7.19325800	19.88432900	3.44304200
H	5.52296000	21.66263300	11.85858800

#### VI (small core, singlet)

H= -1354.429401 au

U	-0.40030300	-0.42752300	-0.26860700
C	-2.81534000	0.68808500	-0.26957000
C	-2.14986300	1.15796000	-1.43506800
C	-1.51192200	0.55493000	-2.53839600
C	-1.14009300	-0.75619600	-2.88560700
C	-1.18963600	-2.01344600	-2.25620900
C	-1.77088300	-2.52149100	-1.06020300
C	-2.60559000	-1.92044200	-0.07559400
C	-3.04426400	-0.61893000	0.23121600
C	1.71670600	1.21130500	-0.34303200
C	1.72026700	0.54987600	-1.61294500
C	2.07724800	0.25871700	0.65218000
C	2.23947900	-1.00115000	0.01430100
C	2.03082600	-0.82447200	-1.38548500
H	-2.85752200	-2.60635500	0.73163400
H	-3.53959600	-0.60825400	1.20017500
Si	-3.54941200	2.06884500	0.79535100
H	-3.71396200	1.60977000	2.20710000
H	-2.08898600	2.24513100	-1.48619000
H	-1.12596500	1.28871000	-3.24155100
H	-0.53909300	-0.77895000	-3.79223200
H	-0.58909400	-2.74943000	-2.78765600
H	-2.56329700	-5.17781200	-1.46423300
Si	-1.49083600	-4.37297400	-0.79818700
H	-1.49834600	-4.70184900	0.66007200
H	-0.17864400	-4.78175900	-1.39203800

C	2.29150400	-1.85766800	-2.44284400
C	2.62860500	-2.28204200	0.69435100
C	2.38535200	0.56773400	2.08502100
C	1.70299900	1.24136000	-2.94353300
C	1.55094500	2.68822700	-0.12151900
H	-4.89078600	2.48593500	0.27527500
H	-2.65982800	3.27261900	0.75847400
H	2.32447400	-3.16090700	0.11762100
H	3.71722000	-2.34554000	0.82062400
H	2.18316400	-2.36760700	1.69045900
H	2.30853900	-0.31843800	2.71850600
H	3.41089000	0.94982000	2.17296000
H	1.71609900	1.32577600	2.50028000
H	1.17401500	2.91069800	0.88129300
H	2.50936300	3.21412100	-0.22754100
H	0.85940000	3.13802000	-0.84057600
H	1.32472700	0.59956700	-3.74357500
H	1.09332100	2.14916500	-2.92863600
H	2.71974800	1.54455900	-3.22758300
H	2.00980400	-2.86388100	-2.11803800
H	1.74545900	-1.64500700	-3.36561500
H	3.35917100	-1.88895300	-2.69759700
N	-0.43213900	-0.52554200	1.97833300
C	-0.62046700	-0.58695700	3.17047200
O	-0.80091400	-0.65102800	4.33854200

#### VI (small core, triplet)

H= -1354.472731 au

U	-0.42133900	-0.39224700	-0.24097700
C	-2.87596500	0.67067000	-0.28875400
C	-2.20133700	1.14969900	-1.44483400
C	-1.52757400	0.54783500	-2.52840800
C	-1.13055000	-0.76045200	-2.86134900
C	-1.17392700	-2.01625900	-2.22726600
C	-1.76023300	-2.53043800	-1.03837200
C	-2.59004100	-1.92993500	-0.05199300
C	-3.06341500	-0.63333100	0.23430600
C	1.77896800	1.21580600	-0.33999700
C	1.77239500	0.57236800	-1.61506300
C	2.08858400	0.23756200	0.64705400
C	2.20841500	-1.02205400	-0.00752100
C	2.03052300	-0.81173500	-1.40915400
H	-2.83124600	-2.61026000	0.76311900
H	-3.56392900	-0.62295600	1.20033400
Si	-3.65130400	2.04682900	0.75304200
H	-3.85559900	1.58771700	2.15936400
H	-2.17548900	2.23696900	-1.51238100
H	-1.13681300	1.28424500	-3.22633200
H	-0.51901800	-0.78163900	-3.76070300
H	-0.56528000	-2.74758500	-2.75627000
H	-2.49574400	-5.20262200	-1.43964900
Si	-1.44869700	-4.37434300	-0.76140600
H	-1.47261900	-4.69724500	0.69796100
H	-0.12114800	-4.76564800	-1.33322500
C	2.26754700	-1.83742200	-2.47808700
C	2.58902500	-2.31787000	0.65042600
C	2.41594000	0.51900100	2.08190300
C	1.73215200	1.27757300	-2.93756400
C	1.63891300	2.69240900	-0.09980100
H	-4.97849300	2.45312500	0.18989100

H	-2.77138800	3.25845000	0.74253900
H	2.25018600	-3.18521700	0.07577000
H	3.67919400	-2.40586500	0.74712200
H	2.16834900	-2.40369800	1.65684600
H	2.28252100	-0.36296400	2.71169400
H	3.46419800	0.83351600	2.17047400
H	1.79748800	1.31653500	2.50165900
H	1.26508800	2.90868500	0.90550200
H	2.60595300	3.20330700	-0.19826100
H	0.95580000	3.16310100	-0.81399800
H	1.34488700	0.64093500	-3.73731000
H	1.11924700	2.18283800	-2.90473600
H	2.74331100	1.58724300	-3.23349100
H	1.95342800	-2.83807000	-2.16688800
H	1.73709900	-1.59745300	-3.40342700
H	3.33608100	-1.89825400	-2.72337300
N	-0.46064000	-0.42841200	2.01096800
C	-0.62314000	-0.49150300	3.20652600
O	-0.77782200	-0.55461100	4.37847200

#### VI (small core, quintet)

H= -1354.412449 au

U	-0.26801200	-0.32419500	-0.12910500
C	-3.04302200	0.62538100	-0.28907900
C	-2.26837700	1.14448700	-1.40448300
C	-1.61678200	0.56470000	-2.48229500
C	-1.25127700	-0.77338500	-2.84590800
C	-1.29294500	-2.00748800	-2.22155600
C	-1.80098800	-2.53062800	-0.96961300
C	-2.63672000	-1.95256600	-0.00780900
C	-3.19068200	-0.64860700	0.24121900
C	1.95382400	1.21105900	-0.31648500
C	1.85818600	0.58443500	-1.59760400
C	2.27009000	0.20829400	0.64369100
C	2.34293700	-1.04418600	-0.03744900
C	2.09945200	-0.80962700	-1.42309500
H	-2.90418800	-2.63393200	0.79822000
H	-3.80679400	-0.67247100	1.13752000
Si	-3.99495300	1.99365700	0.61484800
H	-4.63477900	1.44920400	1.84726100
H	-2.28164300	2.23257200	-1.46483900
H	-1.23968600	1.29604700	-3.19407200
H	-0.72708900	-0.80279600	-3.79848800
H	-0.77456300	-2.76687600	-2.80716300
H	-2.28575200	-5.20609600	-1.63439800
Si	-1.43987300	-4.37177400	-0.72165800
H	-1.72554300	-4.75642800	0.69237000
H	-0.01047000	-4.67688800	-1.04526700
C	2.25238200	-1.82371500	-2.51946700
C	2.75446600	-2.35059800	0.58034700
C	2.62788100	0.44776100	2.08063900
C	1.75062500	1.30495900	-2.91083800
C	1.86843900	2.68743400	-0.05126800
H	-5.04724300	2.56119600	-0.28621200
H	-3.06387500	3.11065800	0.97052600
H	2.39093500	-3.20934100	0.00732400
H	3.84839900	-2.43925800	0.62766800
H	2.38197600	-2.45569800	1.60435100
H	2.40249500	-0.41797100	2.70820800
H	3.70106200	0.65892700	2.18168700



H	2.08625300	1.29844200	2.50297300
H	1.52334800	2.90023700	0.96549600
H	2.84820600	3.17163600	-0.16297200
H	1.18588900	3.19213100	-0.74330600
H	1.30795800	0.67993500	-3.69225200
H	1.14848100	2.21599100	-2.83497000
H	2.74240500	1.61034300	-3.27086800
H	1.93202200	-2.82254300	-2.20624000
H	1.67387400	-1.55721700	-3.40875600
H	3.30168400	-1.90924000	-2.83257400
N	-0.48478900	-0.27520400	2.15952400
C	-0.63856000	-0.27225600	3.35681400
O	-0.79212100	-0.27217500	4.53378500

### VI (large core)

H= -914.920256 au

U	-0.36357000	-0.51381200	-0.24751900
C	-2.75395300	0.75640800	-0.02497500
C	-2.09235000	1.31370100	-1.16503700
C	-1.58540600	0.78346100	-2.37556700
C	-1.29261500	-0.50366400	-2.86741200
C	-1.36330200	-1.82264400	-2.36110800
C	-1.99553300	-2.43777500	-1.23320100
C	-2.75559200	-1.88058500	-0.17179400
C	-3.06445200	-0.58620200	0.31376000
C	1.74327700	1.27351100	-0.58192600
C	1.85491900	0.39114500	-1.70203600
C	2.04256000	0.52712100	0.59525200
C	2.33664300	-0.81823700	0.20429500
C	2.21493900	-0.90345500	-1.21350900
H	-3.06771800	-2.63198200	0.55064900
H	-3.53968800	-0.66375100	1.28985400
Si	-3.41467500	2.04259600	1.19290400
H	-3.45883200	1.48175200	2.57636400
H	-1.98821200	2.39605700	-1.12069400
H	-1.19771000	1.56330000	-3.02674300
H	-0.73719200	-0.46013200	-3.80075200
H	-0.84120000	-2.52956400	-3.00331700
H	-2.95514400	-4.92984200	-2.06957700
Si	-1.88095800	-4.32436700	-1.21991400
H	-2.02925200	-4.84425700	0.17215300
H	-0.56299000	-4.75899000	-1.78157900
C	2.56973000	-2.08963100	-2.06424900
C	2.83051600	-1.90103600	1.11650000
C	2.16269700	1.07289900	1.98742500
C	1.86231200	0.80910600	-3.14124300
C	1.52225400	2.75695700	-0.66420400
H	-4.79926900	2.46945400	0.81426100
H	-2.54324300	3.25961500	1.16843900
H	2.59657800	-2.89984800	0.73625500
H	3.92116900	-1.84375700	1.22576600
H	2.38845300	-1.81868300	2.11159600
H	1.82476200	0.34855000	2.73264700
H	3.20588900	1.32642900	2.21526100
H	1.57334500	1.98458100	2.12295700
H	1.10901200	3.16420700	0.26273800
H	2.46834500	3.28114500	-0.85156300
H	0.83908100	3.02567600	-1.47559800
H	1.60756100	-0.01616800	-3.81108900
H	1.16878100	1.63043000	-3.34071700

H	2.86373300	1.15735000	-3.42688300
H	2.44991100	-3.03237600	-1.52321100
H	1.95384300	-2.14810000	-2.96697400
H	3.61682900	-2.03699900	-2.38941200
N	-0.26162500	-1.25073600	1.95987900
C	-0.47670000	-1.68757000	3.06381800
O	-0.67341400	-2.11495600	4.15340800

**VII**(large core)

H= -1656.133080 au

U	10.84302900	7.89126000	9.81748600
U	11.98184900	7.53694200	2.60735700
Si	10.54922100	3.69938000	9.28960800
Si	7.18946100	9.81486900	8.88016100
C	10.26709000	5.70555800	11.22662000
H	10.97207800	5.00239600	11.66591600
C	9.23970800	7.96641300	12.05179900
H	9.35148300	8.55037800	12.96205400
C	9.87292000	5.36152500	9.89519700
C	8.61640700	8.71384800	11.02215000
H	8.38017000	9.72592600	11.34508700
C	9.91498900	6.73334100	12.13612000
H	10.41337100	6.61152200	13.09435700
C	9.00438300	6.01438500	8.98187600
H	8.95141000	5.49847200	8.02509100
C	8.32124500	7.25275900	8.89906400
H	7.91161900	7.38248100	7.89922000
C	8.18847400	8.42500300	9.68797500
C	12.70051700	10.84050500	8.49718000
H	12.65013300	10.35058600	7.52195600
H	13.59450700	11.47649100	8.50089400
H	11.83472700	11.50423900	8.57964000
C	14.32723700	8.11654100	8.45809100
H	13.89253900	8.37991900	7.49174200
H	14.45512900	7.03048500	8.47604400
H	15.32923400	8.56098100	8.50504400
C	13.48417300	8.60946400	9.59581100
C	12.47546800	8.77745300	13.20500700
H	12.49588800	7.73769500	13.54185900
H	11.55145600	9.23309300	13.57115700
H	13.30704400	9.29295300	13.70294300
C	14.12165200	6.79309500	11.36268500
H	13.53578800	6.21712700	12.08582500
H	15.06429500	7.06589700	11.85392000
H	14.37451200	6.12389400	10.53608200
C	11.52159300	11.23951500	11.44994800
H	11.01172800	11.79154600	10.65589700
H	12.23797000	11.92984400	11.91319100
H	10.77631100	10.98942500	12.21099100
C	12.22397000	10.01913700	10.92830000
C	13.39435200	8.02010400	10.89115100
C	12.75824200	9.84517600	9.61829600
C	12.61920100	8.89217300	11.71749300
Si	14.09974100	11.24457100	3.21898500
Si	14.32577500	4.41514100	4.48712900
O	10.99656400	7.76861500	5.07480200
N	11.20417600	7.98046200	7.45151900
C	11.10846700	7.87192400	6.26877300
C	13.91783800	9.11787500	1.43154000
H	13.76144800	10.00359000	0.81734100

C	13.95481000	6.55036000	0.90819700
H	13.81930600	5.96431100	0.00132500
C	14.04755500	9.41004100	2.82274100
C	14.00383600	5.73583300	2.06348800
H	13.89778600	4.68053800	1.81537900
C	13.92729800	7.94004800	0.64982600
H	13.77604700	8.15263500	-0.40620400
C	14.24172200	8.56907100	3.95747900
H	14.28528600	9.13244300	4.88985400
C	14.29173800	7.18121500	4.21336500
H	14.36067100	6.99333700	5.28463300
C	14.15699600	5.97836300	3.46138500
C	8.64162500	5.91556900	3.45167600
H	8.65465800	6.45258400	4.40489800
H	7.59243000	5.67943200	3.22743100
H	9.15341000	4.95959300	3.60838100
C	8.54440200	9.08973800	3.16356400
H	8.59171000	8.74318000	4.20017200
H	8.98669500	10.09153100	3.13437800
H	7.48204300	9.20600700	2.90921600
C	9.23012400	8.14127300	2.22188700
C	10.77683900	7.17026300	-1.06247900
H	11.34375100	8.05813100	-1.35778300
H	11.43837300	6.30647900	-1.18032200
H	9.96115600	7.05257600	-1.78923100
C	9.89889300	9.86679800	0.38085600
H	10.78406400	9.99738400	-0.25008600
H	9.02247900	10.07452900	-0.24825200
H	9.93017700	10.64746500	1.14779500
C	10.04039500	4.73509100	0.83671300
H	10.08214200	4.10155100	1.72852800
H	9.19184900	4.38103100	0.23529400
H	10.94745700	4.53907500	0.25574600
C	9.89600700	6.19012000	1.18343000
C	9.83123300	8.48919100	0.97752800
C	9.27070500	6.71886100	2.34933000
C	10.24186000	7.28365000	0.33510700
H	7.69579400	11.14021700	9.35532900
H	7.30047700	9.73304900	7.39341200
H	5.74521700	9.71249900	9.25755800
H	13.83274000	4.63430000	5.88784300
H	13.54889700	3.28358600	3.88364700
H	15.74901900	3.95071900	4.60342600
H	15.49589100	11.79718300	3.21707000
H	13.53553700	11.51676200	4.58309500
H	13.31611200	12.03635000	2.21636800
H	10.65411800	3.70061400	7.80081300
H	11.89297300	3.45254100	9.89787200
H	9.64191700	2.58475500	9.70594600

### VIII (large core)

H= -1829.868886 au

U	10.76311300	8.13537400	9.31557600
Si	9.29774400	4.13687100	9.00759300
Si	7.80550800	10.89139000	8.09937200
O	11.76464900	6.33922700	7.74754000
N	11.86362800	6.38572400	5.34456800
C	11.81419500	6.36795300	6.52916100
C	9.47065200	6.24222800	10.82025600
H	9.90341600	5.39105900	11.34388200

C	9.15045200	8.76267900	11.44567600
H	9.41020300	9.34875200	12.32385000
C	9.07124200	5.94858300	9.48270300
C	8.74482600	9.58229300	10.37233100
H	8.77553800	10.63834500	10.63454300
C	9.43269000	7.38927300	11.63513600
H	9.85060700	7.19906100	12.61951300
C	8.50446100	6.76160600	8.47143600
H	8.35976300	6.22047800	7.53802800
C	8.18473900	8.13259400	8.29410400
H	7.88220800	8.31368000	7.26513100
C	8.31396900	9.33269900	9.03403700
C	13.03855500	11.10802700	8.75330800
H	13.09187000	10.89210800	7.68475000
H	13.93672500	11.67770900	9.02527800
H	12.17733200	11.76464100	8.90967100
C	14.26759000	8.28265500	7.96802400
H	13.80532300	8.72439800	7.08104700
H	14.36111000	7.20776900	7.79823300
H	15.28211200	8.69292200	8.05130000
C	13.48074800	8.57649500	9.20786200
C	12.51300700	7.96219500	12.77820900
H	12.31544000	6.88893000	12.84649600
H	11.70266700	8.48536500	13.29284300
H	13.43322000	8.15805800	13.34421500
C	13.84504400	6.29244300	10.41421100
H	13.34120100	5.72126600	11.19905100
H	14.91644200	6.29454300	10.65260600
H	13.71783100	5.74441300	9.47640100
C	11.96196100	10.91065900	11.72240400
H	11.46979400	11.67756000	11.11791600
H	12.80921000	11.39300600	12.22722300
H	11.25992900	10.59888800	12.50006900
C	12.43652500	9.75710400	10.88978600
C	13.31518300	7.69437700	10.31947500
C	12.94491400	9.85189900	9.56667200
C	12.67334800	8.42249700	11.36096900
U	12.13075500	7.40514500	3.11252600
Si	13.95005600	11.24846700	3.67207000
Si	14.89440900	4.34690700	3.99381000
O	11.23258500	9.24876900	4.69625400
N	11.04123800	9.17944900	7.09326800
C	11.13545800	9.20761900	5.91147000
C	13.50502700	9.31895700	1.71799200
H	13.11581200	10.24094300	1.28896100
C	13.62670600	6.84761300	0.87551700
H	13.30106200	6.35537700	-0.03824300
C	13.99344300	9.46931600	3.04819500
C	14.00011400	5.91265000	1.86348500
H	13.87724800	4.88833700	1.51675700
C	13.42514900	8.24537200	0.80901900
H	12.98455100	8.54496600	-0.13768300
C	14.52460000	8.53351300	3.96953000
H	14.75241000	8.98707300	4.93231700
C	14.72875500	7.13199900	4.03473700
H	15.03804000	6.84595600	5.03780000
C	14.47382500	6.01045200	3.20704600
C	9.75268000	4.52594300	3.72867700
H	9.74830500	4.74731000	4.79758200
H	8.81660600	4.00406700	3.49066900

H	10.57144700	3.82376100	3.54581900
C	8.64341800	7.39430700	4.51707000
H	9.10415800	6.94125700	5.39920400
H	8.58806900	8.47241500	4.68327000
H	7.61428000	7.01845800	4.45114200
C	9.40063000	7.06863100	3.26734900
C	10.33084800	7.63031900	-0.32140300
H	10.52193500	8.70381500	-0.40030200
H	11.14289800	7.10737700	-0.83366400
H	9.41031000	7.42382300	-0.88304400
C	9.09873100	9.35972200	2.05947800
H	9.60104800	9.90746800	1.25711500
H	8.02173600	9.39659300	1.85110800
H	9.27217400	9.90781600	2.98994400
C	10.79808500	4.67235100	0.74094300
H	11.26231800	3.88754700	1.34439700
H	9.93075500	4.22398200	0.23899600
H	11.50945400	4.95634700	-0.03879400
C	10.37397900	5.84394100	1.57515300
C	9.57850000	7.93952200	2.14908900
C	9.88361600	5.77299100	2.90655100
C	10.17645900	7.18422000	1.10091500
H	8.67143200	12.04573900	8.49754500
H	7.90496700	10.67762800	6.62353500
H	6.38928800	11.26812500	8.41477600
H	14.81091900	4.43147400	5.48336800
H	13.96225600	3.28463100	3.49952000
H	16.28542000	3.92143600	3.63268900
H	15.18485800	11.98933700	3.25386000
H	13.89030100	11.28383900	5.16582500
H	12.77602900	11.98200100	3.10521000
H	9.36994500	3.98521300	7.52212400
H	10.53660800	3.57547200	9.63079500
H	8.14288300	3.31320000	9.49347500

**NO**

H= -129.825383 au

N	0.00000000	0.00000000	-0.61599200
O	0.00000000	0.00000000	0.53899300

**NO<sup>+</sup>**

H= -335.925821 au

N	0.00000000	0.00000000	-0.57109000
O	0.00000000	0.00000000	0.49970400

**NO<sup>-</sup> (triplet)**

H= -129.804457 au

N	0.00000000	0.00000000	-0.6159900
O	0.00000000	0.00000000	0.5389900

**NO<sup>2-</sup>**

H= -129.377169 au

N	0.00000000	0.00000000	-0.78779100
O	0.00000000	0.00000000	0.68931700

**CO**

H= -113.249933 au

C	0.00000000	0.00000000	-0.64972100
O	0.00000000	0.00000000	0.48729100

**CNO**

H= -167.914783 au

O	0.00000000	0.00000000	1.14314400
C	0.00000000	0.00000000	-0.04093300
N	0.00000000	0.00000000	-1.27136500