

*Supporting Information for*

**DFT Study on 1,7-Octadiene Polymerization Catalyzed by Non-Bridged Half-Titanocene System**

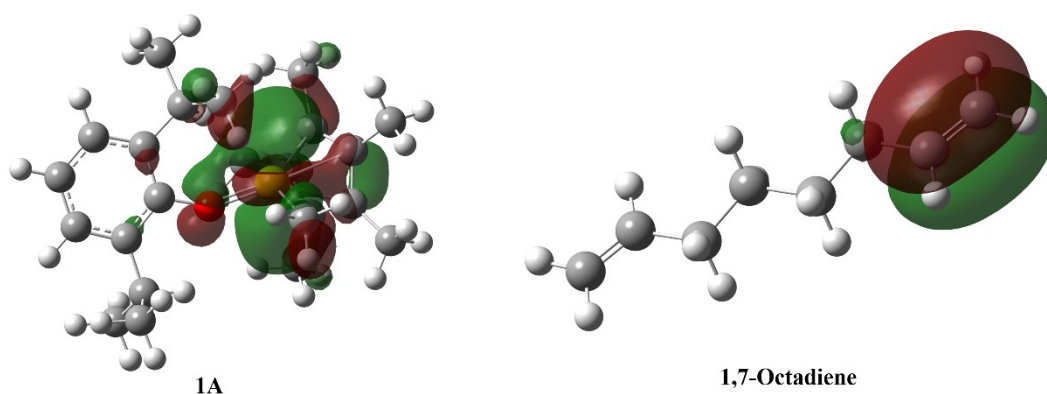
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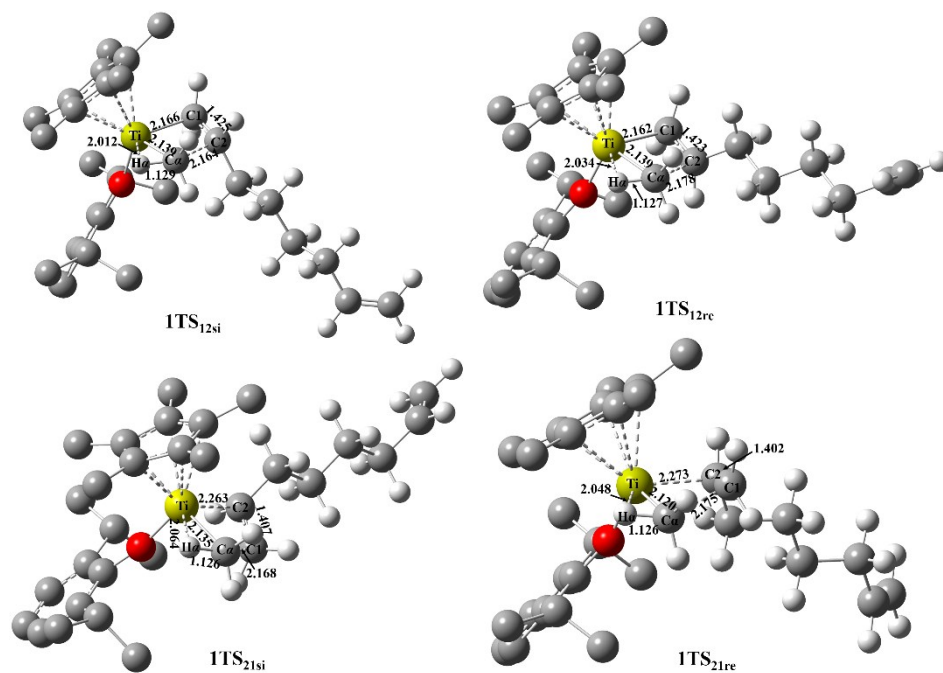
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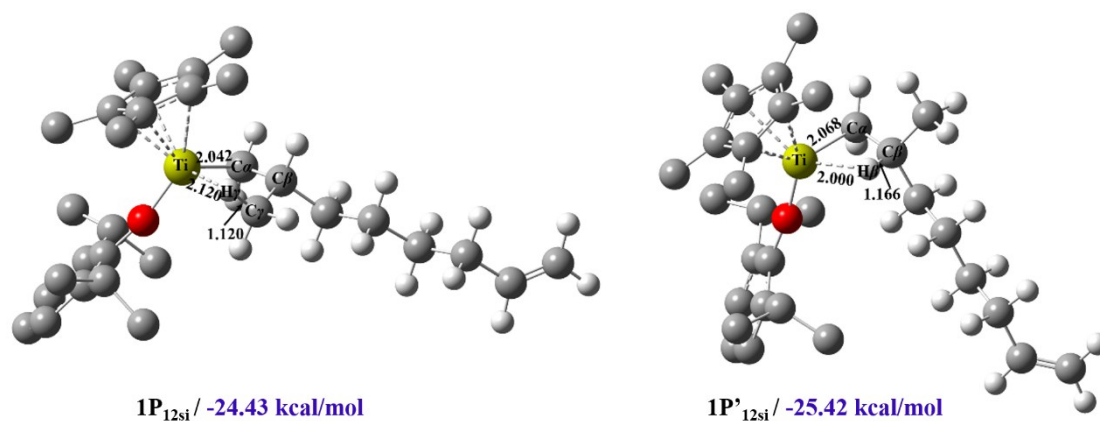
\*Corresponding author. E-mail: hgaohong@dlut.edu.cn (G. H.)



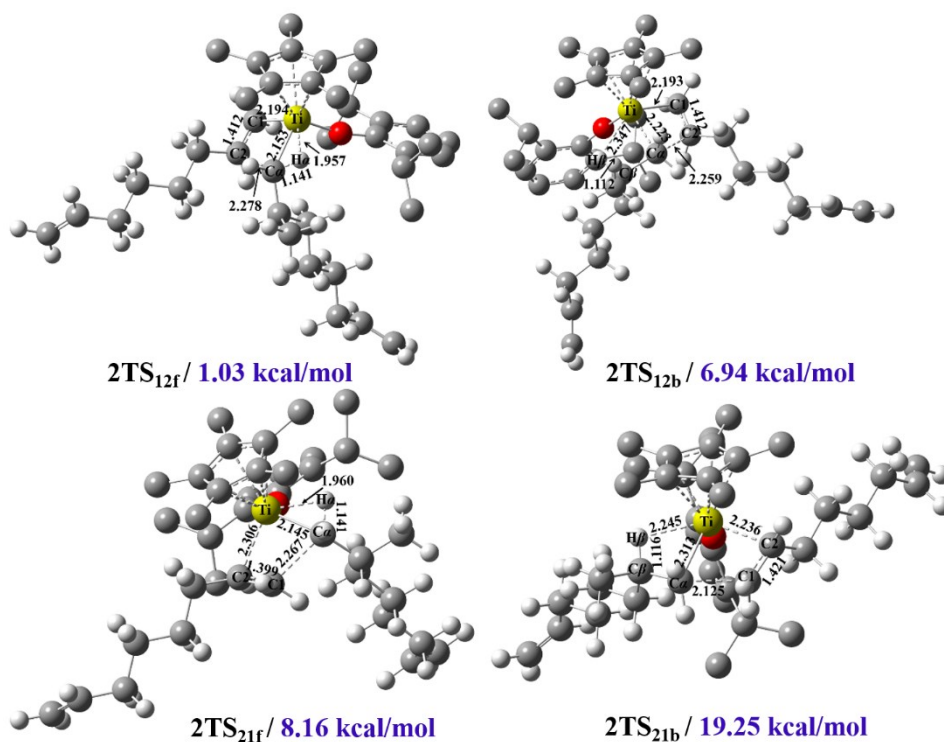
**Fig. S1.** Structures of LUMO of active species **1A** and HOMO of 1,7-octadiene (OD).



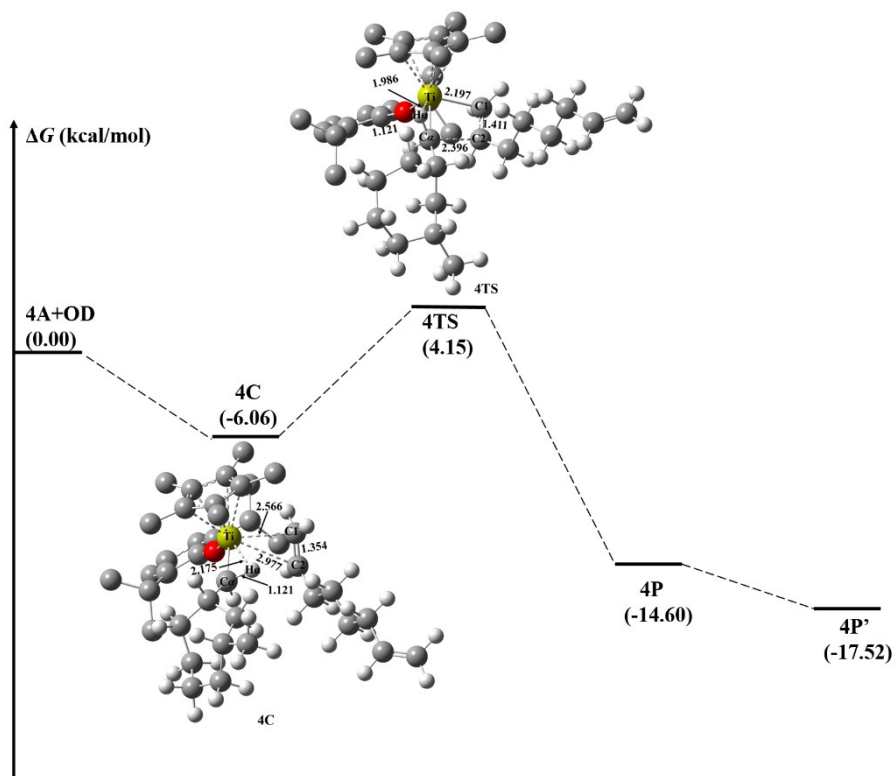
**Fig. S2.** Geometric structures (distance in Å) and their corresponding free energy relative to the energy sum of **1A** and OD of the transition states derived from four insertion modes. Hydrogen atoms of the C<sub>5</sub>Me<sub>5</sub> ligand and phenoxy have been omitted for clarity.



**Fig. S3.** Optimized structures (distances in Å) of direct product (**1P**<sub>12si</sub>) and its isomer (**1P'**<sub>12si</sub>) and their corresponding energies relative to the summation of the energies energy of **1A** and OD. Hydrogen atoms of the C<sub>5</sub>Me<sub>5</sub> ligand and phenoxy have been omitted for clarity.



**Fig. S4.** Geometric structures (distance in Å) and their corresponding free energy relative to the energy sum of **2A** and 1,7-octadiene of the transition states derived from 1,2-*f*-, 1,2-*b*-, 2,1-*f*- and 2,1-*b*-insertion. Hydrogen atoms of the C<sub>5</sub>Me<sub>5</sub> ligand and phenoxyl have been omitted for clarity.



**Fig. S5.** Computed energy profiles (energy in kcal/mol) and geometric structures (distance in Å) for repeated insertion of OD into **4A**. Hydrogen atoms of the C<sub>5</sub>Me<sub>5</sub> ligand and phenoxyl have been omitted for clarity.

**Table S1** Optimized Cartesian coordinates (Å) and zero-point energy corrected energy (a.u.) of cationic species **1A**, **2A**, **3A**, **4A** and **7A**.

Atom	x	y	z
<b>1A, -1029.9712169</b>			
Ti	-0.98543800	-0.17346000	-0.50103000
O	0.75669800	-0.34095600	-0.18322700
C	-2.73692100	0.87028100	0.72233100
C	-3.40079400	0.09011100	-0.28417000
C	-3.07113300	-1.27616900	-0.07312900
C	-2.17102300	-1.34140700	1.05256000
C	-2.00214100	-0.01668100	1.56921500
C	2.00315900	0.22656300	-0.08210100
C	2.06166700	1.63891400	-0.08527600
C	4.37978500	0.05378900	0.04125900
C	3.13908000	-0.59578900	-0.01506300
C	-2.91043900	2.35090300	0.92342500
C	-4.33295100	0.62050300	-1.33589900
C	-3.66322600	-2.45201100	-0.78954800
C	-1.62322100	-2.60425800	1.66018400
C	0.76365600	2.43688400	-0.13520800
C	0.05792800	2.34571900	-1.51147700
C	0.91348000	3.91541100	0.25323000
C	3.03832900	-2.11449600	-0.01636400
C	3.67617600	-2.72890900	1.24470700
C	3.65195100	-2.71263500	-1.29818800
C	3.32402100	2.23056800	-0.02951400
C	4.47592900	1.44225900	0.03100700
C	-1.23454800	0.35087300	2.80925900
H	0.09535500	1.99089400	0.62397700
H	1.97429900	-2.37344300	-0.00794000
C	-1.15149900	-1.20675600	-2.28342100
H	-2.07661600	-1.06121500	-2.84682700
H	-0.29076500	-0.87461100	-2.87968600
H	-1.02473300	-2.27964000	-2.08783600
H	-4.60060100	-2.74428600	-0.30089600
H	-3.89660100	-2.22790800	-1.83267100
H	-3.00298700	-3.32195900	-0.76988500
H	-2.35579700	-3.03168600	2.35564200
H	-1.41187500	-3.36701000	0.90587100
H	-0.70502300	-2.42221600	2.22270000
H	-1.86198300	0.19958700	3.69578700
H	-0.33899800	-0.26267400	2.93444000
H	-0.92453800	1.39850500	2.80834700
H	-3.81762800	2.53783600	1.51088100

H	-2.07736300	2.79807000	1.47014500
H	-3.02918000	2.88845400	-0.02134500
H	-5.35951200	0.65103700	-0.95053100
H	-4.07665700	1.63837600	-1.64188800
H	-4.34182000	-0.00927800	-2.22865500
H	3.41939900	3.31052200	-0.02821000
H	5.45065200	1.91757400	0.07437400
H	5.28560200	-0.54231400	0.09268200
H	3.22997700	-2.32422600	2.15869500
H	3.53684800	-3.81462300	1.24882200
H	4.75302100	-2.53619900	1.28622800
H	3.52811400	-3.80028900	-1.30783200
H	3.17669200	-2.30760100	-2.19718800
H	4.72411100	-2.50029300	-1.36332900
H	0.65023200	2.84596100	-2.28450400
H	-0.03964200	1.31777400	-1.91179600
H	-0.92654300	2.82586100	-1.49196100
H	1.38953000	4.02215500	1.23126100
H	1.51412400	4.46076100	-0.48128100
H	-0.06664300	4.39984300	0.29597600
<b>2A, -1342.8923076</b>			
Ti	1.17985500	-0.80575700	-0.06295200
O	0.42817200	0.80308000	-0.05754800
C	2.45962300	-1.21514600	1.83987500
C	2.44162200	-2.45039300	1.10514300
C	3.11774700	-2.23676800	-0.13480800
C	3.50880900	-0.85995000	-0.18630100
C	3.12931100	-0.23482600	1.04996500
C	0.02178800	2.11117000	0.04172800
C	-0.70241300	2.51374000	1.18476600
C	-0.11750900	4.31003700	-0.90711700
C	0.33428700	2.99153100	-1.01861600
C	1.92394600	-1.02243400	3.23238200
C	1.95660900	-3.77135900	1.63952400
C	3.49634900	-3.29089300	-1.13261200
C	4.28201900	-0.20925900	-1.29951300
C	-1.05047100	1.55414400	2.31536100
C	-2.56158500	1.24808100	2.34208700
C	-0.57075600	2.07210100	3.68476800
C	1.09844800	2.53247200	-2.25409100
C	2.23973300	3.49170100	-2.63936400
C	0.13898400	2.31157600	-3.44179800
C	-1.12872500	3.84528500	1.23441600
C	-0.84300200	4.73678600	0.20340400

C	3.43581200	1.17920800	1.45577100
H	-0.52905200	0.60766000	2.12558800
H	1.55818500	1.56475300	-2.02197800
H	4.46634500	-3.72534700	-0.86143000
H	2.77555400	-4.11114800	-1.16583300
H	3.59631300	-2.88555800	-2.14226700
H	5.35851100	-0.34068400	-1.13407600
H	4.04646100	-0.64694300	-2.27272500
H	4.09401200	0.86555900	-1.35688700
H	3.48705400	1.85033500	0.59541900
H	2.68802000	1.58046800	2.14334100
H	4.40725400	1.22167300	1.96269900
H	2.67122500	-1.34699300	3.96697100
H	1.69402200	0.02358100	3.44376600
H	1.02140200	-1.61261400	3.41710800
H	2.75077400	-4.24932400	2.22586400
H	1.09348800	-3.66015800	2.30127300
H	1.68282200	-4.46494400	0.84213500
H	-1.69569700	4.18896700	2.09402500
H	-1.18514600	5.76505800	0.26502100
H	0.09931500	5.01459700	-1.70352500
H	2.92087000	3.66623900	-1.80012800
H	2.81840600	3.07510700	-3.47011200
H	1.86207600	4.46503700	-2.96681100
H	0.68337000	1.93688300	-4.31521100
H	-0.64952100	1.59364600	-3.19309800
H	-0.34875400	3.24897600	-3.72827700
H	-3.14188000	2.15412000	2.54345100
H	-2.90428100	0.84184800	1.38534000
H	-2.79499600	0.52225000	3.12831900
H	0.50136000	2.29507800	3.68036800
H	-1.09352500	2.98931400	3.97250400
H	-0.76509100	1.32857200	4.46463400
C	-0.49466700	-2.26098600	-1.14290000
C	0.67540000	-1.63387200	-1.88930400
H	0.37943400	-0.82552800	-2.56357500
H	1.32639000	-2.34891600	-2.38724300
C	-1.84687500	-1.56386900	-1.41528000
H	-1.69988400	-0.47744500	-1.38516400
H	-2.12284900	-1.80849600	-2.44941100
C	-2.99233000	-1.94528300	-0.46927200
H	-3.18186700	-3.02442800	-0.51920100
H	-2.69562900	-1.73144900	0.56914500
C	-4.29373700	-1.19697000	-0.78916700

H	-4.11680600	-0.11352900	-0.73409300
H	-4.59099700	-1.40461200	-1.82494600
C	-5.45424700	-1.57398100	0.15089700
H	-5.65103700	-2.65101200	0.07969100
H	-5.14258100	-1.37984600	1.18856800
C	-6.71613900	-0.80870600	-0.14500700
H	-6.64964700	0.27581200	-0.04510700
C	-7.87211800	-1.35575600	-0.52024200
H	-7.98542200	-2.43182700	-0.63134600
H	-8.75068400	-0.75135500	-0.72413300
C	-0.55394800	-3.79054400	-1.28538600
H	-0.87336200	-4.03857800	-2.30231100
H	0.42439600	-4.24751100	-1.12210800
H	-1.26288200	-4.24014000	-0.58652600
H	-0.32946200	-2.11616200	0.00175400

Atom	x	y	z
<b>3A, -1655.7949964</b>			
Ti	-0.90481900	-1.30598500	-0.02055900
O	-1.97869500	0.09277400	0.21363500
C	-0.24432500	-3.65949800	0.12016400
C	0.20398900	-2.95800100	1.27974100
C	-0.95121400	-2.46408500	1.97454400
C	-2.10833900	-2.82401200	1.21999000
C	-1.66689400	-3.54965200	0.05874500
C	-2.96645200	1.00098100	0.51365500
C	-4.15020400	0.98787100	-0.26081200
C	-3.76989900	2.84784700	1.82067400
C	-2.75584700	1.91755500	1.56781200
C	0.60657400	-4.47727600	-0.80539400
C	1.62018700	-2.87564800	1.78342800
C	-0.94264300	-1.78108800	3.31348000
C	-3.53622400	-2.58531000	1.62495700
C	-4.36214800	0.00900300	-1.40899400
C	-4.10194400	0.69306300	-2.76721400
C	-5.75537900	-0.64684000	-1.38741200
C	-1.47277200	1.94938500	2.38814400
C	-1.74550900	1.88519800	3.90321500
C	-0.62759800	3.19208500	2.04233800
C	-5.12596500	1.94155900	0.04477400
C	-4.94270300	2.86549700	1.07102000
C	-2.55531000	-4.20610500	-0.95882900
H	-3.62699300	-0.79649000	-1.30128500

H	-0.88231200	1.06408700	2.12279500
H	-0.88817000	-2.53083000	4.11240500
H	-0.08282500	-1.11719500	3.44068900
H	-1.84825300	-1.19491400	3.47691900
H	-3.86823600	-3.37740400	2.30691600
H	-3.66547000	-1.63044400	2.14000000
H	-4.20974600	-2.59379300	0.76536400
H	-3.48660100	-3.65452500	-1.10883000
H	-2.06266100	-4.30548100	-1.92874200
H	-2.82639000	-5.21517000	-0.62454400
H	0.56363400	-5.53203900	-0.50652000
H	0.26468200	-4.42777600	-1.84257100
H	1.65588600	-4.17710700	-0.77494500
H	1.82738600	-3.71571800	2.45761700
H	2.35161800	-2.91803300	0.97401000
H	1.80332900	-1.95951700	2.35181700
H	-6.04476000	1.96354100	-0.53211700
H	-5.71410400	3.59823400	1.28608600
H	-3.63638700	3.57293500	2.61728700
H	-2.36646200	1.02449900	4.16952900
H	-0.80387500	1.81376000	4.45732800
H	-2.26142200	2.78350400	4.25561800
H	0.32041300	3.17967600	2.59095900
H	-0.40739700	3.24186700	0.97225700
H	-1.15684900	4.11138500	2.31285900
H	-4.81749200	1.50425700	-2.93658200
H	-3.09799900	1.12725900	-2.81478100
H	-4.20736200	-0.02321100	-3.58928600
H	-5.96728400	-1.11456100	-0.42073900
H	-6.55104100	0.07739500	-1.58623300
H	-5.82141000	-1.41626100	-2.16362000
C	3.21881100	-0.78295900	-2.45525700
C	1.78517800	-1.33449500	-2.60886500
H	1.78917900	-2.39230600	-2.32116000
H	1.51917500	-1.31455100	-3.67309300
C	3.73243700	-0.87342300	-1.00438600
H	2.99195200	-0.43317500	-0.32086700
H	3.81170200	-1.93546800	-0.72565400
C	5.07954800	-0.18350000	-0.74185600
H	5.86513000	-0.65624200	-1.34325200
H	5.02386500	0.86139900	-1.07898800
C	5.49194700	-0.21823200	0.73544000
H	4.72147800	0.28080000	1.34156100
H	5.53040600	-1.25883800	1.08468800



C	6.85555300	0.44693000	1.00268100
H	7.63517200	-0.07040400	0.42998200
H	6.82188000	1.47944600	0.62413400
C	7.22360300	0.46068300	2.46180600
H	6.54925000	1.01506700	3.11696900
C	8.28364500	-0.14952600	2.99180500
H	8.98561800	-0.70948500	2.37797900
H	8.49689700	-0.10501100	4.05559400
C	4.13501000	-1.53873100	-3.43427300
H	4.19153200	-2.60395300	-3.17876200
H	3.76451100	-1.46146900	-4.46160800
H	5.15218700	-1.14003900	-3.42320200
H	3.22121300	0.27198500	-2.75812400
C	0.60049200	-0.63866300	-1.88138600
H	0.89910600	-0.66136700	-0.76446200
C	-0.68382600	-1.45451700	-2.06587900
H	-1.47825500	-0.90273200	-2.57267800
H	-0.53044500	-2.42715100	-2.52912700
C	0.40981800	0.86305800	-2.22260800
H	0.61515600	0.97431400	-3.29533500
H	-0.64637700	1.12270100	-2.08747100
C	1.24793200	1.87516000	-1.42694700
H	2.31728900	1.67166000	-1.54087100
H	1.02892300	1.76327400	-0.35402800
C	0.96753000	3.32310400	-1.85289400
H	1.12714700	3.41715600	-2.93571400
H	-0.08958200	3.56409500	-1.67938700
C	1.85026500	4.35323600	-1.12276200
H	2.90526300	4.10007200	-1.30655100
H	1.69499800	4.27659000	-0.03914900
C	1.58940300	5.76588000	-1.57163000
H	1.76479900	5.96833900	-2.62918200
C	1.16333500	6.75330200	-0.78424900
H	0.97938000	6.59885900	0.27678800
H	0.99120200	7.75494600	-1.16603800
<b>4A, -1655.7949964</b>			
O	1.05415300	-0.16674500	-0.09098500
C	-1.29065300	3.12899500	-0.25610100
C	0.09748100	3.13516200	-0.61010900
C	0.86671400	2.84466300	0.56707100
C	-0.05125200	2.60567300	1.63178800
C	-1.38531600	2.77101500	1.12294900
C	-2.41682000	3.58358700	-1.13654300
C	0.65531500	3.49811600	-1.95840600

C	2.36612000	2.85353300	0.66342700
C	0.30055200	2.30672300	3.06362400
C	-2.63945700	2.75178600	1.95487900
C	2.25864400	-0.82519600	-0.13237100
C	2.90462500	-0.95715800	-1.38294200
C	4.11536000	-1.65560400	-1.40553700
C	4.66133200	-2.19815600	-0.24360800
C	4.00269900	-2.04578000	0.97352000
C	2.79019800	-1.35327900	1.06402000
C	2.29368700	-0.40415200	-2.66435100
C	2.08075500	-1.22297500	2.40557700
H	-2.54493200	4.66886100	-1.04129600
H	-3.36942000	3.12301200	-0.86494400
H	-2.22579200	3.37360500	-2.19169700
H	0.78132800	4.58547000	-2.03124200
H	-0.00740800	3.19259700	-2.77204800
H	1.63553700	3.04786200	-2.13211400
H	2.73007200	2.20417100	1.46227100
H	2.72125600	3.86897000	0.87616400
H	2.83988300	2.52987400	-0.26630500
H	0.28221800	3.23220400	3.65228800
H	1.29993900	1.87916500	3.16144900
H	-0.41008400	1.61953500	3.53277700
H	-3.52487500	2.51425700	1.36243200
H	-2.80298900	3.73919300	2.40359400
H	-2.58070100	2.03319100	2.77676200
Ti	-0.33569800	0.93558600	0.02640200
C	3.32478100	0.27831200	-3.58080900
H	3.89324600	1.04710100	-3.04775500
H	4.04090300	-0.43737400	-3.99586000
H	2.81860500	0.75223100	-4.42786000
C	1.53065900	-1.50978400	-3.42374700
H	0.76267900	-1.97241100	-2.79532800
H	1.04684600	-1.10323000	-4.31849900
H	2.21487900	-2.30252500	-3.74346400
H	4.63961200	-1.78031300	-2.34716900
H	5.60120300	-2.73936700	-0.28785100
H	4.43710400	-2.47395600	1.87153000
C	-2.00961200	-2.00759900	-0.49364200
C	-1.64437200	0.33109100	-1.45508200
H	-2.29955100	1.03754400	-1.95931400
H	-1.07567700	-0.26763600	-2.17199700
H	-2.17871600	-2.28480900	-1.54131500
C	-5.23450500	-2.25921300	-0.30821200

C	-4.81569600	-0.94064400	-0.97830100
C	-3.80963600	-0.12237300	-0.14513300
C	-4.16616100	-3.35841500	-0.23066200
C	-2.32216600	-0.49369000	-0.36792100
C	-2.80979000	-2.97970100	0.40373600
H	-5.59090800	-2.02767200	0.70539300
H	-4.42413800	-1.12140200	-1.98789900
H	-4.06516100	-0.24423000	0.91395200
H	-3.96696500	-3.74448400	-1.24082600
H	-6.10077100	-2.66528000	-0.84336600
H	-5.71346500	-0.32623300	-1.11033700
H	-3.92571400	0.94304600	-0.36630400
H	-4.59055700	-4.19904100	0.33113800
H	-1.85261300	-0.20119600	0.65841500
H	-0.93539200	-2.14354200	-0.32353900
H	1.56253500	0.36203900	-2.37995500
H	1.22399800	-0.55149000	2.26873100
C	2.98524500	-0.59572300	3.48369400
H	2.42451500	-0.44212900	4.41152300
H	3.83456800	-1.24342600	3.72125400
H	3.39113100	0.36916300	3.16210000
C	1.52788400	-2.58243900	2.87847300
H	2.33871800	-3.29710200	3.05140100
H	0.97618100	-2.47050200	3.81784200
H	0.85530100	-3.02032000	2.13459600
C	-1.98387400	-4.25332400	0.65124000
H	-1.75900000	-4.76425200	-0.29241400
H	-1.03146800	-4.02664100	1.14204400
H	-2.52791500	-4.95805200	1.28694700
H	-2.99237800	-2.50412400	1.37998700

Atom

x

y

z

**7A, -1655.8228367**

O	1.05415300	-0.16674500	-0.09098500
C	-1.29065300	3.12899500	-0.25610100
C	0.09748100	3.13516200	-0.61010900
C	0.86671400	2.84466300	0.56707100
C	-0.05125200	2.60567300	1.63178800
C	-1.38531600	2.77101500	1.12294900
C	-2.41681900	3.58358700	-1.13654300
C	0.65531600	3.49811600	-1.95840600
C	2.36612000	2.85353300	0.66342700
C	0.30055200	2.30672300	3.06362400
C	-2.63945700	2.75178600	1.95487900
C	2.25864400	-0.82519600	-0.13237100

C	2.90462500	-0.95715800	-1.38294200
C	4.11536000	-1.65560400	-1.40553700
C	4.66133200	-2.19815700	-0.24360800
C	4.00269900	-2.04578000	0.97352000
C	2.79019800	-1.35327900	1.06402000
C	2.29368700	-0.40415200	-2.66435100
C	2.08075500	-1.22297500	2.40557700
H	-2.54493100	4.66886100	-1.04129600
H	-3.36942000	3.12301200	-0.86494400
H	-2.22579200	3.37360500	-2.19169700
H	0.78132900	4.58547000	-2.03124200
H	-0.00740800	3.19259700	-2.77204800
H	1.63553700	3.04786200	-2.13211400
H	2.73007200	2.20417100	1.46227100
H	2.72125700	3.86897000	0.87616400
H	2.83988300	2.52987400	-0.26630500
H	0.28221800	3.23220400	3.65228800
H	1.29993900	1.87916500	3.16144900
H	-0.41008400	1.61953500	3.53277700
H	-3.52487500	2.51425700	1.36243200
H	-2.80298800	3.73919300	2.40359400
H	-2.58070100	2.03319100	2.77676200
Ti	-0.33569800	0.93558600	0.02640200
C	3.32478100	0.27831200	-3.58080900
H	3.89324600	1.04710100	-3.04775500
H	4.04090300	-0.43737400	-3.99586000
H	2.81860500	0.75223100	-4.42786000
C	1.53065900	-1.50978400	-3.42374700
H	0.76267900	-1.97241100	-2.79532800
H	1.04684600	-1.10323000	-4.31849900
H	2.21487900	-2.30252500	-3.74346400
H	4.63961200	-1.78031400	-2.34716900
H	5.60120300	-2.73936800	-0.28785100
H	4.43710400	-2.47395700	1.87153000
C	-2.00961200	-2.00759900	-0.49364200
C	-1.64437200	0.33109100	-1.45508200
H	-2.29955100	1.03754400	-1.95931400
H	-1.07567700	-0.26763600	-2.17199700
H	-2.17871600	-2.28480900	-1.54131500
C	-5.23450500	-2.25921200	-0.30821200
C	-4.81569600	-0.94064300	-0.97830100
C	-3.80963600	-0.12237200	-0.14513300
C	-4.16616100	-3.35841400	-0.23066200
C	-2.32216600	-0.49369000	-0.36792100

C	-2.80979000	-2.97970100	0.40373600
H	-5.59090800	-2.02767100	0.70539300
H	-4.42413800	-1.12140100	-1.98789900
H	-4.06516100	-0.24422900	0.91395200
H	-3.96696500	-3.74448300	-1.24082600
H	-6.10077100	-2.66527900	-0.84336600
H	-5.71346500	-0.32623200	-1.11033700
H	-3.92571400	0.94304700	-0.36630400
H	-4.59055700	-4.19904000	0.33113800
H	-1.85261300	-0.20119600	0.65841500
H	-0.93539200	-2.14354200	-0.32353900
H	1.56253500	0.36203900	-2.37995500
H	1.22399800	-0.55149000	2.26873100
C	2.98524500	-0.59572300	3.48369400
H	2.42451500	-0.44212900	4.41152300
H	3.83456800	-1.24342600	3.72125400
H	3.39113100	0.36916300	3.16210000
C	1.52788400	-2.58243900	2.87847300
H	2.33871800	-3.29710200	3.05140100
H	0.97618100	-2.47050200	3.81784200
H	0.85530100	-3.02032000	2.13459600
C	-1.98387400	-4.25332400	0.65124000
H	-1.75900100	-4.76425200	-0.29241400
H	-1.03146800	-4.02664100	1.14204400
H	-2.52791600	-4.95805200	1.28694700
H	-2.99237800	-2.50412400	1.37998700

**Table S2** Optimized Cartesian coordinates (Å) and zero-point energy corrected energy (a.u.) of **1C<sub>12si</sub>**, **1TS<sub>12si</sub>**, **1P<sub>12si</sub>**, **1C<sub>12re</sub>**, **1TS<sub>12re</sub>**, **1P<sub>12re</sub>**, **1C<sub>21re</sub>**, **1TS<sub>21re</sub>**, **1P<sub>21re</sub>**, **1C<sub>21si</sub>**, **1TS<sub>21si</sub>** and **1P<sub>21si</sub>**, as well as the imaginary frequency (cm<sup>-1</sup>) of **1TS<sub>12si</sub>**, **1TS<sub>12re</sub>**, **1TS<sub>21re</sub>** and **1TS<sub>21si</sub>**.

Atom	x	y	z
<b>1C<sub>12si</sub>, -1342.882024</b>			
Ti	-1.50803700	-0.69832300	-0.26346000
O	-0.14243700	0.40302900	0.04820900
C	-3.38337800	0.50744100	-1.06316700
C	-3.82005800	-0.85502800	-1.04040200
C	-3.79242200	-1.29698300	0.31343000
C	-3.34503500	-0.20563900	1.13113100
C	-3.10939400	0.91543000	0.28142500
C	0.72063800	1.44663500	0.29126200
C	1.16654000	2.22158000	-0.80604800
C	2.05009200	2.74846200	1.81423500
C	1.14961700	1.69604300	1.61573400

C	-3.35751600	1.40578000	-2.26565700
C	-4.35087700	-1.62867500	-2.21084100
C	-4.32692900	-2.60989400	0.81603400
C	-3.26444900	-0.21377600	2.63297800
C	0.72068400	1.95134500	-2.23784700
C	1.85199900	1.29804600	-3.05795200
C	0.20387500	3.22157200	-2.94064900
C	0.69699300	0.86480900	2.81030500
C	-0.02294000	1.72252700	3.87031800
C	1.88007400	0.11367600	3.45464400
C	2.06758400	3.25765900	-0.53940400
C	2.50921900	3.52417300	0.75378900
C	-2.75111900	2.30931900	0.71058000
H	-0.10774300	1.23902600	-2.20148600
H	-0.01561600	0.11477200	2.44835400
C	-1.13288300	-1.37455600	-2.19877500
H	-1.62544400	-2.34061800	-2.36461800
H	-1.44058100	-0.69490500	-2.99800100
H	-0.04486100	-1.50207200	-2.25684400
H	-5.40793800	-2.52914800	0.98245900
H	-4.17790700	-3.42325500	0.09989100
H	-3.88130100	-2.90611600	1.76902900
H	-4.23414300	0.06767500	3.06181400
H	-3.01779700	-1.20249800	3.03002600
H	-2.52661400	0.49639700	3.01121900
H	-2.27486600	2.32558400	1.69200400
H	-2.07350000	2.79801500	0.00636000
H	-3.65739100	2.92350400	0.77506400
H	-4.30604000	1.95240100	-2.33880900
H	-2.56057100	2.15074100	-2.20772700
H	-3.23402100	0.84644200	-3.19525900
H	-5.42446700	-1.43764800	-2.32898600
H	-3.86596900	-1.34386300	-3.14699800
H	-4.22644900	-2.70697700	-2.08253000
H	2.43062300	3.86629500	-1.36144600
H	3.20905900	4.33399000	0.93438700
H	2.39980000	2.96198600	2.81964300
H	-0.86640200	2.27579500	3.44610600
H	-0.39780700	1.09356700	4.68476100
H	0.65596700	2.45810300	4.31244400
H	1.53014800	-0.54542900	4.25642700
H	2.42345800	-0.49024300	2.72204600
H	2.59776600	0.81310000	3.89456500
H	2.71608300	1.96600200	-3.13641000

H	2.19455500	0.36528800	-2.59906800
H	1.51074100	1.07226700	-4.07373100
H	-0.58764300	3.71138900	-2.36371500
H	1.00043000	3.95622800	-3.09284300
H	-0.19707900	2.97091200	-3.92811800
C	0.21207500	-3.10910000	0.23058700
H	0.13948800	-3.63881500	-0.72066200
C	-0.94667500	-2.81510000	0.87368600
H	-0.93194200	-2.38699500	1.87740400
H	-1.87534600	-3.26627300	0.53688500
C	1.59564300	-2.83855000	0.71136900
H	1.57495000	-2.24494800	1.63039800
H	2.00729500	-3.82468800	0.98367400
C	2.52647100	-2.20507400	-0.34360000
H	2.47001700	-2.78749900	-1.27321400
H	2.16521200	-1.19676600	-0.57895500
C	3.98500000	-2.13630100	0.12717500
H	4.04106100	-1.56954500	1.06656600
H	4.34647300	-3.14707300	0.35569100
C	4.91837300	-1.48893800	-0.91304900
H	4.88564600	-2.06466000	-1.84657300
H	4.53713200	-0.48370400	-1.14795600
C	6.34099900	-1.38609200	-0.43168200
H	6.49843900	-0.77871700	0.46084400
C	7.38652700	-1.98094200	-1.00551300
H	7.27679700	-2.59416900	-1.89715900
H	8.39224600	-1.87307300	-0.61109300
<b>1TS<sub>12si</sub>, -1342.8678659, i303.99</b>			
Ti	0.84863000	-1.05686100	0.06062500
O	0.59470000	0.70578500	-0.00109400
C	2.76605400	-1.48977400	1.31103000
C	2.20520500	-2.78976500	1.05231500
C	2.26686600	-3.02232400	-0.34625700
C	2.84319000	-1.86455700	-0.96662900
C	3.18193100	-0.93109200	0.06608300
C	0.69842800	2.07608500	0.04173700
C	0.51433500	2.73051300	1.28096400
C	1.05247600	4.16671400	-1.08305700
C	0.97265600	2.77204200	-1.15654700
C	3.00886600	-0.88943700	2.66922100
C	1.77335800	-3.78284700	2.09388500
C	1.89182300	-4.30425800	-1.03314500
C	3.18022000	-1.72133200	-2.42423600
C	0.16617000	1.95788400	2.54701900

C	-1.36525200	1.84301900	2.70489900
C	0.79888100	2.54502700	3.82030500
C	1.12554300	2.04813600	-2.48828600
C	2.25140700	2.62012300	-3.36824100
C	-0.21331100	2.03952800	-3.25629100
C	0.60743700	4.12588900	1.28825200
C	0.87302000	4.84054800	0.12226500
C	3.91522200	0.36852800	-0.11007000
H	0.56406700	0.94252600	2.43376600
H	1.38754600	1.00669900	-2.26876200
C	-0.79194400	-1.77413400	1.23029300
H	-0.93599200	-2.80596800	1.54846300
H	0.04090900	-1.36967700	1.87678500
H	-1.65763400	-1.16886400	1.48471400
H	2.68842100	-5.04602300	-0.89949500
H	0.97564100	-4.74337700	-0.62684400
H	1.75982400	-4.17461600	-2.10973800
H	4.17409500	-2.13953300	-2.62477600
H	2.47252500	-2.25026700	-3.06746800
H	3.20047600	-0.67513400	-2.73827100
H	3.81175100	0.76218700	-1.12323100
H	3.56249200	1.13798800	0.58111300
H	4.98600500	0.22246000	0.07617500
H	3.98532900	-1.21174500	3.05140700
H	3.01755800	0.20259400	2.63882600
H	2.26010400	-1.20188200	3.40244000
H	2.63662700	-4.36359400	2.44040200
H	1.33917400	-3.30180900	2.97484700
H	1.04257900	-4.49643000	1.70390300
H	0.46963600	4.66353300	2.22013400
H	0.94009400	5.92348500	0.15359800
H	1.25801500	4.73517400	-1.98389400
H	3.20331400	2.66674100	-2.82986400
H	2.38963700	1.99358700	-4.25536300
H	2.02106300	3.62900000	-3.72370800
H	-0.12385600	1.47426700	-4.19065700
H	-1.01771100	1.59714100	-2.65941500
H	-0.51866200	3.05963600	-3.51091400
H	-1.81259800	2.83285800	2.84164400
H	-1.82859000	1.39378300	1.82024800
H	-1.62340400	1.23471800	3.57885000
H	1.88044700	2.67370900	3.71330600
H	0.36971300	3.51781300	4.07863500
H	0.61660200	1.88001100	4.67039500



C	-1.34948800	-1.92691700	-0.85551000
H	-1.59184700	-2.96464100	-0.63826200
C	-0.22349600	-1.71655200	-1.70241900
H	-0.24610400	-0.83533500	-2.34308000
H	0.23423400	-2.59438200	-2.14327200
C	-2.53778200	-0.97760900	-0.91039000
H	-2.23102100	0.03104700	-0.61019300
H	-2.78532900	-0.90171200	-1.97888000
C	-3.80116100	-1.42237600	-0.16082400
H	-4.06072900	-2.44354600	-0.47218800
H	-3.62159600	-1.47008500	0.92050900
C	-4.99111800	-0.49048300	-0.42894800
H	-4.72869100	0.53212700	-0.12364100
H	-5.18961500	-0.44669400	-1.50750500
C	-6.27541300	-0.92692800	0.30066300
H	-6.55742900	-1.93714400	-0.02136400
H	-6.06358200	-0.98824300	1.37882200
C	-7.42428600	0.01745800	0.06776800
H	-7.27641800	1.04149500	0.41394000
C	-8.57215900	-0.30786200	-0.52622500
H	-8.76395800	-1.31667600	-0.88487000
H	-9.36663300	0.41798600	-0.67003000
<b>1P<sub>12si</sub>, -1342.8907234</b>			
Ti	-0.33129500	0.90617200	-0.00248200
O	-1.34535200	-0.55418700	-0.02925300
C	-1.31730000	2.70545600	1.12232100
C	-0.04690000	3.18866000	0.65701900
C	-0.06673300	3.18511200	-0.76862600
C	-1.33127900	2.66265900	-1.18716700
C	-2.11622100	2.39111800	-0.01583300
C	-2.34199800	-1.49675100	0.02638100
C	-2.81491700	-1.91130400	1.29122700
C	-3.83348000	-3.00007100	-1.10035800
C	-2.83337900	-2.02629100	-1.18768600
C	-1.75339900	2.63359000	2.56025400
C	1.05128500	3.75045700	1.51903500
C	0.99087300	3.75948500	-1.66313200
C	-1.79751000	2.53028700	-2.60903700
C	-2.22454600	-1.37333500	2.58853800
C	-1.18671700	-2.35999700	3.16419300
C	-3.29252200	-1.02726600	3.64150300
C	-2.26514300	-1.60122500	-2.53585400
C	-3.34661800	-1.39531100	-3.61129800
C	-1.19985600	-2.61015700	-3.01479600

C	-3.81187300	-2.89208800	1.31123200
C	-4.32065200	-3.43102500	0.13168200
C	-3.54571800	1.92926600	0.00064900
H	-1.69547900	-0.44149000	2.35248400
H	-1.76105200	-0.63897300	-2.39528300
C	1.65341100	0.10430800	1.19366000
H	0.94836200	0.82199800	1.68520700
H	1.22248500	-0.90238700	1.21550900
H	2.47139700	0.12254100	1.91671200
H	0.87373700	4.84832100	-1.72416400
H	2.00168500	3.56675600	-1.29273600
H	0.92157600	3.37092500	-2.68120700
H	-2.22283400	3.48085400	-2.95399300
H	-0.97917400	2.27320100	-3.28610700
H	-2.57497100	1.77069000	-2.71546000
H	-3.78169200	1.29470400	-0.85638300
H	-3.78396000	1.36282800	0.90352000
H	-4.21919000	2.79391600	-0.03414800
H	-2.14479300	3.60698000	2.88053600
H	-2.54710700	1.89957300	2.71326100
H	-0.92885300	2.38552100	3.23510900
H	0.90967800	4.83023100	1.64843100
H	1.06192600	3.30933200	2.51929300
H	2.04011300	3.60935000	1.07455000
H	-4.19490500	-3.24243500	2.26415300
H	-5.09559400	-4.18998900	0.17278200
H	-4.23531200	-3.43185000	-2.01098800
H	-4.12541500	-0.70274300	-3.27566700
H	-2.89707500	-0.98848400	-4.52275500
H	-3.83475000	-2.33494000	-3.88749800
H	-0.75195200	-2.28166600	-3.95878800
H	-0.39956700	-2.72894400	-2.27687700
H	-1.64499400	-3.59693900	-3.17929900
H	-1.66215000	-3.30908600	3.43150700
H	-0.39821400	-2.58405700	2.43778700
H	-0.72020500	-1.95278200	4.06785800
H	-4.05009500	-0.34565500	3.24130900
H	-3.81063200	-1.92001400	4.00420200
H	-2.82715300	-0.55149200	4.51082100
C	2.20565900	0.49727400	-0.21908600
H	2.62496900	1.50561800	-0.12585900
C	1.14406700	0.51279100	-1.35786400
H	0.95187600	-0.50048500	-1.72994500
H	1.44742700	1.15762700	-2.17976200

C	3.36089900	-0.47303000	-0.59655300
H	2.96825400	-1.49858300	-0.60893000
H	3.64747900	-0.24225100	-1.62864700
C	4.60861200	-0.39320500	0.29509300
H	4.94540200	0.65115200	0.35958200
H	4.37601500	-0.70923600	1.32070800
C	5.75777900	-1.26343600	-0.23575900
H	5.41962800	-2.30590600	-0.31177900
H	6.01666700	-0.94942600	-1.25483700
C	7.01908100	-1.19885500	0.64649900
H	7.37375900	-0.16227000	0.70804600
H	6.74778900	-1.49980000	1.66967000
C	8.12702900	-2.08351300	0.14122300
H	7.90247300	-3.15032700	0.09961300
C	9.32557600	-1.65641700	-0.25566700
H	9.59401600	-0.60261400	-0.22947600
H	10.08665200	-2.34268600	-0.61419500
<b>1C<sub>12res</sub> -1342.8829827</b>			
Ti	1.11994400	-0.94779700	0.01486600
O	0.28923400	0.62919700	0.02693100
C	2.82386000	-0.95883600	1.64852200
C	2.84287700	-2.28099200	1.10059900
C	3.18820400	-2.17543200	-0.27789100
C	3.40583300	-0.78795800	-0.57703500
C	3.19202600	-0.03798000	0.61616700
C	-0.10924300	1.94120300	0.11698900
C	-0.68670600	2.38818300	1.32852300
C	-0.38952100	4.11021600	-0.88024700
C	0.05007900	2.78801600	-1.00400800
C	2.59936300	-0.60722000	3.09090700
C	2.68149800	-3.55548000	1.87467900
C	3.45664900	-3.33207300	-1.20081000
C	3.89574000	-0.23346800	-1.88662500
C	-0.88935100	1.46749400	2.52527900
C	-2.37398400	1.07409000	2.66981700
C	-0.35698500	2.07709500	3.83604000
C	0.62946900	2.30646800	-2.32846600
C	1.82691900	3.15928400	-2.79084200
C	-0.45585100	2.26674900	-3.42485300
C	-1.10327600	3.72196200	1.38836200
C	-0.95914300	4.57912000	0.30041200
C	3.40953500	1.43719400	0.79647600
H	-0.32603100	0.54881600	2.33944600
H	0.99448200	1.28289800	-2.18349100

C	-0.09799900	-2.12039800	1.22850100
H	0.05251000	-3.18712000	1.02679000
H	0.02569900	-1.95479000	2.30239000
H	-1.12080700	-1.83535800	0.95402400
H	4.49694100	-3.66154300	-1.09175800
H	2.82390800	-4.19533500	-0.97729400
H	3.31567800	-3.07169900	-2.25278800
H	4.99015800	-0.15974000	-1.87433800
H	3.63403600	-0.87278200	-2.73423100
H	3.50932300	0.76913400	-2.08489400
H	3.32535000	1.98075700	-0.14634600
H	2.69528600	1.87742400	1.49631700
H	4.41528400	1.62132100	1.19308400
H	3.55851100	-0.59768400	3.62358900
H	2.15522700	0.38366300	3.20970400
H	1.95604400	-1.33094300	3.59603200
H	3.64987100	-3.86548500	2.28600100
H	1.99297600	-3.44358000	2.71489200
H	2.31848200	-4.37495400	1.24924500
H	-1.55237400	4.09494900	2.30331400
H	-1.29236800	5.60967900	0.37167800
H	-0.28686200	4.78395800	-1.72532100
H	2.61074100	3.20691500	-2.02838700
H	2.26195700	2.74515400	-3.70661000
H	1.52493500	4.18753000	-3.01133000
H	-0.05704000	1.84518000	-4.35402300
H	-1.32311900	1.67336200	-3.11600400
H	-0.82157100	3.27348100	-3.64969400
H	-2.99557300	1.95372300	2.86664900
H	-2.75223400	0.59878300	1.75910400
H	-2.50865400	0.37490900	3.50178500
H	0.69100900	2.38158900	3.74572400
H	-0.92992300	2.95907600	4.13824500
H	-0.43265300	1.34870300	4.64984500
C	-0.71310600	-1.49604100	-2.23095600
C	0.52840300	-2.03011300	-2.10011500
H	1.37398500	-1.54750200	-2.58847100
H	0.66434500	-3.05920200	-1.77247900
H	-0.79555100	-0.50492400	-2.67758300
C	-2.00205800	-2.16274800	-1.88187900
H	-2.38467300	-2.57453500	-2.83093000
H	-1.82519500	-3.02489700	-1.22892400
C	-3.07365900	-1.22209500	-1.29931500
H	-2.69961700	-0.76665400	-0.37367900

H	-3.24425100	-0.39442100	-2.00082200
C	-4.39787300	-1.94435500	-1.02240400
H	-4.22843700	-2.77356300	-0.32337900
H	-4.76557600	-2.39748100	-1.95320800
C	-5.48003100	-1.01300500	-0.44445200
H	-5.12583900	-0.57513200	0.49758200
H	-5.63250200	-0.17656900	-1.14271600
C	-6.78923400	-1.71873400	-0.21257800
H	-7.26680400	-2.13819800	-1.09911300
C	-7.37856300	-1.86536600	0.97377500
H	-8.32452400	-2.38714900	1.08098500
H	-6.94043600	-1.46048300	1.88346000
<b>1TS<sub>12re</sub>, -1342.8669007, i306.44</b>			
Ti	-0.14555000	0.73506400	0.16114900
O	-1.39823500	-0.50091300	-0.12462100
C	-0.91802800	2.14706500	1.83876600
C	0.45259700	2.54032600	1.64192100
C	0.57004500	3.07906600	0.33433900
C	-0.71691800	3.00474900	-0.29609300
C	-1.64316000	2.46040000	0.65102900
C	-2.54119200	-1.26284900	-0.18765900
C	-2.86520400	-2.09017700	0.91125300
C	-4.48599800	-1.98944800	-1.39213100
C	-3.33525800	-1.19523700	-1.35406400
C	-1.51243300	1.64287800	3.12554500
C	1.52679400	2.51736900	2.69224600
C	1.79837800	3.72233900	-0.24170200
C	-1.06946500	3.55967000	-1.64756300
C	-1.95017700	-2.19124200	2.12480300
C	-0.88222100	-3.28388500	1.90156700
C	-2.69829400	-2.42675500	3.44745500
C	-2.92802700	-0.33895600	-2.54616700
C	-4.11800400	0.30223000	-3.28037000
C	-2.06339900	-1.16086500	-3.52650200
C	-4.02807900	-2.86068000	0.81168200
C	-4.83320200	-2.81319100	-0.32417100
C	-3.12705500	2.31411500	0.46415700
H	-1.42827100	-1.23163600	2.22233200
H	-2.30850300	0.48123200	-2.16412600
C	1.49002700	-0.37917700	0.97240500
H	2.36240200	0.14821500	1.35429700
H	0.67202500	-0.25560700	1.73811700
H	1.66926800	-1.45174200	0.94483800
H	1.85030000	4.77206500	0.07235800

H	2.71943700	3.24153000	0.09913800
H	1.79673300	3.72023900	-1.33416300
H	-1.36016300	4.61339500	-1.55773300
H	-0.22962600	3.51588200	-2.34519600
H	-1.91080300	3.03060200	-2.10193300
H	-3.40240300	2.26085000	-0.59107600
H	-3.51911200	1.42010500	0.95507600
H	-3.64498300	3.18026800	0.89339300
H	-1.82050300	2.48941300	3.75159700
H	-2.39853600	1.02745100	2.95401900
H	-0.80000500	1.05517300	3.71095100
H	1.47261000	3.42445700	3.30595800
H	1.42649600	1.66605000	3.37153500
H	2.52878200	2.48463800	2.25644900
H	-4.30916800	-3.50895000	1.63437700
H	-5.73156900	-3.42010400	-0.37737800
H	-5.12096100	-1.96396800	-2.27107300
H	-4.76801900	0.85404500	-2.59414200
H	-3.75629500	0.99871000	-4.04362000
H	-4.73152800	-0.44308600	-3.79561100
H	-1.71336300	-0.53773200	-4.35705600
H	-1.19145900	-1.59783800	-3.02795900
H	-2.64313900	-1.98731400	-3.95008500
H	-1.35328600	-4.26858300	1.81849300
H	-0.31761800	-3.11221000	0.97928600
H	-0.17760300	-3.31867500	2.73988600
H	-3.48948400	-1.68687700	3.60333600
H	-3.15497300	-3.42034800	3.48796600
H	-2.00074900	-2.36244400	4.28851000
C	1.76605900	-0.24113700	-1.18387500
C	0.88209800	0.72498700	-1.74100900
H	0.08387800	0.34936400	-2.38003100
H	1.31265600	1.67225600	-2.04952100
H	1.46059200	-1.27985800	-1.29045600
C	3.26631400	-0.00885400	-1.18641200
H	3.51278600	0.11920300	-2.25120500
H	3.50043700	0.95414800	-0.71757800
C	4.15167900	-1.13066800	-0.62595500
H	4.00980900	-1.23347400	0.45574900
H	3.84465800	-2.08716000	-1.07154200
C	5.64034200	-0.89098200	-0.91330600
H	5.94934500	0.07177000	-0.48514300
H	5.79382000	-0.80766100	-1.99789000
C	6.54749100	-2.00262600	-0.35305300

H	6.41459000	-2.07519500	0.73389400
H	6.22264600	-2.96558600	-0.77459100
C	8.00197700	-1.78078200	-0.67068500
H	8.25897900	-1.75561100	-1.73058100
C	8.96456400	-1.61069900	0.23531200
H	9.99917600	-1.45286600	-0.05333200
H	8.75517500	-1.63256100	1.30256900
<b>1P<sub>12re</sub>, -1342.8898743</b>			
Ti	-0.46982900	1.03152800	-0.00455900
O	-1.20590800	-0.58585200	-0.05847500
C	-2.32202200	2.29383700	0.63195000
C	-1.17782800	2.97579800	1.15306200
C	-0.39699400	3.44753800	0.04908300
C	-1.03552700	3.03230100	-1.15570300
C	-2.22273900	2.30482500	-0.79276900
C	-2.03837600	-1.67222500	0.04510200
C	-2.39932100	-2.12479500	1.33409900
C	-3.32105000	-3.40354000	-1.00456900
C	-2.47424500	-2.29879600	-1.14287500
C	-3.47013800	1.73130300	1.42223000
C	-0.89906700	3.23230200	2.60998700
C	0.83862000	4.29839500	0.13319900
C	-0.64424900	3.42824400	-2.54926000
C	-1.82305800	-1.47886400	2.58836600
C	-0.46578500	-2.12231700	2.94772800
C	-2.77388300	-1.50947700	3.79597800
C	-1.98740200	-1.82740800	-2.50752800
C	-3.02688600	-2.00007000	-3.62709000
C	-0.66565600	-2.53566000	-2.87613500
C	-3.24419600	-3.23667600	1.40529100
C	-3.70666700	-3.86718400	0.25144600
C	-3.25805800	1.77520300	-1.74508800
H	-1.63771200	-0.42001100	2.35903000
H	-1.77208600	-0.75596800	-2.42715600
C	1.75974700	0.74603100	1.15186900
H	1.98682600	1.81633200	1.19084300
H	0.78801500	0.56604600	1.67531500
H	2.44258700	0.23897100	1.83682800
H	0.57729600	5.35510700	-0.00059200
H	1.33361300	4.21537100	1.10412000
H	1.56742600	4.04932300	-0.64338400
H	-1.17368300	4.34437100	-2.83820300
H	0.42528500	3.63308100	-2.63345600
H	-0.89898500	2.65960100	-3.28291900

H	-2.82967200	1.52320500	-2.71788900
H	-3.75751200	0.88585000	-1.35355000
H	-4.02910100	2.53633500	-1.91705400
H	-4.30804600	2.43897500	1.41628200
H	-3.83586600	0.78920300	1.00562400
H	-3.20311500	1.55656300	2.46665700
H	-1.40228400	4.15150100	2.93307400
H	-1.26666700	2.42504200	3.24944900
H	0.16704700	3.36311700	2.81181800
H	-3.54525600	-3.61774300	2.37493400
H	-4.36542300	-4.72612600	0.33224100
H	-3.68323900	-3.91121400	-1.89179700
H	-3.98489300	-1.53960600	-3.36646600
H	-2.66418400	-1.53321600	-4.54821900
H	-3.21143300	-3.05425300	-3.85620400
H	-0.28131800	-2.16475500	-3.83260500
H	0.10151300	-2.37706200	-2.11126600
H	-0.81906400	-3.61551500	-2.97197000
H	-0.59839300	-3.17957300	3.19782900
H	0.24030200	-2.07048500	2.11217500
H	-0.01584800	-1.62681500	3.81535400
H	-3.75576700	-1.09418900	3.54985600
H	-2.92308200	-2.52685600	4.17023000
H	-2.35222800	-0.92629000	4.62083300
C	1.92418400	0.16050200	-0.28803100
C	1.05528500	0.88766600	-1.35565200
H	0.84321000	0.24010600	-2.21020900
H	1.52917100	1.80980400	-1.69811500
H	1.63439600	-0.89603700	-0.24805400
C	3.42060200	0.23006800	-0.70446200
H	3.47363200	-0.06104200	-1.75960900
H	3.75265300	1.27612400	-0.65775800
C	4.37140000	-0.66287000	0.10589900
H	4.39490600	-0.35204300	1.15885200
H	3.99877700	-1.69660400	0.09517300
C	5.80520700	-0.63347400	-0.44422200
H	6.17901500	0.39854500	-0.44673900
H	5.79832100	-0.96041200	-1.49278900
C	6.77692200	-1.51780900	0.36030700
H	6.80708700	-1.17932900	1.40379100
H	6.38532900	-2.54595900	0.37435700
C	8.16935900	-1.51923500	-0.21103900
H	8.26525100	-1.89980300	-1.22897200
C	9.25805100	-1.08895300	0.42624600



H	10.23890300	-1.11233100	-0.03866900
H	9.21043100	-0.70408400	1.44257800
<b>1C<sub>21re</sub>, -1342.8782786</b>			
Ti	-0.91525800	-1.14581500	-0.45599100
O	-1.25070800	0.60489300	-0.41598700
C	-1.46310800	-1.45444000	1.81110900
C	-2.47159200	-2.09425500	1.02444100
C	-1.87652500	-3.21258800	0.35395200
C	-0.49547100	-3.24098100	0.69866100
C	-0.23909600	-2.15253800	1.60123900
C	-1.67138100	1.87608100	-0.09280400
C	-0.78791200	2.74230600	0.58900400
C	-3.38159500	3.56580400	-0.13131900
C	-2.97409200	2.27449400	-0.47920100
C	-1.69138200	-0.32257000	2.77077700
C	-3.93087200	-1.74302900	1.02582700
C	-2.60786500	-4.27437900	-0.41160600
C	0.45835200	-4.33548600	0.30168900
C	0.64990700	2.36258000	0.91797100
C	1.03137300	2.65882600	2.38074100
C	1.61977500	3.07714000	-0.04711800
C	-3.87590200	1.36855900	-1.30678700
C	-3.63381300	1.61099500	-2.81242800
C	-5.37017900	1.50694100	-0.96915100
C	-1.25459200	4.02408300	0.90266600
C	-2.53810200	4.43443100	0.55745300
C	1.04434700	-1.87398900	2.33451100
H	0.75699800	1.28279600	0.76167400
H	-3.59121500	0.33498600	-1.09215300
C	-1.99830700	-1.73251000	-2.13972700
H	-1.73276700	-2.72991000	-2.50455800
H	-3.08199900	-1.69864800	-1.99850900
H	-1.72868800	-0.98029800	-2.89303800
H	-2.96578200	-5.04678500	0.28029200
H	-3.48003500	-3.88038000	-0.93729900
H	-1.96631400	-4.76822300	-1.14565300
H	0.16181400	-5.27805600	0.77638900
H	0.46821700	-4.51645500	-0.77829300
H	1.48114900	-4.12886900	0.62281300
H	0.97390100	-2.25164400	3.36164700
H	1.90240000	-2.36508100	1.87163800
H	1.26092400	-0.80396600	2.40326000
H	-2.13809800	-0.70426500	3.69687100
H	-0.75805000	0.17476700	3.04021300

H	-2.36814700	0.43456700	2.36753300
H	-4.43951700	-2.28128700	1.83559300
H	-4.09509400	-0.67618700	1.19273300
H	-4.42342900	-2.02278500	0.09191400
H	-0.59761500	4.71419500	1.42239900
H	-2.87845000	5.43234900	0.81543700
H	-4.37493500	3.90068800	-0.40911500
H	-2.58107400	1.47180500	-3.07735600
H	-4.23366000	0.92290000	-3.41750600
H	-3.91286300	2.63346300	-3.08747600
H	-5.94467300	0.74254300	-1.50188800
H	-5.55916500	1.38948100	0.10273700
H	-5.77309300	2.47723600	-1.27532400
H	1.04221100	3.73342500	2.58612900
H	0.33309900	2.19800700	3.08579300
H	2.03688400	2.28168000	2.59595900
H	1.40317100	2.82959900	-1.09163600
H	1.53614300	4.16368800	0.05461900
H	2.65879900	2.80514200	0.16838000
C	1.10442700	-1.23315900	-1.85974600
H	0.61869800	-2.09364500	-2.31865500
H	0.94527100	-0.26361700	-2.32885700
C	2.11323200	-1.42135100	-0.97414700
H	2.30864500	-2.43812300	-0.63518300
C	3.06502200	-0.37803600	-0.49460100
H	3.08429900	-0.37125100	0.60317000
H	2.74711500	0.61319100	-0.82988700
C	4.50050200	-0.67485100	-1.00231500
H	4.49676700	-0.69314400	-2.09904900
H	4.80395700	-1.67742000	-0.67343100
C	5.51579600	0.36131400	-0.50240500
H	5.51388800	0.38114800	0.59509800
H	5.20669300	1.36259200	-0.83165600
C	6.94687900	0.07973900	-0.99920300
H	6.93529200	0.03834800	-2.09833200
H	7.27060000	-0.90885100	-0.65061900
C	7.93111200	1.12470300	-0.54582700
H	7.74305100	2.14003800	-0.89775000
C	8.98200400	0.89350500	0.24064000
H	9.21043000	-0.10341800	0.61095100
H	9.65992900	1.68844000	0.53590800
<b>1TS<sub>21re</sub>, -1342.8623604, i294.65</b>			
Ti	-0.89013000	-1.05767900	-0.30047900
O	-0.65678300	0.71482600	-0.21784400

C	-2.38531400	-1.11898400	1.49628600
C	-3.03882800	-1.72735400	0.38291300
C	-2.35551700	-2.95218600	0.07371400
C	-1.28796700	-3.10076500	1.00288400
C	-1.28196500	-1.95630500	1.86328200
C	-0.83541400	2.06488900	-0.00124700
C	-0.12324400	2.70006200	1.04018200
C	-1.89523500	4.13855600	-0.61030800
C	-1.72798300	2.77095800	-0.84476000
C	-2.84780000	0.11904900	2.20925600
C	-4.30226800	-1.23079400	-0.26540500
C	-2.79476400	-3.97509300	-0.93513200
C	-0.42786700	-4.32216500	1.15909000
C	0.87836300	1.97323900	1.92844100
C	0.59325300	2.17205800	3.43006200
C	2.31962800	2.41336600	1.59641500
C	-2.43387400	2.08782400	-2.00840700
C	-1.54076200	2.11742900	-3.26732500
C	-3.82579600	2.66317800	-2.31946900
C	-0.33130500	4.07325200	1.21938100
C	-1.20710400	4.78948200	0.41130400
C	-0.36732400	-1.74866700	3.03835900
H	0.79770500	0.90188400	1.71700400
H	-2.58426100	1.03813400	-1.73072900
C	-1.08577300	-1.48513000	-2.36774600
H	-1.34454700	-2.36463000	-2.95365500
H	-2.06295600	-1.08242500	-1.97870200
H	-0.64323000	-0.71055400	-2.99431800
H	-3.50680100	-4.67394400	-0.47985000
H	-3.29801700	-3.52207300	-1.79330700
H	-1.95816400	-4.57123200	-1.31022600
H	-0.98042500	-5.09059500	1.71332600
H	-0.14316300	-4.76856000	0.20199800
H	0.48352200	-4.12017500	1.72657400
H	-0.74817400	-2.29152400	3.91213100
H	0.64451400	-2.11740300	2.84766100
H	-0.29282700	-0.69623700	3.31791600
H	-3.62765300	-0.13846300	2.93606000
H	-2.03734100	0.60324200	2.75562900
H	-3.26875900	0.85770700	1.52287800
H	-5.17403900	-1.60670600	0.28402500
H	-4.36645900	-0.13974800	-0.26241800
H	-4.40299500	-1.57450600	-1.29827500
H	0.20722300	4.58942500	2.00789700

H	-1.35198100	5.85299300	0.57285300
H	-2.57265000	4.70643600	-1.23830400
H	-0.55011200	1.69536100	-3.06915200
H	-2.00189500	1.55776100	-4.08873600
H	-1.39333700	3.14814300	-3.60559900
H	-4.32581500	2.04471200	-3.07156900
H	-4.46007600	2.69629200	-1.42809500
H	-3.76879600	3.67638300	-2.72855500
H	0.72971200	3.21486500	3.73187100
H	-0.43028500	1.88882700	3.69573400
H	1.28260900	1.56945100	4.03079300
H	2.55352500	2.26335600	0.53856800
H	2.46305600	3.47569100	1.81811500
H	3.04464100	1.85001400	2.19403500
C	0.73429300	-2.41467300	-1.62276500
H	0.33170900	-3.42116900	-1.62841300
H	1.12587800	-2.07257800	-2.57567300
C	1.23105300	-1.86226000	-0.43361600
H	1.28207000	-2.53446700	0.41901400
C	2.28015800	-0.76243700	-0.47878600
H	2.27663400	-0.19894500	0.45816100
H	2.04179200	-0.04516800	-1.27413400
C	3.69554100	-1.33667900	-0.71002100
H	3.70717900	-1.90206400	-1.65176500
H	3.92568100	-2.05988700	0.08408000
C	4.77827000	-0.25080600	-0.74610100
H	4.76751500	0.31426500	0.19465600
H	4.54447100	0.47094800	-1.54112700
C	6.19221200	-0.81963300	-0.97373100
H	6.19049700	-1.39978700	-1.90857900
H	6.44080000	-1.52273500	-0.16895600
C	7.24433700	0.25388900	-1.05156500
H	7.12983100	0.97421000	-1.86299500
C	8.27129200	0.38063500	-0.21140300
H	8.42723000	-0.31612400	0.60924000
H	9.00032300	1.17830700	-0.31648300
<b>1P<sub>21re</sub>, -1342.8872883</b>			
Ti	-0.76400800	-1.07762600	-0.18327500
O	-0.65851400	0.70253800	-0.13480000
C	-2.42468900	-1.19237900	1.44276300
C	-2.91989200	-1.87639500	0.29568700
C	-2.11660400	-3.04950800	0.09261500
C	-1.13307100	-3.09587100	1.12352500
C	-1.29632200	-1.93138000	1.93749200

C	-0.93798300	2.04517800	-0.02839900
C	-0.29652600	2.79801300	0.97951200
C	-2.09130300	3.99549600	-0.83236700
C	-1.84364200	2.62430600	-0.94825900
C	-3.02961800	0.03217700	2.06746900
C	-4.13442200	-1.49443100	-0.50512600
C	-2.37997400	-4.12729500	-0.92347600
C	-0.19593000	-4.23563100	1.39176200
C	0.70214500	2.18695300	1.95431000
C	0.31331100	2.43992400	3.42406600
C	2.12952200	2.70057300	1.67487300
C	-2.48076300	1.81817900	-2.07323900
C	-1.69415700	2.00643400	-3.38771700
C	-3.97226900	2.13626600	-2.28151800
C	-0.58922300	4.16511500	1.04471100
C	-1.47519400	4.76301000	0.15365200
C	-0.49848200	-1.60554200	3.16833800
H	0.70412800	1.10397400	1.79535300
H	-2.41972300	0.75702000	-1.80012400
C	-0.31343100	-1.56344900	-2.51240400
H	-0.42841100	-2.07918700	-3.46865400
H	-1.37095600	-1.57778800	-2.14451200
H	-0.03046000	-0.52944200	-2.72603200
H	-3.08773800	-4.85945000	-0.51625300
H	-2.82369900	-3.73545000	-1.84286400
H	-1.47359100	-4.67695900	-1.19041900
H	-0.72970600	-5.03911500	1.91367900
H	0.21351700	-4.66926200	0.47452200
H	0.63921600	-3.93819400	2.02930200
H	-0.91927000	-2.12523900	4.03794100
H	0.54459100	-1.91828900	3.07428300
H	-0.51044000	-0.53709700	3.39262800
H	-3.83492800	-0.25736200	2.75314200
H	-2.29769600	0.60104500	2.64347900
H	-3.45767700	0.70728900	1.32275700
H	-5.02253900	-1.99298600	-0.09760000
H	-4.32518100	-0.41957600	-0.47550800
H	-4.05483600	-1.79517800	-1.55385100
H	-0.10984900	4.77195200	1.80655300
H	-1.68410000	5.82579900	0.22425800
H	-2.77485700	4.47294600	-1.52665700
H	-0.63403300	1.76114900	-3.26273400
H	-2.10621200	1.37841300	-4.18540000
H	-1.74703900	3.04756600	-3.72155000

H	-4.40486400	1.45487300	-3.02121800
H	-4.54101300	2.03915300	-1.35128600
H	-4.12319200	3.15280700	-2.65650400
H	0.34911800	3.50478900	3.67378900
H	-0.69996400	2.08796300	3.64486800
H	1.00853700	1.92545800	4.09567600
H	2.43475200	2.49629100	0.64441100
H	2.19618900	3.78184500	1.83255800
H	2.84978800	2.22267700	2.34756200
C	0.76348200	-2.32979100	-1.66588900
H	0.46170500	-3.37605500	-1.58781800
H	1.65882900	-2.29815200	-2.29561600
C	1.17599400	-1.75991500	-0.26789900
H	1.49156600	-2.58314400	0.37186900
C	2.25956500	-0.67439100	-0.32001000
H	2.30185700	-0.17501900	0.65465600
H	1.99443100	0.10711600	-1.04454000
C	3.66656800	-1.21720500	-0.64377700
H	3.66297800	-1.72826300	-1.61685200
H	3.93450500	-1.98027000	0.09980400
C	4.73830500	-0.11912600	-0.66068900
H	4.75237300	0.39713200	0.30781000
H	4.47145600	0.63993500	-1.40934400
C	6.15003900	-0.65773000	-0.96246000
H	6.12456100	-1.18835000	-1.92615800
H	6.43147600	-1.39913800	-0.20419800
C	7.18872900	0.43014600	-1.01682900
H	7.04067300	1.19132800	-1.78441800
C	8.24131500	0.52426500	-0.20453100
H	8.43067200	-0.21303100	0.57250600
H	8.95845400	1.33497600	-0.28995900

**1C<sub>21si</sub>, -1342.8788741**

Ti	0.57754200	1.03511300	-0.34329500
O	1.57831100	-0.43795200	-0.40522500
C	1.22752400	1.53712600	1.85859600
C	1.77354600	2.54626500	1.00562400
C	0.68994600	3.30989000	0.46112500
C	-0.52516900	2.74551000	0.94479800
C	-0.19248700	1.65054500	1.81267900
C	2.45388200	-1.47611200	-0.18960500
C	2.01484700	-2.60064400	0.54490500
C	4.61860400	-2.46259000	-0.51843400
C	3.75401200	-1.38553700	-0.73849600
C	2.02028900	0.59765900	2.72099300

C	3.23465300	2.83934100	0.82492800
C	0.81521300	4.58001500	-0.32560400
C	-1.89433900	3.31605800	0.69849900
C	0.58929600	-2.72088800	1.06786200
C	0.51221900	-3.27287200	2.50297000
C	-0.26379100	-3.57930800	0.10943600
C	4.18220600	-0.19850300	-1.59143800
C	3.93254200	-0.49644400	-3.08552900
C	5.64170600	0.22870900	-1.35780700
C	2.92517300	-3.64739900	0.72431200
C	4.21535400	-3.58249600	0.20487300
C	-1.15070100	0.84699500	2.64828800
H	0.15808700	-1.71262700	1.08602300
H	3.54905300	0.65077300	-1.31800600
C	1.12888800	2.01149900	-2.09796200
H	0.38805200	2.76579600	-2.38607400
H	2.11117600	2.49069000	-2.06942400
H	1.15847200	1.21651100	-2.85394200
H	0.89340400	5.43198600	0.36087600
H	1.70541000	4.59029300	-0.95796000
H	-0.05384100	4.75680100	-0.96406900
H	-2.04143400	4.21270400	1.31276600
H	-2.03661300	3.61806600	-0.34361400
H	-2.68750900	2.61438700	0.95982400
H	-1.16287500	1.23474100	3.67416600
H	-2.17350500	0.90519400	2.27274600
H	-0.86909200	-0.20792400	2.70993200
H	2.34973200	1.11503200	3.63019500
H	1.42908800	-0.26517900	3.03326000
H	2.91321000	0.22354200	2.21449500
H	3.56978300	3.54372000	1.59663700
H	3.84764800	1.94015600	0.91941600
H	3.44677600	3.29632200	-0.14434100
H	2.61912900	-4.52907300	1.27783500
H	4.90507100	-4.40621700	0.35978200
H	5.62372100	-2.42683400	-0.92461500
H	2.88589300	-0.75620800	-3.27353300
H	4.18569400	0.37295300	-3.70145400
H	4.54809000	-1.33789400	-3.42027000
H	5.85195000	1.15355000	-1.90425900
H	5.84924400	0.40476300	-0.29739200
H	6.35267300	-0.52175200	-1.71682700
H	0.82930300	-4.31872300	2.55404300
H	-0.51902200	-3.23414000	2.86971500

H	-0.26402000	-3.17162800	-0.90710900
H	0.13049700	-4.59860600	0.05007600
H	-1.30046800	-3.64827900	0.45987100
C	-1.37916400	0.14559800	-1.62296000
H	-1.65194900	1.03789800	-2.18322800
H	-0.56954200	-0.46631000	-2.01959500
C	-2.22214600	-0.37452700	-0.69800600
H	-1.95412700	-1.32807900	-0.24117700
C	-3.56544400	0.16840600	-0.33834500
H	-3.67849400	0.20837900	0.75220400
H	-3.69142800	1.18227900	-0.73182600
C	-4.68183700	-0.75212500	-0.90108400
H	-4.58680700	-0.80335300	-1.99256300
H	-4.53567300	-1.77302100	-0.52529600
C	-6.08363100	-0.25759800	-0.52043200
H	-6.22334700	0.76598600	-0.89360800
H	-6.17284800	-0.20407100	0.57222000
C	-7.20244200	-1.16101700	-1.07391800
H	-7.09293100	-1.22660700	-2.16646500
H	-7.08111800	-2.17925400	-0.68398700
C	-8.57720500	-0.64905000	-0.73599700
H	-8.83158300	0.33272600	-1.13785300
C	-9.47224400	-1.29897500	0.00754000
H	-9.26320100	-2.28145700	0.42489200
H	-10.45097600	-0.87953900	0.21927600
H	1.14303400	-2.70254500	3.19165400
<b>1TS<sub>21si</sub>, -1342.8566387, i325.66</b>			
Ti	0.32273700	0.95718000	-0.23898200
O	1.45196000	-0.42010000	-0.31820900
C	0.87004000	1.51947400	1.96597500
C	1.39664900	2.52236900	1.10285900
C	0.28955800	3.24184500	0.53170900
C	-0.91215300	2.68543800	1.04688400
C	-0.56049600	1.59686600	1.91209800
C	2.44728800	-1.35755000	-0.17001000
C	2.17235800	-2.52628400	0.57547800
C	4.68420300	-2.10042900	-0.62958300
C	3.69815800	-1.12125000	-0.78544500
C	1.66842700	0.61370400	2.86039000
C	2.85193300	2.86099500	0.93175600
C	0.39110700	4.47494900	-0.32028800
C	-2.27789400	3.27774200	0.83999800
C	0.79936700	-2.79186300	1.17974800
C	0.85942000	-3.43619600	2.57605900



C	-0.05311200	-3.65108500	0.22120300
C	3.94516700	0.11362500	-1.64236700
C	3.58192600	-0.17309400	-3.11539000
C	5.37747500	0.66382800	-1.53453600
C	3.20072200	-3.46713400	0.69413900
C	4.44403900	-3.26120200	0.10209000
C	-1.48230700	0.80749100	2.80213500
H	0.29780600	-1.82376100	1.29594700
H	3.27479500	0.90212200	-1.28234600
C	0.34933200	1.73154900	-2.22807700
H	-0.24255400	2.62783200	-2.41335000
H	1.29515000	2.04170100	-1.70146000
H	0.68387600	1.28947700	-3.16375700
H	0.49032200	5.36355000	0.31472200
H	1.26313500	4.45591300	-0.98034200
H	-0.49758300	4.62128000	-0.93981800
H	-2.35657500	4.21391800	1.40592900
H	-2.47414300	3.52286200	-0.20806700
H	-3.07512700	2.62106300	1.18645900
H	-1.30278400	1.07419500	3.85010000
H	-2.53233700	1.01481400	2.59356300
H	-1.32815100	-0.27278600	2.71634400
H	1.93777400	1.14343100	3.78239000
H	1.10152100	-0.27361100	3.14958800
H	2.59709500	0.27945200	2.39156400
H	3.15287600	3.60024000	1.68440700
H	3.49376600	1.98648200	1.06087500
H	3.06576100	3.29756200	-0.04768100
H	3.02551600	-4.37726800	1.25778100
H	5.22591600	-4.00648800	0.20884500
H	5.65571100	-1.95456600	-1.08908400
H	2.55228000	-0.53280300	-3.21401300
H	3.69545600	0.72794700	-3.72818800
H	4.23832000	-0.94498800	-3.52976300
H	5.45418200	1.61519700	-2.07043700
H	5.66909200	0.83420200	-0.49361300
H	6.11124100	-0.01341500	-1.98192400
H	1.24770600	-4.45839000	2.53832300
H	-0.14537200	-3.49314300	3.00705400
H	-0.13992700	-3.18986500	-0.76833200
H	0.40139500	-4.63715900	0.08161400
H	-1.06127100	-3.80158600	0.62293100
C	-1.07267100	0.10236300	-2.07124700
H	-1.67533900	0.67411800	-2.77133900

H	-0.37457600	-0.59374800	-2.52255800
C	-1.57646200	-0.14736000	-0.78096600
H	-1.22910200	-1.07880600	-0.32632700
C	-3.00047300	0.25075000	-0.43960400
H	-3.12910600	0.32976000	0.64231500
H	-3.22638200	1.23644100	-0.86243600
C	-4.02057000	-0.77555900	-0.97936500
H	-3.91620000	-0.85152100	-2.07020500
H	-3.77894200	-1.76947000	-0.57893600
C	-5.46802000	-0.41590100	-0.62155500
H	-5.70769100	0.57831000	-1.02392300
H	-5.57159800	-0.33939400	0.46885200
C	-6.49124300	-1.43954000	-1.15033500
H	-6.37054900	-1.52450000	-2.24058500
H	-6.27104400	-2.42987400	-0.73254600
C	-7.91209000	-1.05936600	-0.83085000
H	-8.25939500	-0.11644300	-1.25591500
C	-8.74467600	-1.77693700	-0.07689200
H	-8.44316000	-2.72458800	0.36389600
H	-9.76120600	-1.45088800	0.12095700
H	1.49351100	-2.86340600	3.25971100

**1P<sub>21si</sub>, -1342.8830711**

Ti	-0.20729700	-0.85827200	-0.09796800
O	-1.39453600	0.45855000	-0.28100100
C	-0.77505100	-1.42806500	2.07221100
C	-1.45439800	-2.33922500	1.21229600
C	-0.46516200	-3.13494600	0.55317700
C	0.82285300	-2.75397000	1.04981400
C	0.63801800	-1.69235000	1.98162500
C	-2.50033500	1.26906900	-0.21583100
C	-2.42230800	2.45133600	0.55383500
C	-4.76174900	1.75179300	-0.85854600
C	-3.65514400	0.90111000	-0.94380500
C	-1.42810400	-0.47628600	3.03488900
C	-2.94560200	-2.48363000	1.09604000
C	-0.73885400	-4.27690100	-0.38836100
C	2.11052500	-3.45867600	0.72712600
C	-1.12852600	2.86708500	1.24323200
C	-1.34789300	3.56418000	2.59650200
C	-0.28553500	3.75558900	0.30287200
C	-3.66325600	-0.32100300	-1.85454000
C	-3.14551600	0.05510600	-3.26011500
C	-5.03176500	-1.01522200	-1.95072300
C	-3.56473000	3.25730200	0.60207200

C	-4.72395300	2.91316500	-0.08923000
C	1.67000000	-1.08298500	2.88828900
H	-0.55060200	1.95665600	1.43799300
H	-2.96537500	-1.05422300	-1.42959900
C	0.42579400	-1.43288300	-2.39153700
H	1.03927700	-2.29120600	-2.10038200
H	-0.62460900	-1.61214400	-2.05336600
H	0.29799200	-1.47408300	-3.47571100
H	-0.90435300	-5.20007000	0.18007000
H	-1.63362700	-4.11089400	-0.99483300
H	0.09912700	-4.46576300	-1.06441600
H	2.15121300	-4.41724000	1.25867100
H	2.21039100	-3.68697200	-0.33892000
H	2.98407000	-2.87978000	1.02730400
H	1.50318000	-1.42741400	3.91589600
H	2.68384200	-1.37329800	2.61138700
H	1.62235200	0.00975800	2.90349500
H	-1.71037300	-1.00915300	3.95131500
H	-0.75610300	0.33421500	3.32525900
H	-2.33636500	-0.03083800	2.62188600
H	-3.32173400	-3.10758900	1.91617300
H	-3.45828300	-1.52053400	1.15851300
H	-3.24285000	-2.96700400	0.16262700
H	-3.54664400	4.17116000	1.18594800
H	-5.59761900	3.55504700	-0.03525200
H	-5.66691600	1.50598700	-1.40295900
H	-2.14953600	0.50842800	-3.21617100
H	-3.09837300	-0.82721800	-3.90825200
H	-3.81378600	0.78161300	-3.73291800
H	-4.94018600	-1.94835000	-2.51571300
H	-5.43734800	-1.25234000	-0.96262700
H	-5.76595600	-0.39688000	-2.47596900
H	-1.81797100	4.54556600	2.48051700
H	-0.38602200	3.72917100	3.09232500
H	-0.07852700	3.25288700	-0.64765200
H	-0.81375000	4.68692600	0.07409500
H	0.67004700	4.01757500	0.77009600
C	1.08405500	-0.06277100	-2.01498700
H	1.99677200	-0.02699200	-2.61736700
H	0.43377300	0.74369600	-2.36047100
C	1.53710200	0.14552400	-0.52325600
H	1.33473400	1.18469100	-0.23799100
C	3.00124400	-0.20005400	-0.27039400
H	3.17564300	-0.25619900	0.80832900

H	3.23232500	-1.19521800	-0.67278900
C	3.99622300	0.82371000	-0.85514700
H	3.85480400	0.91487100	-1.94123300
H	3.77464600	1.81470700	-0.43591000
C	5.45927000	0.46069600	-0.56931400
H	5.67964700	-0.52903000	-0.99360200
H	5.61235700	0.37085400	0.51417000
C	6.45911400	1.48912300	-1.13191300
H	6.28851800	1.58809800	-2.21447600
H	6.26036300	2.47456600	-0.69236400
C	7.89266200	1.10360600	-0.88366300
H	8.21790500	0.16503400	-1.33515400
C	8.76116100	1.81076600	-0.16101100
H	8.48252100	2.75351400	0.30462500
H	9.78501600	1.48056700	-0.01432200
H	-1.97762500	2.96725500	3.26339100

**Table S3** Optimized Cartesian coordinates (Å) and zero-point energy corrected energy (a.u.) of **2C<sub>12f</sub>**, **2TS<sub>12f</sub>**, **2P<sub>12f</sub>**, **2C<sub>12b</sub>**, **2TS<sub>12b</sub>**, **2P<sub>12b</sub>**, **2C<sub>21f</sub>**, **2TS<sub>21f</sub>**, **2P<sub>21f</sub>**, **2C<sub>21b</sub>**, **2TS<sub>21b</sub>** and **2P<sub>21b</sub>**, as well as the imaginary frequency (cm<sup>-1</sup>) of **2TS<sub>12f</sub>**, **2P<sub>12b</sub>**, **2TS<sub>21f</sub>**, and **2TS<sub>21b</sub>**.

Atom	x	y	z
<b>2C<sub>12f</sub>, -1655.7750764</b>			
Ti	-0.06471800	-1.16723300	-0.08532800
O	1.61958700	-0.58034600	0.05783700
C	-1.49322400	-3.07928400	0.42819400
C	-1.50379600	-2.95036400	-0.98861700
C	-0.16132600	-3.10871000	-1.45365800
C	0.67465800	-3.38191400	-0.31893700
C	-0.14816600	-3.35295200	0.84243000
C	2.98494700	-0.48123700	0.22224600
C	3.52117200	-0.54482200	1.53217100
C	5.18850200	-0.20624900	-0.70485300
C	3.80767800	-0.30255200	-0.91407600
C	-2.71340000	-3.14852600	1.30178500
C	-2.73349500	-2.83498900	-1.84104800
C	0.26972400	-3.15059100	-2.89163400
C	2.12416900	-3.77021500	-0.35933700
C	2.63618000	-0.64935800	2.76743800
C	2.35791000	0.75449600	3.34684200
C	3.20427700	-1.57782500	3.85590300
C	3.26222200	-0.18354700	-2.33169400
C	3.84586400	-1.25468000	-3.27475700
C	3.51890300	1.22454200	-2.90764900

C	4.90794100	-0.43637400	1.67320600
C	5.74090900	-0.27399200	0.56931700
C	0.28602900	-3.69685400	2.23971300
H	1.67956500	-1.08095800	2.45432400
H	2.18028300	-0.33053300	-2.28696800
H	0.17883600	-4.17354400	-3.27729500
H	-0.34572000	-2.50704400	-3.52383000
H	1.31158000	-2.84894100	-3.01715900
H	2.21360500	-4.86208700	-0.41396900
H	2.63472600	-3.35673800	-1.23020000
H	2.66818800	-3.43814000	0.52745400
H	1.35056900	-3.51412400	2.39620500
H	-0.26754500	-3.14223900	3.00305900
H	0.10796100	-4.76235100	2.43219200
H	-3.09411600	-4.17758400	1.32087400
H	-2.50498500	-2.87260600	2.33864200
H	-3.52292000	-2.51516900	0.93154000
H	-3.21263200	-3.81749200	-1.93406000
H	-3.47509700	-2.15371400	-1.41379900
H	-2.50410000	-2.49375700	-2.85217100
H	5.34465400	-0.47595400	2.66536900
H	6.81497700	-0.19424300	0.70413200
H	5.84161700	-0.06946800	-1.56113000
H	3.68847000	-2.26888100	-2.89388600
H	3.38160500	-1.18533600	-4.26412800
H	4.92384600	-1.12424700	-3.41125200
H	3.05056500	1.32814600	-3.89220700
H	3.12260500	2.00659500	-2.25393400
H	4.59071000	1.41075200	-3.03015700
H	3.28673200	1.21262200	3.70135600
H	1.93533700	1.42867500	2.59372300
H	1.66597300	0.70071200	4.19478800
H	3.45719100	-2.56524300	3.45675100
H	4.10741800	-1.16541200	4.31523000
H	2.47092300	-1.71035500	4.65790900
C	-1.04694500	1.41935700	-1.66591900
C	-0.76263800	-0.10176100	-1.77016800
H	0.07732300	-0.26765600	-2.46460400
H	-1.63133300	-0.58021500	-2.22757500
C	0.08862800	2.23288400	-1.01216500
H	0.34589800	1.79670500	-0.03649800
H	0.99499900	2.12489000	-1.62085600
C	-0.20928800	3.72569300	-0.80491500
H	-0.34341800	4.21956600	-1.77448600

H	-1.16667700	3.84236500	-0.27356800
C	0.89378900	4.45324900	-0.02468000
H	1.01857100	3.98150300	0.96124200
H	1.85380900	4.33071100	-0.54294500
C	0.61616800	5.95662100	0.16405300
H	0.52616400	6.43976300	-0.81677300
H	-0.35903500	6.07363500	0.66078200
C	1.67707800	6.65081200	0.97485000
H	1.80767400	6.28943500	1.99638400
C	2.45169400	7.64265400	0.53556100
H	2.35597800	8.03738900	-0.47346300
H	3.20438100	8.10357300	1.16803200
C	-1.38792600	1.95050400	-3.07445400
H	-0.51251900	1.89587300	-3.73201600
H	-2.18817400	1.36165900	-3.53381900
H	-1.72195100	2.99174900	-3.04353200
H	-1.95263300	1.54905100	-1.05641400
C	-2.04532000	0.71109600	1.62251300
H	-1.81491500	1.66374300	1.14607300
C	-1.00571400	-0.07478400	1.99426500
H	0.00002200	0.34149700	1.99307600
H	-1.17554700	-0.97518600	2.57923400
C	-3.49377000	0.44708700	1.86497800
H	-3.63927200	-0.54964500	2.29304100
H	-3.80275700	1.16548200	2.64158300
C	-4.39654700	0.66112000	0.63266000
H	-4.10532900	-0.04146300	-0.16000500
H	-4.22557600	1.66738800	0.22830700
C	-5.88538900	0.48555200	0.95801000
H	-6.05515500	-0.51889200	1.37008400
H	-6.17416200	1.19237300	1.74621100
C	-6.79576700	0.69651000	-0.26643600
H	-6.48630800	-0.00144000	-1.05945800
H	-6.64881400	1.70814500	-0.66475600
C	-8.25219900	0.48324400	0.04926300
H	-8.52328500	-0.51520200	0.39549600
C	-9.20006100	1.41417200	-0.05583700
H	-8.97596400	2.42194200	-0.39827200
H	-10.23652600	1.20372900	0.18921600
<b>2TS<sub>12f</sub>, -1655.7715552, i213.39</b>			
Ti	-0.25605900	-1.34938700	-0.04146000
O	1.41233700	-0.72811100	0.13870200
C	-1.70088400	-3.37595600	0.17957500
C	-1.64542200	-2.99077200	-1.18400700

C	-0.27304200	-3.07573400	-1.61124700
C	0.50985600	-3.51912700	-0.50158100
C	-0.36497400	-3.65615800	0.61905000
C	2.77281800	-0.54392900	0.25697600
C	3.35340400	-0.66506800	1.54402600
C	4.91852100	-0.02521500	-0.69947100
C	3.54563500	-0.23095700	-0.88575300
C	-2.93962900	-3.64894700	0.98197800
C	-2.81546600	-2.71695700	-2.08647300
C	0.19970700	-2.91596700	-3.03060800
C	1.96873800	-3.87370200	-0.51699800
C	2.51577300	-0.97064100	2.77913000
C	2.07248000	0.33911500	3.46546800
C	3.21858200	-1.89762300	3.78673500
C	2.97072900	-0.10969200	-2.29299100
C	3.59574900	-1.14375300	-3.25294200
C	3.16121700	1.30806900	-2.87151400
C	4.72919600	-0.44886000	1.66073700
C	5.51083300	-0.12832300	0.55379900
C	0.01260900	-4.18829900	1.97251700
H	1.61596800	-1.49692300	2.44372800
H	1.89480700	-0.30836100	-2.23805500
H	0.05404100	-3.85515500	-3.57862200
H	-0.35569800	-2.14277200	-3.56889100
H	1.26035200	-2.66913500	-3.08694400
H	2.08779400	-4.95284300	-0.67248900
H	2.50531400	-3.36532500	-1.31890900
H	2.46608900	-3.62046800	0.42219800
H	1.06014300	-3.99184700	2.21188400
H	-0.60164500	-3.76303900	2.77110500
H	-0.12864400	-5.27602500	2.00380500
H	-3.11894100	-4.73103900	1.00861500
H	-2.85923500	-3.32266700	2.02295000
H	-3.82937000	-3.18922300	0.54792200
H	-3.13679900	-3.64013200	-2.58372800
H	-3.67899600	-2.32800200	-1.54044400
H	-2.56844100	-2.00102100	-2.87553700
H	5.19825000	-0.53126200	2.63519900
H	6.57725100	0.03785100	0.66897500
H	5.53466700	0.22066300	-1.55873900
H	3.50759200	-2.16650800	-2.87428800
H	3.11406300	-1.09736100	-4.23538300
H	4.66190600	-0.94785200	-3.40257000
H	2.67274200	1.39175700	-3.84830600

H	2.75002700	2.07926100	-2.21517000
H	4.22236700	1.53377600	-3.01570800
H	2.94267700	0.89050700	3.83606700
H	1.54200500	1.00016100	2.77164400
H	1.41865500	0.13349400	4.32063100
H	3.58273700	-2.81279000	3.30917100
H	4.07140800	-1.41100400	4.26947900
H	2.52196700	-2.18148900	4.58213800
C	-1.15302100	1.72478300	-1.22918500
C	-1.36724200	0.21813800	-1.01368200
H	-0.60629000	-0.32225300	-1.67002300
H	-2.33813500	-0.08984900	-1.40603000
C	0.12570900	2.27780200	-0.57043800
H	0.15637800	1.97215200	0.48416100
H	1.00146100	1.80997300	-1.03234100
C	0.26576700	3.80646200	-0.63024500
H	0.37736300	4.13438900	-1.67106600
H	-0.65824500	4.27378200	-0.26008900
C	1.45719200	4.32548300	0.18631500
H	1.33797800	4.02423200	1.23688800
H	2.38272000	3.84907600	-0.16316500
C	1.62240400	5.85515100	0.11217100
H	1.77508000	6.15960400	-0.93082100
H	0.68337200	6.32499000	0.44124200
C	2.75865700	6.36178100	0.95894100
H	2.67704500	6.16714700	2.02961300
C	3.83039600	7.00650200	0.49795100
H	3.95279900	7.22642600	-0.56029300
H	4.62077800	7.34792200	1.15956500
C	-1.21405600	2.02913500	-2.74132300
H	-0.35681400	1.59205600	-3.26683500
H	-2.12818400	1.62921700	-3.19205800
H	-1.20178500	3.10633500	-2.92490800
H	-2.01245700	2.22859300	-0.76869300
C	-1.95916600	0.13637000	1.18498100
H	-1.59920200	1.15928400	1.18534000
C	-1.17186600	-0.80922100	1.87808400
H	-0.29758100	-0.43214900	2.40357100
H	-1.67328600	-1.64430900	2.35402200
C	-3.46409800	-0.03297900	1.07856800
H	-3.70525300	-0.98498200	0.59671600
H	-3.80452200	-0.14283900	2.11909100
C	-4.26193300	1.11028400	0.43739700
H	-4.03794500	1.18656100	-0.63337700



H	-3.95614900	2.06447100	0.88785200
C	-5.77586300	0.92912100	0.61648600
H	-6.08400100	-0.02902200	0.17444000
H	-6.01610000	0.86417800	1.68546700
C	-6.59819200	2.06826500	-0.01476200
H	-6.33739500	2.14063400	-1.08154800
H	-6.31427400	3.02419100	0.44280700
C	-8.08253900	1.86109700	0.12542600
H	-8.48577000	0.96747200	-0.35337500
C	-8.90826700	2.67248000	0.78577200
H	-8.55126400	3.57558300	1.27573400
H	-9.97265900	2.47037000	0.85572400
<b>2P<sub>12f</sub>, -1655.7926734</b>			
Ti	1.66743700	-0.72827100	-0.70164100
O	1.65200800	0.42191000	0.65887000
C	2.64799200	-2.04389600	-2.48772700
C	2.84212900	-0.65238300	-2.76175500
C	3.66277800	-0.10440900	-1.72710100
C	3.93406900	-1.14547900	-0.78766800
C	3.31475400	-2.35298800	-1.26691900
C	2.00181100	1.33026500	1.62958400
C	2.36486100	0.83773400	2.90538700
C	2.32632200	3.59889000	2.34342000
C	1.96604300	2.70925600	1.32483400
C	1.93537600	-3.03028700	-3.36807600
C	2.35707400	0.08917000	-3.97848500
C	4.22099500	1.28855700	-1.66910400
C	4.84187300	-1.03014700	0.40478200
C	2.30631200	-0.65022400	3.22827300
C	0.89506300	-1.03329500	3.72387000
C	3.37601400	-1.10838800	4.23345900
C	1.47493800	3.23424600	-0.01854500
C	2.34020500	4.37746500	-0.57921200
C	0.00047200	3.67685000	0.09031000
C	2.72114000	1.77799900	3.87674100
C	2.70723800	3.14425000	3.60275200
C	3.49314500	-3.72094400	-0.67669900
H	2.48587900	-1.19729500	2.29602800
H	1.52087700	2.40760800	-0.73871200
H	5.23233400	1.30127300	-2.09389500
H	3.62114500	1.99831400	-2.24273300
H	4.29293700	1.65749500	-0.64334800
H	5.88643800	-1.13940800	0.08811600
H	4.74934900	-0.06071700	0.90064500

H	4.64440300	-1.80829700	1.14504900
H	3.55721400	-3.69497200	0.41372600
H	2.67962100	-4.39627600	-0.95017800
H	4.42398000	-4.16674300	-1.04816100
H	2.65912100	-3.56141200	-3.99830700
H	1.39797500	-3.78804300	-2.79105600
H	1.22314700	-2.54501100	-4.03964200
H	3.11547800	0.04936300	-4.76980200
H	1.44032100	-0.34135100	-4.38839400
H	2.16939200	1.14608100	-3.76956500
H	3.01035400	1.43840200	4.86518600
H	2.98686000	3.85470900	4.37434500
H	2.30441100	4.66594500	2.14810000
H	3.39867100	4.10536300	-0.62439400
H	2.00968800	4.63877500	-1.58985100
H	2.25570900	5.28394400	0.02765100
H	-0.37751200	4.01131700	-0.88203400
H	-0.63843200	2.86430600	0.44812000
H	-0.10012800	4.51084200	0.79235600
H	0.66258600	-0.51658900	4.66076300
H	0.12514500	-0.75972100	2.99544700
H	0.82798600	-2.11103000	3.90963200
H	4.38116200	-0.80651400	3.92315400
H	3.19804300	-0.70455800	5.23490000
H	3.36000900	-2.19919400	4.32375200
C	-2.11794000	-0.39045700	-2.16000100
C	-0.82366300	-1.08112300	-1.66559900
H	-0.04803500	-0.27252900	-1.82798100
H	-0.55648100	-1.87575100	-2.37283500
C	-2.45463400	0.87363500	-1.34637700
H	-2.39398900	0.64684800	-0.27463200
H	-1.68345300	1.63360300	-1.54168800
C	-3.84084400	1.47196400	-1.63058600
H	-3.91147300	1.77959800	-2.68107600
H	-4.60645400	0.69615800	-1.48718500
C	-4.16582600	2.67542000	-0.73576100
H	-4.11571600	2.37049100	0.31903500
H	-3.39989900	3.45123800	-0.86646400
C	-5.55029500	3.28667500	-1.02306600
H	-5.59744600	3.61918300	-2.06765400
H	-6.31077400	2.49953000	-0.91030300
C	-5.88154600	4.43655600	-0.11044100
H	-5.92446900	4.20122900	0.95424900
C	-6.11045100	5.68853800	-0.50667200

H	-6.08250100	5.96882800	-1.55736000
H	-6.34426800	6.47847700	0.20068600
C	-2.00111800	-0.10121000	-3.66482400
H	-1.20741800	0.62993100	-3.86592200
H	-1.77609700	-1.01169000	-4.23069400
H	-2.93097400	0.30823700	-4.06553600
H	-2.92587700	-1.12064200	-2.02249800
C	-0.77501700	-1.68352200	-0.23026400
H	-0.92433800	-0.88145100	0.50261800
C	0.61592100	-2.33979500	0.01771600
H	0.78493100	-2.52321500	1.08288000
H	0.70314000	-3.28218000	-0.52800200
C	-1.89219700	-2.75260600	-0.00740200
H	-2.10414800	-3.25351800	-0.96209300
H	-1.48723000	-3.52842600	0.65186600
C	-3.19337500	-2.23290500	0.62436000
H	-3.65280600	-1.46050300	-0.00353600
H	-2.95429100	-1.74678400	1.58047600
C	-4.21220900	-3.35521700	0.86670200
H	-4.45378100	-3.84154500	-0.08861700
H	-3.76333700	-4.13127400	1.49997900
C	-5.51185900	-2.85721400	1.52759200
H	-5.94599900	-2.06725700	0.89617100
H	-5.27973800	-2.39296000	2.49435600
C	-6.52350300	-3.95427800	1.72286000
H	-6.87283300	-4.44637500	0.81388100
C	-6.99749000	-4.35734800	2.90161400
H	-6.67936500	-3.89489500	3.83339000
H	-7.72608900	-5.15840100	2.98091400

**2C<sub>12b</sub>, -1655.777264**

Ti	-0.75542800	-1.33793900	-0.28589600
O	-1.66100500	0.06203800	0.36125800
C	-2.26069000	-2.74149900	-1.46229600
C	-1.00624400	-3.41642200	-1.57879700
C	-0.58528000	-3.78890900	-0.27279500
C	-1.58903900	-3.36310000	0.65857400
C	-2.63136200	-2.72682200	-0.07609000
C	-2.61018100	0.88592500	0.93090200
C	-3.51239000	1.58757200	0.09966300
C	-3.59813700	1.86103200	2.90119700
C	-2.64172400	1.00925400	2.34237100
C	-3.11303000	-2.28400600	-2.61026300
C	-0.32258700	-3.82113000	-2.85129300
C	0.59982500	-4.66710000	0.01962100

C	-1.61270900	-3.66355500	2.13174700
C	-3.49916700	1.49559800	-1.42069200
C	-3.03717500	2.82856800	-2.04443700
C	-4.87267800	1.09267200	-1.99415700
C	-1.63391800	0.28973500	3.22805000
C	-2.17736000	-0.09122500	4.61543100
C	-0.34516000	1.12891600	3.36438100
C	-4.44634900	2.42581500	0.72210100
C	-4.49592800	2.56683100	2.10370900
C	-3.94003400	-2.25406600	0.48831300
H	-2.77743000	0.72454300	-1.70673100
H	-1.38026100	-0.65085300	2.72473200
H	0.38926800	-5.69023300	-0.31504000
H	1.50368400	-4.34254100	-0.50548600
H	0.82231700	-4.72624100	1.08739800
H	-2.07094000	-4.64513700	2.30495500
H	-0.61210600	-3.69741200	2.57077400
H	-2.20186400	-2.93264500	2.69024300
H	-3.83830900	-1.87633600	1.50808600
H	-4.38293800	-1.45734200	-0.11113200
H	-4.65572400	-3.08485100	0.51364000
H	-3.67920900	-3.13298000	-3.01332200
H	-3.83662300	-1.52668800	-2.30706800
H	-2.51753900	-1.87229300	-3.42894500
H	-0.50781400	-4.88467500	-3.04642000
H	-0.69650500	-3.26850100	-3.71507200
H	0.76182800	-3.68416700	-2.80542000
H	-5.14800400	2.97935600	0.10610100
H	-5.23032700	3.22310500	2.55990300
H	-3.64315700	1.97565600	3.97841300
H	-3.12105700	-0.64095800	4.54510400
H	-1.45289800	-0.72247500	5.13982700
H	-2.34674700	0.78763300	5.24477700
H	0.41535100	0.59585000	3.94616000
H	0.07632600	1.38327000	2.38627500
H	-0.55998300	2.07006500	3.88032400
H	-3.74841800	3.63105900	-1.82388300
H	-2.06245200	3.13522100	-1.65582000
H	-2.96274000	2.74165500	-3.13368900
H	-5.25240900	0.16839700	-1.54679700
H	-5.62439300	1.86835100	-1.81911500
H	-4.80449500	0.94602500	-3.07712900
C	0.22417000	0.79083500	-2.51421900
C	0.06503700	-0.69112100	-2.10415800

H	1.05885200	-1.13624600	-1.86667300
H	-0.29292000	-1.24697500	-2.97152800
C	0.93143800	1.65677300	-1.45321700
H	0.37288700	1.58476000	-0.50975200
H	1.93120600	1.23735900	-1.26626200
C	1.09465900	3.14443500	-1.80169400
H	1.75971100	3.25466600	-2.66650200
H	0.12540200	3.56097900	-2.10749000
C	1.65529800	3.96806800	-0.63463400
H	0.97566500	3.89183500	0.22645500
H	2.61379500	3.54161200	-0.30765400
C	1.86735100	5.45351600	-0.98326100
H	2.56965000	5.53805700	-1.82188100
H	0.91096600	5.87057200	-1.33236700
C	2.37027000	6.26179800	0.18221800
H	1.71191600	6.30281800	1.05169100
C	3.53752400	6.90435100	0.22350500
H	4.22367300	6.89578100	-0.62051800
H	3.84777300	7.47169900	1.09583100
C	0.94487400	0.85785600	-3.87724800
H	1.97694200	0.49527600	-3.79499600
H	0.43433300	0.24078100	-4.62354500
H	0.97913000	1.87971600	-4.26529500
H	-0.78363800	1.20052200	-2.65945700
C	2.06563200	-0.74352700	0.81405100
H	1.91145700	0.32970000	0.91989400
C	1.16688600	-1.58174000	1.38215900
H	0.41221200	-1.19127600	2.06227000
H	1.35184300	-2.64929500	1.39784100
C	3.31335300	-1.16305400	0.10829900
H	3.31681400	-2.24688500	-0.05363000
H	3.36198600	-0.67785200	-0.87501700
C	4.56933600	-0.74785100	0.91699400
H	4.53097000	-1.21910500	1.90688400
H	4.55089500	0.33673800	1.08534600
C	5.87081000	-1.13842300	0.20443300
H	5.88448400	-2.22124400	0.02598300
H	5.90161200	-0.66110900	-0.78451500
C	7.12798500	-0.74458300	1.00333200
H	7.11191200	-1.23771700	1.98320300
H	7.09756400	0.33823200	1.19491100
C	8.40278400	-1.09188100	0.28197800
H	8.55488400	-0.59936400	-0.67950200
C	9.32506100	-1.94417300	0.72855800

H	9.21692200	-2.45466200	1.68296600
H	10.22722500	-2.15705000	0.16330600
<b>2TS<sub>12b</sub>, -1655.7621438, i247.25</b>			
Ti	0.26834500	-1.55144700	-0.02095300
O	-1.16488400	-0.74700800	0.71920900
C	-0.36260500	-3.39813000	-1.35112600
C	1.06500400	-3.33663600	-1.52860800
C	1.67981000	-3.60823800	-0.28582500
C	0.64209800	-3.82116700	0.68430400
C	-0.61507700	-3.73997800	0.01318000
C	-2.28542100	-0.02805400	1.08613100
C	-3.49779000	-0.17790700	0.37188300
C	-3.28937000	1.65682900	2.49411400
C	-2.17442400	0.87833100	2.17259400
C	-1.34827800	-3.37609700	-2.48998800
C	1.76593700	-3.20966200	-2.85170900
C	3.15440600	-3.77688400	-0.06220600
C	0.81639000	-4.28876100	2.10170200
C	-3.70390700	-1.20414400	-0.73369200
C	-4.00242200	-0.56330700	-2.10341800
C	-4.82777300	-2.19490900	-0.36210500
C	-0.90586700	0.96635100	3.00962300
C	-0.91590200	-0.12075800	4.10677200
C	-0.65211800	2.35056100	3.62925700
C	-4.57657400	0.63729200	0.74019200
C	-4.48139200	1.55197200	1.78117600
C	-1.93087800	-4.08579100	0.65212900
H	-2.77631400	-1.77124700	-0.82814000
H	-0.06522500	0.76331900	2.33997400
H	3.45500300	-4.79702300	-0.33186500
H	3.74946700	-3.09560900	-0.67645000
H	3.44102100	-3.63119700	0.98174100
H	0.73154300	-5.38170000	2.14673200
H	1.79405900	-4.02841200	2.51261000
H	0.05023500	-3.87809200	2.76511200
H	-2.16922300	-3.43797500	1.50123300
H	-2.75569100	-4.02226400	-0.05647000
H	-1.89860000	-5.11558800	1.02574700
H	-1.16219900	-4.22911100	-3.15335000
H	-2.37823500	-3.45537200	-2.14210200
H	-1.27169600	-2.47216500	-3.10231100
H	1.91009700	-4.20422500	-3.29217400
H	1.18979500	-2.62424700	-3.57214800
H	2.75794100	-2.75790600	-2.76080900

H	-5.51319100	0.54247000	0.19945500
H	-5.33277300	2.17091300	2.04612400
H	-3.22517900	2.35898900	3.31763500
H	-1.05354500	-1.12200000	3.68472700
H	0.01862600	-0.11043800	4.67888700
H	-1.73870600	0.05355300	4.80751400
H	0.33754200	2.37195800	4.09661400
H	-0.69037500	3.14525700	2.87782700
H	-1.37745000	2.59057600	4.41268500
H	-4.91342600	0.04245700	-2.06995100
H	-3.18859900	0.08511100	-2.43938800
H	-4.15279600	-1.33838000	-2.86258900
H	-4.66311700	-2.64671800	0.61991000
H	-5.80164000	-1.69663800	-0.33602600
H	-4.89691600	-2.99728100	-1.10544100
C	0.11223400	0.45409400	-1.84746000
C	1.41996300	-0.08481100	-1.23093200
H	2.13859800	0.72701200	-1.21284600
H	1.88337400	-0.89134400	-1.80958300
C	-0.20455900	1.83862600	-1.23671000
H	-0.26981200	1.73642900	-0.14703700
H	0.66171900	2.48673500	-1.43394500
C	-1.47363100	2.54227800	-1.73351500
H	-1.42014500	2.70137100	-2.81773000
H	-2.34532400	1.90343400	-1.54976500
C	-1.69547500	3.89489000	-1.04165500
H	-1.76286100	3.73846400	0.04384300
H	-0.82646200	4.54486700	-1.20847600
C	-2.96509400	4.61885200	-1.52774800
H	-2.89943200	4.79588700	-2.60862700
H	-3.82680200	3.95322600	-1.36909500
C	-3.20231500	5.92293000	-0.81511000
H	-3.34192700	5.85524000	0.26510300
C	-3.24135500	7.12040200	-1.39928600
H	-3.10922700	7.23639300	-2.47271300
H	-3.41369000	8.02900100	-0.83032700
C	0.25852900	0.49680500	-3.38529100
H	1.05456300	1.19190000	-3.67178600
H	0.50835700	-0.48520800	-3.79579200
H	-0.66922600	0.83082200	-3.85734700
H	-0.75633800	-0.21291400	-1.65368500
C	2.19219800	-0.09278400	0.89170100
H	1.70566400	0.86943100	1.02921300
C	1.67251600	-1.18320500	1.62303400

H	0.93242900	-0.98416100	2.39301200
H	2.35493400	-1.99208300	1.84964000
C	3.66862100	-0.03032100	0.51820700
H	4.22375000	-0.56061400	1.30152800
H	3.86733800	-0.58298800	-0.40771000
C	4.21429800	1.40142300	0.40039200
H	4.03046800	1.93198200	1.34416500
H	3.66295500	1.95623000	-0.37206200
C	5.71305600	1.43851800	0.07612200
H	6.26987900	0.88442800	0.84265400
H	5.89375900	0.91524700	-0.87337800
C	6.27442500	2.87011400	-0.01488500
H	6.12100300	3.38707600	0.94055500
H	5.69769300	3.42628300	-0.76928900
C	7.73493200	2.89988200	-0.37783500
H	7.99391600	2.46752000	-1.34551300
C	8.70316600	3.39875200	0.39026000
H	8.49130800	3.84211000	1.36066500
H	9.74244100	3.39097800	0.07630400

**2P<sub>12b</sub>, -1655.7963315**

Ti	-0.58462500	-0.93724800	-1.04354200
O	-0.33579000	-1.15217900	0.71404400
C	-2.60789400	-2.04299500	-1.32226500
C	-2.48731200	-1.17856600	-2.45629800
C	-1.38280900	-1.62860700	-3.24534400
C	-0.79384300	-2.74523200	-2.58410300
C	-1.55549900	-3.00499000	-1.39055100
C	-0.43933800	-1.63883600	1.99799700
C	-1.42123000	-1.09798600	2.85841600
C	0.31339600	-3.14532300	3.71308600
C	0.45599400	-2.65393200	2.41146800
C	-3.70712200	-2.01886200	-0.29860800
C	-3.44044600	-0.06633000	-2.80012800
C	-0.96320400	-1.09907600	-4.58573000
C	0.30539400	-3.60805400	-3.12980300
C	-2.28719500	0.08842800	2.45640200
C	-1.64584700	1.39593500	2.96722000
C	-3.74520600	-0.02071200	2.93660700
C	1.57935800	-3.14784200	1.50899200
C	1.90843400	-4.63990200	1.68649300
C	2.84281500	-2.28627100	1.71923800
C	-1.50779800	-1.62800800	4.15073800
C	-0.66023800	-2.64700300	4.57535700
C	-1.39084900	-4.18428800	-0.47512300



H	-2.30862100	0.13512300	1.36016800
H	1.25503900	-3.00950800	0.47194000
H	-1.29848200	-1.78225400	-5.37553800
H	-1.40127800	-0.12250700	-4.79769500
H	0.12321700	-1.01298000	-4.67878800
H	-0.12437100	-4.41595200	-3.73483500
H	0.98643300	-3.04742900	-3.77353300
H	0.89633200	-4.07485800	-2.33827000
H	-0.38586900	-4.60652600	-0.53061700
H	-1.59307200	-3.93150300	0.56823100
H	-2.09338200	-4.97507300	-0.76565800
H	-4.53139700	-2.66605900	-0.62332300
H	-3.36732500	-2.38488700	0.67258500
H	-4.12130200	-1.01753700	-0.15800400
H	-4.33353400	-0.47725400	-3.28649300
H	-3.78216700	0.47556600	-1.91336400
H	-2.99949700	0.65767700	-3.48768100
H	-2.24758200	-1.23175000	4.83815500
H	-0.75037400	-3.04523900	5.58110300
H	0.97869400	-3.92799200	4.06063100
H	1.01667400	-5.26825500	1.59857300
H	2.62661700	-4.95668300	0.92343200
H	2.36789000	-4.84545600	2.65813800
H	3.64374500	-2.59913700	1.04030800
H	2.63803300	-1.22532300	1.54728600
H	3.21268200	-2.39112100	2.74444700
H	-1.57742800	1.38759600	4.05978200
H	-0.63285600	1.52700600	2.57335900
H	-2.24640200	2.26295100	2.67562000
H	-4.20541400	-0.96688400	2.63717600
H	-3.82117100	0.05675300	4.02532500
H	-4.34092400	0.79679000	2.51755200
C	-0.09476000	1.99469200	-2.07509900
C	1.40294300	1.63711500	-2.18443600
H	1.96664200	2.55566600	-1.98954200
H	1.63416000	1.35290100	-3.21892900
C	-0.38178200	2.92421200	-0.87817100
H	0.13555600	2.55102000	0.01511900
H	0.09012800	3.88767300	-1.11481900
C	-1.86118500	3.16042200	-0.54147000
H	-2.42770800	3.38953600	-1.45202200
H	-2.29854200	2.23499600	-0.13347000
C	-2.06782500	4.30614200	0.45929000
H	-1.48347400	4.11349300	1.36863000

H	-1.66728300	5.23357000	0.03099900
C	-3.54553800	4.52674600	0.83287200
H	-4.12803400	4.73472100	-0.07367100
H	-3.94671600	3.59086000	1.25311500
C	-3.73824300	5.64291500	1.82427600
H	-3.24221800	5.51522400	2.78764500
C	-4.44613300	6.74982200	1.60087800
H	-4.95756800	6.92009600	0.65609500
H	-4.54637600	7.52539800	2.35393200
C	-0.60810300	2.58367400	-3.39678900
H	-0.07203100	3.51677000	-3.60400600
H	-0.42107300	1.90704800	-4.23458200
H	-1.67509800	2.81611700	-3.37179300
H	-0.68733800	1.03886400	-1.91872500
C	1.89662600	0.50568100	-1.26262100
H	1.54022100	0.70315400	-0.23689000
C	1.36070100	-0.86381700	-1.75527900
H	1.88606400	-1.69187300	-1.26202000
H	1.50086300	-0.97314600	-2.83414500
C	3.44733200	0.46472700	-1.18138300
H	3.73911300	-0.45499600	-0.66123300
H	3.84708100	0.37907500	-2.20135900
C	4.09653800	1.65697600	-0.46277000
H	3.66071100	1.75548100	0.54193000
H	3.87098300	2.59386600	-0.98845500
C	5.62009400	1.51304500	-0.34144300
H	5.86206300	0.58619700	0.19459500
H	6.05709300	1.40990800	-1.34419300
C	6.28301100	2.69985600	0.38343600
H	5.86483500	2.79604600	1.39350000
H	6.02519600	3.62585800	-0.15233100
C	7.78007500	2.57046600	0.46624500
H	8.30681500	2.52601700	-0.48825100
C	8.48147600	2.49850400	1.59744500
H	7.99935300	2.54093500	2.57168900
H	9.56302800	2.40276800	1.59449000
<b>2C<sub>21f</sub>, -1655.775165</b>			
Ti	0.87312400	-1.24680500	-0.73638200
O	1.12332600	-0.20617500	0.70127800
C	0.27740000	-3.53514100	-1.38338400
C	1.57060600	-3.30097100	-1.92674200
C	2.45941200	-3.02296100	-0.84220400
C	1.71417800	-3.12106000	0.38104300
C	0.36418500	-3.42262900	0.04255200

C	1.40957200	0.28287600	1.95911300
C	0.38312200	0.30574100	2.93487300
C	2.96141500	1.24055100	3.53359200
C	2.71148000	0.76349800	2.24172000
C	-0.90887900	-4.04161600	-2.15401400
C	1.94771000	-3.47214600	-3.36963700
C	3.94505200	-2.83546000	-0.95376100
C	2.27834900	-3.06499000	1.77125900
C	-1.04892500	-0.11296700	2.63327600
C	-1.93880500	1.13539000	2.45229200
C	-1.64291500	-1.04774000	3.70398100
C	3.83315400	0.81546800	1.21213200
C	5.08084000	0.02869100	1.66157400
C	4.22005200	2.27413800	0.88975700
C	0.69611200	0.80323500	4.20387900
C	1.97348600	1.26065100	4.51171400
C	-0.74613100	-3.71560900	1.01154300
H	-1.04220400	-0.66474200	1.68758100
H	3.46364400	0.35978900	0.29120700
H	4.44388100	-3.81241100	-0.93916200
H	4.22830600	-2.33822400	-1.88390300
H	4.34939100	-2.25324800	-0.12345000
H	2.54557400	-4.07536500	2.10403800
H	3.18088600	-2.45460600	1.82276200
H	1.56602200	-2.65747100	2.49188600
H	-0.58723900	-3.22941800	1.97548700
H	-1.72290500	-3.40459100	0.63182900
H	-0.80424400	-4.79531800	1.19854400
H	-0.85986900	-5.13542900	-2.22519100
H	-1.85750300	-3.79847300	-1.66926500
H	-0.93494900	-3.66021900	-3.17862900
H	2.03094500	-4.53991500	-3.60690700
H	1.20245200	-3.04787800	-4.04909700
H	2.91266200	-3.01718700	-3.60024400
H	-0.07756800	0.83717400	4.96409300
H	2.19433000	1.63830600	5.50502700
H	3.95325600	1.61094900	3.77297900
H	4.84604700	-1.01051600	1.91231500
H	5.83552900	0.02663000	0.86808700
H	5.54131900	0.47842600	2.54662200
H	4.96140500	2.30570500	0.08425700
H	3.35259600	2.86470700	0.58246000
H	4.65974500	2.76665800	1.76297600
H	-1.98556600	1.71298800	3.38079200

H	-1.54607600	1.80256100	1.67769100
H	-2.96505000	0.85590900	2.18784300
H	-1.00271900	-1.91630500	3.88681500
H	-1.77917300	-0.53437900	4.66032400
H	-2.62866100	-1.40956700	3.39230100
C	1.67407200	1.06444200	-2.80984400
C	2.09352800	-0.29736800	-2.19256600
H	3.02491800	-0.16278600	-1.62092500
H	2.33887200	-0.97801900	-3.01098900
C	1.22394600	2.11893100	-1.77803100
H	0.43440300	1.70014900	-1.13695100
H	2.06080300	2.32860300	-1.10072900
C	0.70447400	3.43642900	-2.37244300
H	1.51125400	3.94825900	-2.91016800
H	-0.07180600	3.22114400	-3.12159600
C	0.13515100	4.38697800	-1.31081000
H	-0.69493600	3.89316300	-0.78367400
H	0.89910600	4.59141900	-0.54917600
C	-0.35965900	5.72422900	-1.89373800
H	0.47255500	6.23877100	-2.38984500
H	-1.10559000	5.51166900	-2.67443400
C	-0.96605000	6.62800500	-0.85446100
H	-1.84739900	6.23883000	-0.34145700
C	-0.50467000	7.83367100	-0.52231100
H	0.36813000	8.26416600	-1.00806300
H	-0.98479200	8.44001400	0.23984600
C	2.83177500	1.58450000	-3.68705700
H	3.69780700	1.84901100	-3.06924100
H	3.15233200	0.82396300	-4.40588300
H	2.53950800	2.47194300	-4.25580900
H	0.82925900	0.87894200	-3.49343800
C	-1.24419500	-0.68027300	-1.93834700
H	-0.52706500	0.01450100	-2.37323700
C	-2.02311800	-0.28890400	-0.90143500
H	-1.79322800	0.65620200	-0.40898900
H	-1.50249200	-1.55469500	-2.52600700
C	-3.24622700	-0.99857900	-0.42045400
H	-3.34012900	-1.97549000	-0.90706400
H	-3.17667600	-1.16678300	0.66156400
C	-4.51568100	-0.15259900	-0.69949100
H	-4.59720600	0.02778200	-1.77845200
H	-4.40688000	0.83126000	-0.22513300
C	-5.79049300	-0.83529400	-0.18672500
H	-5.89259200	-1.82125300	-0.66014100

H	-5.70348000	-1.01786900	0.89216900
C	-7.05987000	-0.00476900	-0.45664700
H	-6.97218600	0.97286000	0.03342300
C	-8.31251500	-0.69600900	0.01159800
H	-8.53552300	-1.65156800	-0.46516200
C	-9.13653700	-0.22969600	0.94963600
H	-10.02780500	-0.77308300	1.24806800
H	-8.95588200	0.72006300	1.44814100
H	-7.12928600	0.18953300	-1.53712700
<b>2TS<sub>216</sub>, -1655.760189, i234.28</b>			
Ti	-0.34851500	-1.34135300	-0.53148600
O	0.72544100	-0.61350500	0.69787300
C	-2.28810300	-2.88092000	-0.97433600
C	-1.09738300	-3.46660800	-1.48434600
C	-0.19624900	-3.67411300	-0.38778000
C	-0.83127000	-3.19881800	0.79910400
C	-2.12084600	-2.69334700	0.43457200
C	1.44253400	-0.24117600	1.81379700
C	0.80196100	0.56130100	2.78838800
C	3.48610500	-0.21536900	3.08353800
C	2.78932600	-0.65178300	1.95042900
C	-3.55108900	-2.71410600	-1.77343100
C	-0.90636500	-3.97086700	-2.88569200
C	1.11210600	-4.41131900	-0.46589400
C	-0.31902300	-3.32856700	2.20529100
C	-0.64489200	1.01884500	2.65565500
C	-0.71437000	2.50769700	2.25784900
C	-1.47063900	0.75502600	3.92943000
C	3.50546900	-1.54452600	0.94339900
C	3.95120600	-2.87395700	1.58747700
C	4.72149900	-0.83835400	0.30948000
C	1.55498000	0.96534400	3.89526500
C	2.88588400	0.58790200	4.04720200
C	-3.17103700	-2.28202600	1.42913600
H	-1.10618200	0.43789000	1.85114300
H	2.80004800	-1.78165100	0.13984800
H	0.93245600	-5.49155500	-0.39977300
H	1.63552100	-4.23190000	-1.40947000
H	1.78541800	-4.14462900	0.34944400
H	-0.70980600	-4.24542700	2.66355000
H	0.77035900	-3.38156700	2.24220500
H	-0.62911300	-2.49048300	2.83398000
H	-2.79020000	-1.57292700	2.17019300
H	-4.04373500	-1.83564900	0.95247800

H	-3.51572900	-3.16468400	1.98166800
H	-3.90727700	-3.69893800	-2.09836600
H	-4.35330800	-2.26034200	-1.19068800
H	-3.41050900	-2.11730600	-2.68061400
H	-1.27956900	-4.99910500	-2.96952100
H	-1.45368600	-3.37140800	-3.61879800
H	0.14627100	-3.99161000	-3.18080400
H	1.08960000	1.58923600	4.65169300
H	3.45086900	0.91561200	4.91407600
H	4.52223700	-0.51319800	3.21103000
H	3.11892500	-3.39652000	2.06949000
H	4.38764200	-3.53989900	0.83550400
H	4.71213300	-2.70449900	2.35546700
H	5.17640600	-1.47368100	-0.45817000
H	4.44742100	0.11419100	-0.15190400
H	5.49086700	-0.62950100	1.05932200
H	-0.28157400	3.13971600	3.04005800
H	-0.15747500	2.70525500	1.33582000
H	-1.75271500	2.82472000	2.11083000
H	-1.42213700	-0.29619900	4.23177500
H	-1.12244900	1.35658000	4.77433800
H	-2.52110500	1.01499100	3.76088900
C	1.61834600	-0.04495700	-2.97728100
C	0.58136000	-1.04294300	-2.44182000
H	1.12240700	-1.77358900	-1.75239000
H	0.19261400	-1.65236300	-3.25819000
C	2.04576600	1.02992300	-1.95894900
H	1.15071500	1.52414500	-1.55749500
H	2.52229300	0.54469000	-1.09990800
C	2.97830800	2.11353500	-2.52075900
H	3.93746700	1.66966000	-2.81446400
H	2.54154500	2.53360900	-3.43825200
C	3.23964000	3.24636100	-1.51881500
H	2.28458300	3.71450000	-1.24050100
H	3.65736600	2.83193000	-0.59167200
C	4.19574100	4.32604600	-2.06005200
H	5.16157000	3.87049200	-2.31208000
H	3.78136800	4.72171000	-2.99944100
C	4.40744600	5.45753000	-1.09067200
H	3.51522900	6.02425300	-0.81920100
C	5.57867000	5.79649400	-0.55199600
H	6.49487600	5.26341900	-0.79631200
H	5.66949100	6.62442800	0.14462100
C	2.81804500	-0.83295300	-3.54681900

H	3.38107700	-1.32802300	-2.74725400
H	2.49074200	-1.59802500	-4.25809300
H	3.50539900	-0.16719700	-4.07437300
H	1.14481200	0.46187500	-3.83109400
C	-1.26159900	0.26327400	-2.23746900
H	-0.55568900	0.91931100	-2.72429100
C	-1.67385000	0.50506500	-0.92267600
H	-1.05077400	1.22101600	-0.38189100
H	-1.92213800	-0.28218400	-2.90795700
C	-3.13174500	0.53105000	-0.50242900
H	-3.70345300	-0.22401400	-1.04610500
H	-3.22719100	0.31035900	0.56484600
C	-3.75525700	1.91943800	-0.77148700
H	-3.69026700	2.14057300	-1.84527700
H	-3.16174800	2.69037600	-0.26215100
C	-5.21535000	2.00794200	-0.30954800
H	-5.80832600	1.23656800	-0.82067800
H	-5.27860500	1.78378900	0.76345900
C	-5.84620400	3.38956400	-0.57025100
H	-5.27348600	4.16166300	-0.04144400
C	-7.29121500	3.45642400	-0.15451400
H	-7.96690900	2.77277200	-0.67076600
C	-7.78084600	4.26808300	0.78253800
H	-8.83515700	4.27105000	1.04180900
H	-7.14564200	4.96878400	1.31994300
H	-5.76233900	3.61590100	-1.64359100
<b>2P<sub>21b</sub> -1655.7932349</b>			
Ti	0.03609300	-1.57964300	-0.45368700
O	1.12597300	-0.62895500	0.59298400
C	-1.35092500	-3.60353500	-0.75772000
C	-0.18333600	-3.69742200	-1.57266400
C	0.96317200	-3.69906100	-0.71265300
C	0.50523000	-3.56436800	0.63137500
C	-0.93021600	-3.48263900	0.59982400
C	1.94219200	-0.08880900	1.55577900
C	1.34963100	0.38205800	2.75179600
C	4.12221500	0.58556400	2.31067200
C	3.33222400	-0.00162500	1.31589700
C	-2.75685900	-3.80246400	-1.24488800
C	-0.17059000	-3.94695100	-3.05571100
C	2.38516400	-3.89456600	-1.16021600
C	1.35113300	-3.61637700	1.87224200
C	-0.15205800	0.31355100	3.00016900
C	-0.80231000	1.69855500	2.80175800

C	-0.50159300	-0.26111900	4.38577100
C	3.98267300	-0.49021500	0.02771200
C	5.07704100	-1.54126800	0.29998200
C	4.55611900	0.68346700	-0.79214700
C	2.19442200	0.95476200	3.70742200
C	3.56688800	1.06029100	3.49512300
C	-1.82136200	-3.43760600	1.80802900
H	-0.58438700	-0.36131800	2.25394700
H	3.20740100	-0.96944700	-0.58021800
H	2.57875900	-4.96019400	-1.33435000
H	2.60320100	-3.37419600	-2.09810400
H	3.10037900	-3.55183800	-0.41157000
H	1.43820100	-4.65162300	2.22342700
H	2.36114800	-3.24040500	1.69775900
H	0.91949800	-3.03020800	2.68667900
H	-1.38187600	-2.85173300	2.61934300
H	-2.80128000	-3.01459000	1.58008200
H	-1.98092400	-4.45226200	2.19379900
H	-2.90688000	-4.86165800	-1.48859800
H	-3.49703000	-3.53745300	-0.48932800
H	-2.97971500	-3.23745700	-2.15494900
H	-0.26047800	-5.02181200	-3.25597700
H	-1.00582200	-3.45861800	-3.56600600
H	0.75876000	-3.61256100	-3.52395000
H	1.76966400	1.32904600	4.63338200
H	4.20122100	1.51224400	4.25113500
H	5.19263600	0.67366000	2.15216900
H	4.69846200	-2.37906100	0.89468900
H	5.47174300	-1.93809000	-0.64123600
H	5.91833500	-1.10819600	0.84972100
H	4.97652900	0.32460300	-1.73796700
H	3.78908400	1.43038100	-1.01795100
H	5.35803500	1.19061500	-0.24632500
H	-0.41800200	2.41778700	3.53244900
H	-0.59349800	2.10112600	1.80520200
H	-1.88861900	1.63954700	2.93027100
H	-0.03545300	-1.23867200	4.54745200
H	-0.17484800	0.39733000	5.19627300
H	-1.58591400	-0.37817000	4.48396800
C	0.51917000	0.93815500	-3.18568000
C	-0.02720900	-0.44330700	-2.74683300
H	0.83160000	-0.92737000	-2.19416900
H	-0.09855700	-1.08545100	-3.62896200
C	0.64647000	1.93735900	-2.02024200



H	-0.32070300	2.01486800	-1.50686100
H	1.35598100	1.54353800	-1.27887400
C	1.07543200	3.35397900	-2.43214500
H	2.08974500	3.33395000	-2.84913700
H	0.41931000	3.71363800	-3.23738700
C	1.03624500	4.34672500	-1.26262100
H	0.01514500	4.39325000	-0.85802400
H	1.67307600	3.98155900	-0.44587500
C	1.49125100	5.76484000	-1.65617700
H	2.52146100	5.73052600	-2.03215600
H	0.86472000	6.11471800	-2.49018200
C	1.40046000	6.74423700	-0.51719800
H	0.40198000	6.90559500	-0.10753300
C	2.43184500	7.40165800	0.01277500
H	3.44387900	7.27630400	-0.36582200
H	2.30414600	8.09733000	0.83663300
C	1.83156900	0.74516200	-3.95965500
H	2.63254600	0.39000100	-3.29992500
H	1.71229400	0.01869300	-4.77076300
H	2.16774000	1.68160100	-4.40944600
H	-0.23133800	1.33287300	-3.88699500
C	-1.44627300	-0.43686800	-2.06671300
H	-1.90753100	0.48945200	-2.42795000
C	-1.63856700	-0.42357700	-0.50710400
H	-1.16717900	0.48040000	-0.09447200
H	-2.03918800	-1.25796500	-2.47756700
C	-3.08907900	-0.48708500	-0.05720000
H	-3.59824700	-1.33108600	-0.53399100
H	-3.10339900	-0.68311900	1.02246900
C	-3.89809400	0.79970800	-0.32203500
H	-3.93288200	1.00399900	-1.40109300
H	-3.38036800	1.65261600	0.13788800
C	-5.33178500	0.72005300	0.21826900
H	-5.84791400	-0.13481900	-0.24069400
H	-5.30816700	0.52029100	1.29759000
C	-6.14684700	2.00233600	-0.03630500
H	-5.64884100	2.85628500	0.43991700
C	-7.56364400	1.90075600	0.46138300
H	-8.17329900	1.11963100	0.00460300
C	-8.10140200	2.67541700	1.40333900
H	-9.13141900	2.55346400	1.72428500
H	-7.53268400	3.46844100	1.88392300
H	-6.15245700	2.20517800	-1.11786900

**2C<sub>21b</sub>, -1655.77118**

Ti	0.40934200	1.67936300	0.23161100
O	0.30721800	-0.11252400	0.18590300
C	-0.44720900	2.63277000	-1.73244000
C	-0.48598400	3.71105000	-0.78283600
C	0.85464500	4.03506300	-0.43725200
C	1.72695300	3.20650900	-1.21148900
C	0.92887900	2.34519000	-2.01297700
C	0.04648100	-1.46936000	0.26781600
C	-0.20216000	-2.19712100	-0.92011500
C	-0.31050500	-3.46298500	1.57884600
C	0.01670300	-2.10278800	1.53642000
C	-1.63911400	2.09018000	-2.47063200
C	-1.67694700	4.55049000	-0.42253300
C	1.25764500	5.17693500	0.45429700
C	3.20984800	3.38296900	-1.38680400
C	-0.11847300	-1.57232800	-2.30297500
C	-1.41692300	-1.75813500	-3.11171900
C	1.09233200	-2.12316300	-3.08360700
C	0.35118500	-1.40422200	2.84919600
C	1.51863500	-2.10252700	3.57881200
C	-0.86461400	-1.30495500	3.79200400
C	-0.51470600	-3.55598100	-0.80911100
C	-0.58204700	-4.19048800	0.42570300
C	1.47796900	1.47456300	-3.10967000
H	0.03482600	-0.50191100	-2.16413700
H	0.67168300	-0.38794300	2.60821300
H	1.20450600	6.12433000	-0.09665300
H	0.59455700	5.27863800	1.31910700
H	2.28305000	5.08066100	0.82060700
H	3.39456700	3.95783800	-2.30344400
H	3.66805300	3.94534500	-0.56988700
H	3.73821500	2.43243300	-1.49946000
H	2.19305500	0.72920300	-2.74915300
H	0.68871900	0.95064500	-3.64839800
H	2.00507700	2.10171000	-3.83883800
H	-1.87392900	2.73885200	-3.32396000
H	-1.46233600	1.08748100	-2.86161400
H	-2.52840100	2.04874800	-1.83804000
H	-1.57166300	5.53826000	-0.88761800
H	-2.60918100	4.12068400	-0.78939600
H	-1.77742200	4.71417000	0.65462600
H	-0.71013500	-4.12539100	-1.71236800
H	-0.83443500	-5.24419000	0.48898700
H	-0.34725300	-3.96264600	2.54181500

H	2.38015700	-2.25464500	2.92192300
H	1.84008400	-1.51246300	4.44401600
H	1.22075600	-3.08672800	3.95236300
H	-0.59293100	-0.78102500	4.71494400
H	-1.69842000	-0.77108200	3.32950400
H	-1.22542400	-2.29951500	4.07223200
H	-1.60774700	-2.81231600	-3.33425200
H	-2.28652500	-1.37279600	-2.57061300
H	-1.34899300	-1.23470000	-4.07209500
H	2.02879600	-1.95878400	-2.54035400
H	0.99465100	-3.20014900	-3.25302800
H	1.17663700	-1.64156700	-4.06372300
C	-2.71086400	1.81982600	1.33095500
C	-1.19368100	2.01134600	1.50980000
H	-0.82578400	1.28525100	2.25644100
H	-0.98382200	3.02043000	1.89830600
C	-3.07227200	0.42788900	0.77123700
H	-2.49731900	0.25404100	-0.14749600
H	-2.74518000	-0.34819400	1.47479200
C	-4.56402100	0.22984000	0.46245500
H	-5.15066400	0.29955900	1.38642700
H	-4.91803300	1.04652200	-0.18423400
C	-4.86347700	-1.11558100	-0.21180500
H	-4.31310200	-1.18004900	-1.16142800
H	-4.48634800	-1.93505300	0.41370000
C	-6.36398500	-1.33827000	-0.48037800
H	-6.91525300	-1.31258300	0.46787400
H	-6.74067300	-0.49862300	-1.08384200
C	-6.64566200	-2.63249800	-1.19460100
H	-6.19610400	-2.73714400	-2.18363400
C	-7.37916900	-3.63388700	-0.70867300
H	-7.84945800	-3.57374000	0.27028400
H	-7.54582700	-4.54698200	-1.27226100
C	-3.42746100	2.11959200	2.66451200
H	-3.15654100	1.38492300	3.43150300
H	-3.15833400	3.11116500	3.04314900
H	-4.51438400	2.09691900	2.54823200
H	-3.06145600	2.56303700	0.60584700
C	2.01431600	2.06878600	2.13739100
H	1.52914900	1.44172000	2.87968200
C	3.14163300	1.65325000	1.50937500
H	1.73085100	3.11891500	2.11476600
C	3.80134900	0.32223400	1.65339100
H	3.20757400	-0.33455400	2.29337000

H	3.65945000	2.36236300	0.86832700
C	4.13069600	-0.36808000	0.31319400
H	3.19384900	-0.59205400	-0.21334700
H	4.69767700	0.32405600	-0.32474900
C	4.93705300	-1.65962200	0.50273100
H	5.87172600	-1.42841100	1.03135100
H	4.38122600	-2.35185500	1.14773400
C	5.26205300	-2.36590600	-0.82672700
H	5.79751900	-1.65909800	-1.47848600
H	4.32939900	-2.62744700	-1.34303200
C	6.09728300	-3.60388500	-0.63707200
H	7.08115900	-3.44983300	-0.19195100
C	5.71651500	-4.83927300	-0.96112100
H	4.74566100	-5.03885300	-1.40943900
H	6.36197600	-5.69688000	-0.79843300
H	4.74780200	0.51097200	2.18498800

**2TS<sub>21b</sub>, -1655.7425236, i247.49**

Ti	-0.67036100	1.45111700	-0.30129600
O	-0.00216900	-0.21256000	-0.05069300
C	-0.69985100	2.75525300	1.68679200
C	-0.82140300	3.75648900	0.66472700
C	-2.04113600	3.54996400	-0.02273100
C	-2.72698400	2.46677100	0.61621900
C	-1.90232100	1.97789900	1.67245800
C	0.61724100	-1.43956200	0.15292200
C	0.89862300	-1.84984800	1.48150600
C	1.62518800	-3.47888100	-0.67302600
C	0.98354300	-2.26432100	-0.94961300
C	0.36577500	2.75674400	2.74960300
C	0.05216400	4.97019200	0.54496200
C	-2.60477900	4.41197900	-1.11596100
C	-4.18706900	2.16051100	0.45601200
C	0.53043800	-1.03384500	2.71032500
C	1.78129500	-0.60890300	3.50625200
C	-0.45244100	-1.80270300	3.61700700
C	0.72718800	-1.95104100	-2.42323200
C	-0.24032500	-2.97667200	-3.05658200
C	2.02269600	-1.91233700	-3.26322600
C	1.54305300	-3.07459000	1.68278700
C	1.90973300	-3.89177600	0.62162800
C	-2.36960100	1.00399300	2.71968000
H	0.02959000	-0.12899000	2.36551500
H	0.26915400	-0.96210400	-2.47860700
H	-3.27294100	5.17513500	-0.69777700

H	-1.82350000	4.93991200	-1.66916100
H	-3.19642300	3.83567100	-1.83392000
H	-4.76267600	2.88305500	1.04941500
H	-4.53760400	2.25643300	-0.57487800
H	-4.44498700	1.16405200	0.81363900
H	-2.63869400	0.02673000	2.30949600
H	-1.61842800	0.84681400	3.49246500
H	-3.26275800	1.40493000	3.21289800
H	0.18417000	3.57485800	3.45768900
H	0.38077600	1.82924400	3.32062200
H	1.36902500	2.90608700	2.33913500
H	-0.35644600	5.75590000	1.19384600
H	1.07653100	4.78976800	0.87319600
H	0.07413000	5.38109000	-0.46692500
H	1.75903200	-3.39175900	2.69802400
H	2.40738500	-4.83955700	0.80062000
H	1.90716200	-4.11691300	-1.50410800
H	-1.15964600	-3.10064700	-2.47998100
H	-0.51045200	-2.67118800	-4.07313100
H	0.23371500	-3.96030900	-3.12655600
H	1.79258400	-1.61338400	-4.29165900
H	2.76202300	-1.21676100	-2.86294500
H	2.49229600	-2.89916400	-3.31256500
H	2.32769000	-1.47809400	3.88464700
H	2.47350200	-0.02649600	2.89007300
H	1.50146300	-0.00078300	4.37361800
H	-1.35447300	-2.09820900	3.07261800
H	0.00428800	-2.71301800	4.01672700
H	-0.75344900	-1.18889400	4.47269300
C	1.72669100	2.29598400	-1.05004400
C	0.54219500	2.35957800	-2.04847400
H	0.91473200	2.04601700	-3.01970000
H	0.15865600	3.37632100	-2.13241300
C	2.65399800	1.08464800	-1.26376000
H	2.06586900	0.16906700	-1.28845000
H	3.11353900	1.18963500	-2.25605300
C	3.75370300	0.93121700	-0.20168000
H	4.40470600	1.81387700	-0.19513700
H	3.28797900	0.88313100	0.79359400
C	4.61727300	-0.31982800	-0.41225500
H	3.97838300	-1.21224000	-0.39524300
H	5.07728300	-0.28627500	-1.40861600
C	5.72804600	-0.46911300	0.64464300
H	6.39161400	0.40417300	0.61197400

H	5.26286200	-0.47307000	1.64225800
C	6.53593100	-1.72622100	0.46628700
H	5.97883100	-2.66172300	0.53845200
C	7.84564100	-1.76781900	0.22237100
H	8.44076300	-0.86078100	0.14337500
H	8.37484400	-2.70786800	0.09914400
C	2.53471500	3.61087000	-1.21920700
H	3.06564300	3.57481800	-2.17567200
H	1.90897100	4.50097100	-1.22203200
H	3.27804500	3.71854200	-0.42543800
H	1.39176400	2.28016100	0.01438300
C	-1.19544200	1.34361300	-2.72992700
H	-0.62780800	0.60155300	-3.27973500
C	-2.19663400	0.88226800	-1.83274900
H	-1.37728300	2.26143300	-3.27861300
C	-2.58627000	-0.59763400	-1.82514700
H	-1.69841100	-1.21646000	-1.71574300
H	-3.04118500	1.55606800	-1.74229000
C	-3.61928200	-1.02434500	-0.77574900
H	-3.22896800	-0.82119500	0.23065700
H	-4.53169000	-0.42522000	-0.88703700
C	-3.98169700	-2.51169200	-0.88129100
H	-4.35441100	-2.72403500	-1.89274400
H	-3.07969700	-3.12344000	-0.75066000
C	-5.03707500	-2.95179100	0.15110600
H	-5.93371800	-2.32668400	0.02336400
H	-4.66364800	-2.76179600	1.16590600
C	-5.41564300	-4.40222200	0.01747600
H	-5.85788600	-4.69150300	-0.93692900
C	-5.24169700	-5.32900500	0.95945800
H	-4.80841300	-5.08558200	1.92722200
H	-5.53302600	-6.36331500	0.80442800
H	-2.99797700	-0.82501700	-2.82031800
<b>2P<sub>21b</sub>, -1655.7992057</b>			
Ti	-1.47303800	0.02505100	0.80306300
O	-1.32736500	-1.25445400	-0.43011500
C	-3.19120300	-0.81276800	2.10368500
C	-1.95258200	-0.98548500	2.80133300
C	-1.46303500	0.31547800	3.18336900
C	-2.37393700	1.28334000	2.68155600
C	-3.42957500	0.59201300	1.99338800
C	-1.70003500	-2.16824900	-1.38769500
C	-1.02728300	-3.40500200	-1.44771800
C	-3.08701400	-2.75255900	-3.25915900

C	-2.73731000	-1.81702000	-2.28110500
C	-4.09045500	-1.91319700	1.61397000
C	-1.33511700	-2.29745400	3.20175200
C	-0.29372600	0.57457700	4.08838800
C	-2.30442400	2.76552600	2.91424000
C	0.09827900	-3.76708100	-0.48786000
C	1.44008900	-3.91516400	-1.23250200
C	-0.22536000	-5.03897100	0.31993600
C	-3.41174300	-0.45179300	-2.23642600
C	-4.94073000	-0.52074200	-2.39464900
C	-2.79376300	0.49997900	-3.28123100
C	-1.42609300	-4.30215900	-2.44576600
C	-2.44181200	-3.98550100	-3.34312100
C	-4.64010000	1.23827400	1.37432800
H	0.20696400	-2.94177200	0.22325300
H	-3.22366500	-0.01375000	-1.24011000
H	-0.61307600	0.51132500	5.13591700
H	0.50627500	-0.15534400	3.94652700
H	0.12974100	1.57079900	3.94041200
H	-2.83692100	3.02396200	3.83780600
H	-1.27586200	3.11586000	3.02906600
H	-2.77113500	3.33524900	2.10658500
H	-4.41885900	2.22912100	0.96852800
H	-5.06692800	0.63215400	0.57181400
H	-5.42285200	1.36847200	2.13163300
H	-4.76583200	-2.23082100	2.41748700
H	-4.71252500	-1.59162400	0.77565700
H	-3.52785100	-2.79230400	1.29130900
H	-1.64795600	-2.56210500	4.21932200
H	-1.64166800	-3.11181100	2.54252300
H	-0.24238900	-2.25560800	3.20243400
H	-0.92870100	-5.26425600	-2.52125000
H	-2.73154400	-4.69713500	-4.10977100
H	-3.87330300	-2.51523300	-3.96840200
H	-5.39187400	-1.21184900	-1.67593000
H	-5.38332500	0.47001700	-2.24896000
H	-5.22593800	-0.85374600	-3.39692100
H	-3.22959600	1.50212900	-3.20673500
H	-1.70888100	0.58126300	-3.16053000
H	-2.98180800	0.12631600	-4.29268900
H	1.40741500	-4.74053100	-1.95110500
H	1.69320300	-3.00468400	-1.78470000
H	2.24990700	-4.12321900	-0.52552700
H	-1.17301800	-4.94407000	0.86059300

H	-0.30496900	-5.91731600	-0.32837100
H	0.56587600	-5.24038100	1.04945100
C	3.61713300	-0.99770200	0.81266800
C	2.28576200	-0.36596200	1.27659300
H	2.47853500	0.26034400	2.15966900
H	1.61639900	-1.17132200	1.61504600
C	4.70887600	0.06949600	0.58344500
H	4.30979300	0.87055500	-0.05287700
H	4.94922300	0.54092200	1.54794700
C	6.00057900	-0.44876800	-0.06603800
H	6.47702400	-1.19382600	0.58308200
H	5.75246800	-0.97153100	-1.00106600
C	7.00939600	0.66864200	-0.36281700
H	6.54741900	1.41042700	-1.02982300
H	7.25290500	1.20307200	0.56482500
C	8.31359100	0.15412700	-1.00105000
H	8.79622200	-0.56414800	-0.32639900
H	8.05984700	-0.39959600	-1.91764400
C	9.27785000	1.25961100	-1.33635600
H	8.91841300	2.00328400	-2.04971300
C	10.50192700	1.39257800	-0.82550600
H	10.90328500	0.67591200	-0.11236100
H	11.15195700	2.21657200	-1.10424500
C	4.06417100	-2.06442900	1.82527600
H	4.26952300	-1.61350000	2.80401700
H	3.28955900	-2.82700600	1.96582400
H	4.97283200	-2.57810600	1.50174700
H	3.42973400	-1.50181600	-0.14807800
C	1.54846400	0.46315200	0.21425800
H	1.31065900	-0.17191100	-0.64873000
C	0.27990500	1.13498300	0.74554900
H	2.21639200	1.25155900	-0.16305600
C	-0.51051000	1.95398900	-0.27389100
H	-1.63810500	1.85636600	-0.11104300
H	0.48840600	1.72576500	1.64032800
C	-0.28113300	3.47838300	-0.24156600
H	-0.43117100	3.84388700	0.78076400
H	0.77510200	3.65108500	-0.48183200
C	-1.17390300	4.25490100	-1.21595200
H	-1.02166700	3.87577700	-2.23541500
H	-2.23102900	4.07431600	-0.97448900
C	-0.90950200	5.77276700	-1.19033200
H	0.14987700	5.94728300	-1.42861800
H	-1.07109300	6.15863800	-0.17592800



C	-1.77568100	6.52713000	-2.16318500
H	-1.64158700	6.27365300	-3.21569800
C	-2.67259000	7.45388300	-1.82650600
H	-2.83292500	7.74451400	-0.79054000
H	-3.27051000	7.96760400	-2.57293600
H	-0.35509500	1.56967900	-1.28836200

**Table S4** Optimized Cartesian coordinates (Å) and zero-point energy corrected energy (a.u.) of  $2\mathbf{C}_{\text{cyc}}$ ,  $2\mathbf{TS}_{\text{cyc}}$ , and  $2\mathbf{P}_{\text{cyc}}$ , as well as the imaginary frequency ( $\text{cm}^{-1}$ ) of  $2\mathbf{TS}_{\text{cyc}}$ .

Atom	x	y	z
<b><math>2\mathbf{C}_{\text{cyc}}</math>, -1342.894761</b>			
O	-0.91764300	0.18004300	0.10745000
C	1.92992600	-1.48021400	-2.09190300
C	0.51667100	-1.49717500	-2.33333000
C	-0.09143500	-2.30303900	-1.32737700
C	0.94451900	-2.77345300	-0.45433700
C	2.19248900	-2.26537800	-0.93314600
C	2.96198300	-0.91262300	-3.02711600
C	-0.18266500	-0.91100400	-3.52809900
C	-1.53547700	-2.71164200	-1.28220500
C	0.75514100	-3.77669700	0.64596400
C	3.55059600	-2.59726500	-0.38544700
C	-2.27854200	0.35666800	0.22280100
C	-2.94143000	1.20873700	-0.69185900
C	-4.31970700	1.38648600	-0.53059300
C	-5.02074900	0.74624200	0.48667000
C	-4.34514700	-0.08961700	1.37141900
C	-2.96746200	-0.30618400	1.26692100
C	-2.19705700	1.97445400	-1.77732200
C	-2.25012300	-1.18490900	2.28305200
H	3.14229100	-1.62045900	-3.84559000
H	3.92322200	-0.74892700	-2.53426300
H	2.64619200	0.02590900	-3.49215800
H	-0.21011200	-1.64595800	-4.34238100
H	0.32483600	-0.02495300	-3.92059400
H	-1.21586400	-0.63700900	-3.30516500
H	-1.85153500	-2.98302100	-0.27327600
H	-1.69218000	-3.58900200	-1.92180300
H	-2.20068100	-1.92163500	-1.63716100
H	0.69084600	-4.78418400	0.21670800
H	-0.16582600	-3.60510900	1.20870700
H	1.58665200	-3.77940800	1.35280900
H	4.27512100	-1.79811700	-0.56372600

H	3.94135400	-3.50195100	-0.86718600
H	3.52569500	-2.79180000	0.68899400
Ti	0.73436000	-0.39836700	-0.25917500
C	-2.92391600	1.96927700	-3.13459800
H	-3.16819600	0.95325400	-3.46045400
H	-3.85739000	2.53877300	-3.10101200
H	-2.29424300	2.43210200	-3.90145300
C	-1.91597000	3.42137600	-1.31877400
H	-1.38475900	3.44534100	-0.36106500
H	-1.31877600	3.95987800	-2.06305100
H	-2.85262000	3.97108100	-1.18110500
H	-4.85256500	2.04113200	-1.21225700
H	-6.09020200	0.89965200	0.59138800
H	-4.89938900	-0.58274900	2.16281800
C	1.48975300	-0.73837900	1.68000600
C	1.44535200	1.81085600	-1.23262100
H	1.09928100	1.26098900	-2.10870900
H	0.72150300	2.44740300	-0.73643800
H	0.63136300	-0.72429200	2.35979900
C	2.47342900	3.04590600	2.28831900
C	2.66514100	3.71022400	0.91226500
C	3.47716600	2.91717800	-0.12674900
C	1.66028000	1.73799800	2.31993100
C	2.77582100	1.94407900	-1.02572500
C	2.44051400	0.44000000	1.99742100
H	3.45774500	2.88386400	2.74571500
H	1.69024100	3.98965100	0.49319200
H	4.33084300	2.41522300	0.34836900
H	0.79268200	1.84398000	1.65456600
H	1.97135800	3.77992400	2.92866100
H	3.18980500	4.65759600	1.07582600
H	3.94882400	3.61951600	-0.83499900
H	1.23159000	1.60954200	3.32225700
H	3.44369600	1.34074600	-1.63945800
H	2.00731800	-1.68567800	1.82420200
H	-1.23440200	1.47803400	-1.92863200
H	-1.30779500	-1.50926200	1.83110200
C	-3.03431200	-2.45618100	2.65599600
H	-2.41745300	-3.10422800	3.28713000
H	-3.94059600	-2.22832500	3.22519500
H	-3.33350700	-3.02579700	1.77022100
C	-1.90632500	-0.37046300	3.54819800
H	-2.81991600	-0.02861600	4.04562000
H	-1.34338200	-0.98062600	4.26310900

H	-1.31098800	0.51536000	3.30623600
C	3.37351200	0.04813100	3.16406000
H	2.78609000	-0.19938300	4.05455700
H	3.98097700	-0.82508300	2.90722300
H	4.05742100	0.86189200	3.42604100
H	3.09880900	0.61812100	1.13284000
<b>2TS<sub>cyc</sub>, -1342.8852604, i196.37</b>			
O	0.74438900	-0.07605000	0.03545400
C	-2.92028500	-1.81060400	-0.46139300
C	-1.66920800	-2.50479300	-0.57240000
C	-0.93694900	-1.92633900	-1.65493900
C	-1.70945900	-0.84208800	-2.17268300
C	-2.94364900	-0.78427200	-1.43753300
C	-4.06627400	-2.19158400	0.43197700
C	-1.28012200	-3.74076900	0.18836900
C	0.36238700	-2.43423700	-2.21115500
C	-1.38648400	-0.02024600	-3.39016400
C	-4.11272400	0.09995400	-1.76372100
C	2.11167000	-0.17338700	-0.11632100
C	2.81724800	-1.11031400	0.67716700
C	4.20896100	-1.15425500	0.54623700
C	4.88421300	-0.32130400	-0.34084100
C	4.16438200	0.57144800	-1.12757100
C	2.77046200	0.66927100	-1.04254600
C	2.12740300	-2.04510600	1.66329800
C	2.04547200	1.65629000	-1.95055600
H	-4.78077100	-2.80953900	-0.12546400
H	-4.61962300	-1.32248900	0.79993200
H	-3.74782500	-2.78398100	1.29307000
H	-1.71698200	-4.62769500	-0.28700100
H	-1.63590100	-3.72652000	1.22242000
H	-0.19797800	-3.88432900	0.20929400
H	0.93410200	-1.64521500	-2.70306300
H	0.17001100	-3.21572000	-2.95625200
H	1.00045500	-2.86788400	-1.43824100
H	-1.80987800	-0.49501600	-4.28399600
H	-0.31168300	0.07309300	-3.55131000
H	-1.80774900	0.98735000	-3.33307000
H	-4.76079700	0.26480000	-0.89840700
H	-4.73002800	-0.36542600	-2.54174300
H	-3.80272100	1.07633500	-2.14636900
Ti	-1.03306000	-0.26088600	-0.00240700
C	2.56134800	-3.51337300	1.48660700
H	2.42755100	-3.85486000	0.45494300

H	3.61352300	-3.66216100	1.74685400
H	1.97229100	-4.16339500	2.14202500
C	2.35581700	-1.58717000	3.11847900
H	2.02451300	-0.55584500	3.27583400
H	1.81684100	-2.23403400	3.81951700
H	3.41865900	-1.63009400	3.37756200
H	4.77413000	-1.85627900	1.15095800
H	5.96526700	-0.37292400	-0.42308400
H	4.69482500	1.21014300	-1.82695600
C	-1.92985700	1.68177100	0.24223000
C	-1.47709200	-0.78854500	2.09358400
H	-2.09145100	-1.67872700	2.06281900
H	-0.51720600	-0.90616100	2.59063300
H	-1.43946500	1.46423300	-0.76806600
C	0.14450100	3.20335200	2.62489900
C	-0.20485300	1.87009400	3.29900800
C	-1.69984200	1.49765900	3.22360500
C	-0.04589000	3.26301500	1.10292700
C	-2.13398100	0.45143200	2.22254800
C	-1.49982400	3.11074200	0.59964000
H	-0.44602400	4.00329900	3.09243300
H	0.41076200	1.07150000	2.86961900
H	-2.31586400	2.39517400	3.12941900
H	0.58930000	2.50923300	0.62454800
H	1.19261200	3.43485700	2.84808400
H	0.08319500	1.93582200	4.35324700
H	-2.01021400	1.04241100	4.17674600
H	0.33167700	4.23447600	0.76458100
H	-3.20282200	0.44485100	2.02030500
H	-3.00179500	1.67010600	0.03343400
H	1.05280300	-2.00456900	1.46440400
H	0.97340000	1.59176300	-1.73547200
C	2.24826900	1.30293600	-3.43882100
H	1.65541300	1.96669600	-4.07700700
H	3.29645100	1.41650600	-3.73209500
H	1.96314500	0.26911300	-3.65797600
C	2.49037200	3.11001300	-1.69113100
H	3.54289400	3.25318900	-1.95464900
H	1.90304600	3.80479300	-2.30109100
H	2.37178000	3.39054700	-0.64166800
C	-1.75088600	4.01017500	-0.63453200
H	-1.06357800	3.75941000	-1.45119500
H	-2.77547400	3.91398500	-1.00820300
H	-1.58696600	5.06029900	-0.37461300

H	-2.18441100	3.46817200	1.37802700
<b>2P<sub>cyc</sub>, -1342.9132433</b>			
O	0.99190100	-0.17169100	-0.12967900
C	-1.44369300	3.00336000	0.05410600
C	-0.01645000	3.06410400	-0.03160200
C	0.53119100	2.51927400	1.17741400
C	-0.55809300	2.07963900	1.98535200
C	-1.77920800	2.37472500	1.28867800
C	-2.41151900	3.62662400	-0.90672100
C	0.76668400	3.69982300	-1.14468600
C	1.98668800	2.48734200	1.54729500
C	-0.46161200	1.48728800	3.36474100
C	-3.16935400	2.20594500	1.83962900
C	2.25416800	-0.70900600	-0.07589400
C	3.12780900	-0.48078700	-1.16300600
C	4.39957800	-1.05843000	-1.09300200
C	4.78728600	-1.82982700	0.00047800
C	3.90103300	-2.04058800	1.05389900
C	2.61690700	-1.48563400	1.04663200
C	2.69329700	0.31232000	-2.38919400
C	1.64483700	-1.77367500	2.18382000
H	-2.70110800	4.62155800	-0.54694300
H	-3.33070700	3.04374100	-1.01198500
H	-1.97616400	3.75774800	-1.89944500
H	0.83729400	4.78251300	-0.98221200
H	0.29460200	3.54560900	-2.11828500
H	1.78651600	3.31341100	-1.19908700
H	2.21234200	1.68871000	2.25684100
H	2.27459600	3.43604900	2.01580800
H	2.62898800	2.34256900	0.67584300
H	-0.58701300	2.27358700	4.11927600
H	0.50784200	1.01822100	3.54361300
H	-1.23795100	0.73965800	3.55274600
H	-3.90785500	2.02405700	1.05446000
H	-3.47643500	3.11959100	2.36313600
H	-3.23281400	1.38864900	2.56268900
Ti	-0.50620100	0.77274700	0.04427100
C	3.77459400	1.28337200	-2.89582400
H	4.12648100	1.94877200	-2.10063600
H	4.64570300	0.75537000	-3.29565300
H	3.37486800	1.90107800	-3.70641300
C	2.24014400	-0.64028900	-3.51574900
H	1.43656700	-1.30422200	-3.18023300
H	1.87947400	-0.07340700	-4.38077900

H	3.07068300	-1.27096400	-3.84956400
H	5.09732300	-0.90642900	-1.90988200
H	5.77925500	-2.26957900	0.02981600
H	4.21166700	-2.65046200	1.89627200
C	-2.26946400	-0.97656400	-0.00695300
C	-1.38807600	0.66588400	-1.80546300
H	-1.67875200	1.51983000	-2.41445200
H	-0.75135900	-0.00577500	-2.39461200
H	-1.33478900	-1.53210600	-0.18034300
C	-3.47279300	-3.39234800	-1.77397800
C	-2.80339400	-2.32250000	-2.65247900
C	-3.32761600	-0.90061400	-2.38526000
C	-3.13205000	-3.36393500	-0.27739300
C	-2.62782900	-0.09434200	-1.24925500
C	-3.32308500	-2.02177500	0.46399100
H	-4.56053500	-3.30052300	-1.89591900
H	-1.70954500	-2.36381900	-2.55155700
H	-4.39816100	-0.96224200	-2.15340200
H	-2.09078900	-3.68622500	-0.12947400
H	-3.21141000	-4.38533600	-2.15746800
H	-3.00926000	-2.56893600	-3.69971400
H	-3.25292900	-0.29484300	-3.29372900
H	-3.75016700	-4.11697500	0.22553500
H	-3.35159300	0.65271500	-0.90278000
H	-2.12819200	-0.32559500	0.89643200
H	1.82448800	0.91505500	-2.10442300
H	0.80332700	-1.07622100	2.09029200
C	2.26629400	-1.54713800	3.57424500
H	1.50906600	-1.67495400	4.35472900
H	3.06684400	-2.26327700	3.78237600
H	2.69174200	-0.54272400	3.66924800
C	1.07370600	-3.20202100	2.06489400
H	1.86931100	-3.94820600	2.15766500
H	0.34126500	-3.39568000	2.85641800
H	0.58758300	-3.36046200	1.09649200
C	-3.22314400	-2.23941900	1.98192200
H	-2.23476500	-2.62288400	2.26241300
H	-3.39892300	-1.31038700	2.53652000
H	-3.96594500	-2.96775600	2.31850700
H	-4.32045900	-1.62024900	0.24151800

**Table S4** Optimized Cartesian coordinates (Å) and zero-point energy corrected energy (a.u.) of **3C<sub>12</sub>**, **3TS<sub>12</sub>**, **3P<sub>12</sub>**, **3C<sub>cyc</sub>**, **3TS<sub>cyc</sub>** and **3P<sub>cyc</sub>**, as well as the imaginary frequency (cm<sup>-1</sup>) of **3TS<sub>12</sub>**, and

**3TS<sub>eye</sub>**

Atom	x	y	z
<b>3C<sub>12</sub>, -1968.6798553</b>			
Ti	1.73893100	-1.45798200	0.23201100
O	2.56513900	0.07078700	-0.20006400
C	1.98518500	-3.44253500	1.67408300
C	1.88514300	-3.91418000	0.33648900
C	3.00582000	-3.40120800	-0.40007500
C	3.78709500	-2.60055100	0.47969600
C	3.14353200	-2.60836100	1.76073200
C	3.45869700	1.05705400	-0.56913100
C	4.05655100	1.86790500	0.42643900
C	4.62030800	2.26818900	-2.30207900
C	3.73574200	1.24562200	-1.94509000
C	1.14276500	-3.88991600	2.83078900
C	0.88672400	-4.93002400	-0.14610200
C	3.37500600	-3.75147300	-1.81586100
C	5.11221600	-1.97382300	0.15393800
C	3.80293500	1.70766600	1.92170700
C	3.12379400	2.95711600	2.51983400
C	5.10886000	1.41431200	2.69025500
C	3.09276700	0.41295800	-3.04592200
C	4.13750800	-0.28369800	-3.93949300
C	2.12925800	1.26425400	-3.89862200
C	4.93435900	2.87259600	0.00107300
C	5.21919500	3.07934300	-1.34395500
C	3.68831500	-2.02498900	3.03205600
H	3.12605300	0.85956100	2.06331700
H	2.50293100	-0.37278200	-2.56621800
H	4.10553400	-4.56958500	-1.81886700
H	2.51556500	-4.09100100	-2.39933300
H	3.83500400	-2.91279500	-2.34566900
H	5.92453600	-2.67305900	0.38727600
H	5.19518900	-1.71732800	-0.90456700
H	5.28881800	-1.06151800	0.72575800
H	4.37841700	-1.20263900	2.84588500
H	2.89734400	-1.66390800	3.69448000
H	4.24164700	-2.79713600	3.58146200
H	1.59793300	-4.77194600	3.29844600
H	1.05828800	-3.12214900	3.60308600
H	0.13289500	-4.17287400	2.52223700
H	1.17501300	-5.92933700	0.20190300
H	-0.12030100	-4.73838900	0.23690100
H	0.83512100	-4.97841500	-1.23616600

H	5.40310900	3.50807900	0.74575100
H	5.90195200	3.86797900	-1.64378600
H	4.84053700	2.43279400	-3.35233900
H	4.83219400	-0.89140500	-3.35056400
H	3.64579200	-0.93396600	-4.67092100
H	4.73481200	0.44227000	-4.49909200
H	1.61425700	0.64452400	-4.64105000
H	1.37798900	1.76548800	-3.27889600
H	2.67107700	2.04521300	-4.44098600
H	3.78419100	3.82825200	2.46223800
H	2.19866200	3.20674500	1.99669300
H	2.88730500	2.79255000	3.57649200
H	5.65197400	0.55825500	2.27761400
H	5.78863200	2.27118300	2.65681200
H	4.89488700	1.21017000	3.74456700
C	-2.85788900	1.00753100	2.87206400
C	-1.59910200	0.11236800	2.81589600
H	-1.92443100	-0.92618800	2.97210900
H	-0.96319600	0.35866700	3.67773800
C	-3.90325700	0.58408300	1.82127100
H	-3.43572800	0.58748600	0.82688300
H	-4.19104400	-0.46031700	2.01538700
C	-5.17243000	1.44663100	1.75486100
H	-5.72277900	1.37647500	2.70072200
H	-4.89630600	2.50448600	1.63897900
C	-6.10062900	1.03122800	0.60641200
H	-5.57981700	1.17297900	-0.35196000
H	-6.31577500	-0.04331800	0.68251500
C	-7.43703200	1.79621400	0.57144800
H	-7.98503300	1.61978600	1.50519300
H	-7.22720900	2.87502900	0.52866500
C	-8.29266800	1.40247500	-0.60249500
H	-7.88720600	1.64041600	-1.58748300
C	-9.47128700	0.78340600	-0.52167900
H	-9.91805800	0.53082700	0.43736800
H	-10.04023100	0.51824200	-1.40783000
C	-3.43216400	0.96703900	4.29913000
H	-3.77241300	-0.04340500	4.55727100
H	-2.67655600	1.26123700	5.03509600
H	-4.28242900	1.64409800	4.41534300
H	-2.56273100	2.04616800	2.66785200
C	-0.68495500	0.16017000	1.55517900
H	-1.29002100	-0.13211900	0.68685900
C	0.40221700	-0.92788600	1.76993200



H	1.04714200	-0.64518500	2.61753400
H	-0.09786900	-1.85466700	2.07140200
C	-0.11060800	1.57644700	1.30165900
H	-0.02508100	2.09995700	2.26341600
H	0.90893200	1.49279500	0.91539900
C	-0.90675600	2.45197200	0.31925500
H	-1.95283700	2.53593400	0.63616600
H	-0.92850100	1.95886600	-0.66446300
C	-0.31825500	3.85889200	0.15157100
H	-0.30586100	4.36440200	1.12707000
H	0.72953000	3.78691100	-0.16921800
C	-1.09326500	4.72687900	-0.85814500
H	-2.14354000	4.78519900	-0.53514000
H	-1.09596100	4.23847900	-1.84158600
C	-0.53310400	6.11736100	-0.98836600
H	-0.53299200	6.71611800	-0.07629500
C	-0.04369300	6.64600200	-2.10993600
H	-0.02746500	6.08841500	-3.04404000
H	0.34941000	7.65761200	-2.14168400
C	0.31138200	-1.97948900	-1.72012500
C	-0.42450400	-0.88059700	-2.01177400
H	1.35307900	-2.01425500	-2.05092000
H	-0.15996000	-2.92882300	-1.49354100
H	0.10424100	0.01696100	-2.33206600
C	-1.91426500	-0.77886100	-2.02479200
H	-2.20909500	0.10716100	-1.44524400
H	-2.16860100	-0.50691900	-3.06357600
C	-2.72496100	-2.00503400	-1.59585100
H	-2.37722600	-2.89052100	-2.14422800
H	-2.55336700	-2.20608800	-0.52958600
C	-4.22731000	-1.81784800	-1.85236200
H	-4.57440500	-0.90727200	-1.34752600
H	-4.39472100	-1.65857500	-2.92546100
C	-5.07851100	-3.01196700	-1.38325100
H	-4.72956200	-3.93143300	-1.87067600
H	-4.92191500	-3.14974300	-0.30243300
C	-6.54670100	-2.82092500	-1.65927700
C	-7.28762400	-3.62515400	-2.42139200
H	-7.01267700	-1.94812500	-1.19941800
H	-8.34383000	-3.43816200	-2.58931300
H	-6.86727900	-4.50626200	-2.90144200
<b>3TS<sub>12</sub>, -1968.6747858, i212.33</b>			
Ti	1.77877100	1.12006000	-0.31143200
O	2.52803300	-0.48047400	0.00397800

C	1.75921100	3.04277300	-1.79169600
C	2.33842700	3.52955900	-0.59269200
C	3.52808300	2.77169200	-0.33144500
C	3.72487200	1.86527700	-1.41654300
C	2.61414700	2.00381400	-2.30412300
C	3.39999200	-1.54577600	0.09693000
C	3.45594200	-2.50470300	-0.94041800
C	5.09936200	-2.72458700	1.33564900
C	4.21498800	-1.64593100	1.25289700
C	0.57337500	3.61871800	-2.51366500
C	1.92247000	4.75475700	0.16635500
C	4.49179500	3.02724800	0.79288500
C	4.93542100	1.00218900	-1.62383300
C	2.57054100	-2.46595200	-2.18036200
C	1.62521900	-3.68482600	-2.22350300
C	3.39529600	-2.40584600	-3.48245100
C	4.09828100	-0.65032800	2.39964200
C	5.41099500	-0.42305400	3.16809400
C	2.97560700	-1.08284900	3.36790300
C	4.36216300	-3.56320400	-0.79444800
C	5.17983400	-3.67760500	0.32305500
C	2.45378600	1.33805500	-3.64380000
H	1.95218000	-1.56332400	-2.12880000
H	3.81926700	0.31550000	1.96479300
H	5.14743000	3.87167700	0.54594800
H	3.98062100	3.28011500	1.72619500
H	5.13404100	2.16467000	0.98322700
H	5.73853000	1.59404800	-2.07970300
H	5.31967500	0.59338100	-0.68650800
H	4.73088700	0.16158800	-2.28784900
H	2.91633600	0.35070400	-3.67427700
H	1.40331700	1.22779300	-3.92621300
H	2.93307200	1.94632200	-4.42103400
H	0.90437200	4.32706400	-3.28279200
H	-0.01623400	2.85060700	-3.02312200
H	-0.09377200	4.16243600	-1.84044300
H	2.47623100	5.62022500	-0.21911300
H	0.86018600	4.97662500	0.05877800
H	2.15419400	4.68737100	1.23266800
H	4.42328300	-4.31395700	-1.57610900
H	5.87450500	-4.50716300	0.40925900
H	5.73618700	-2.82329500	2.20752600
H	6.23717100	-0.17077000	2.49593100
H	5.28792800	0.39945400	3.87976500

H	5.70622300	-1.30302600	3.74768500
H	2.83999000	-0.34658700	4.16829000
H	2.02043100	-1.21183000	2.84821900
H	3.22461100	-2.04125500	3.83462300
H	2.18938100	-4.61225400	-2.36391300
H	1.05285300	-3.78523400	-1.29851800
H	0.92273600	-3.59817700	-3.05954900
H	4.10532800	-1.57345600	-3.48688400
H	3.97491900	-3.32285600	-3.62592200
H	2.73539300	-2.29874500	-4.34986100
C	-3.18834200	-1.47450400	-2.23167000
C	-1.94710400	-0.55989600	-2.11061900
H	-2.21687100	0.43214400	-2.50035400
H	-1.16129800	-0.94704800	-2.77505300
C	-4.41993100	-0.86494700	-1.52963000
H	-4.15173500	-0.57284900	-0.50502800
H	-4.69572600	0.06624500	-2.04652300
C	-5.64748800	-1.78467300	-1.45026300
H	-5.99799100	-2.03268400	-2.45954300
H	-5.35836100	-2.73819800	-0.98492000
C	-6.80746400	-1.16599400	-0.65905800
H	-6.47142200	-0.93422500	0.36185500
H	-7.09307000	-0.20691200	-1.11092500
C	-8.04873600	-2.07571100	-0.59073000
H	-8.40888100	-2.28483300	-1.60581500
H	-7.75048700	-3.04314900	-0.15931500
C	-9.16334600	-1.48527700	0.22990000
H	-8.93075400	-1.29309600	1.27878100
C	-10.37704000	-1.18044900	-0.22948200
H	-10.65503100	-1.35575800	-1.26640800
H	-11.14101300	-0.75221900	0.41251800
C	-3.45868000	-1.75887900	-3.71888200
H	-3.70049600	-0.83439400	-4.25736100
H	-2.58334000	-2.20697300	-4.20135000
H	-4.29506200	-2.44915800	-3.85373600
H	-2.95949900	-2.43479000	-1.74763100
C	-1.33051800	-0.39957800	-0.69189000
H	-2.13170100	-0.03970800	-0.03684000
C	-0.29074200	0.72808100	-0.74901700
H	0.44774700	0.44087100	-1.57092300
H	-0.76032500	1.65647800	-1.08460100
C	-0.80203900	-1.74101200	-0.11793400
H	-0.71635600	-2.46938200	-0.93182900
H	0.21591100	-1.61498100	0.26931800

C	-1.67945800	-2.34262200	0.99317400
H	-2.70257000	-2.48376300	0.62154200
H	-1.76193200	-1.62720300	1.82529000
C	-1.14302200	-3.67624500	1.52721400
H	-1.07804700	-4.39823400	0.70138400
H	-0.11703900	-3.54196300	1.89592100
C	-2.00722900	-4.27159500	2.65511200
H	-3.03425100	-4.39546400	2.28044200
H	-2.06320100	-3.56298400	3.49143900
C	-1.49163700	-5.59616700	3.14927800
H	-1.44868500	-6.39576300	2.40814500
C	-1.08830100	-5.84521000	4.39514200
H	-1.11793500	-5.08049000	5.16834700
H	-0.72400100	-6.82356000	4.69350900
C	1.24195600	1.76973100	1.71329600
C	-0.03879900	1.22880800	1.46764000
H	1.94658700	1.14274400	2.25425200
H	1.32938500	2.83269200	1.90124400
H	-0.15267500	0.16714900	1.66904300
C	-1.32319900	2.01455400	1.63777400
H	-2.13944800	1.53557400	1.09004200
H	-1.57299100	1.86155600	2.70018400
C	-1.32085700	3.51699000	1.34598400
H	-0.55279900	4.01919000	1.94578200
H	-1.06001900	3.68793400	0.29334600
C	-2.68370500	4.16134100	1.63904100
H	-3.45954400	3.66485200	1.04020000
H	-2.95227400	3.99176200	2.68943500
C	-2.70892400	5.67443300	1.35286900
H	-1.95479200	6.17953100	1.96972800
H	-2.41934700	5.83831700	0.30321500
C	-4.05928100	6.29209400	1.60004000
C	-4.31035100	7.24546400	2.49679900
H	-4.87779000	5.90575700	0.99101600
H	-5.30772400	7.65159500	2.63424700
H	-3.52506300	7.66125600	3.12421000

**3P<sub>12</sub>, -1968.6978635**

Ti	-2.23835300	-1.07096400	-0.56425900
O	-3.00534400	0.36708200	0.15641800
C	-2.03382900	-2.55181700	-2.43080600
C	-2.62467200	-3.31700300	-1.38616300
C	-3.86470300	-2.69232700	-1.03584000
C	-4.07126700	-1.57613500	-1.91357600
C	-2.93017800	-1.47759000	-2.76104400

C	-3.84376300	1.39381100	0.51705700
C	-3.85962000	2.57672200	-0.25404200
C	-5.48627600	2.28192800	2.02905900
C	-4.64685400	1.22379200	1.67012600
C	-0.76922600	-2.89187100	-3.17100200
C	-2.11774300	-4.62166100	-0.84803100
C	-4.84671400	-3.20427200	-0.02032100
C	-5.30718700	-0.72468300	-1.96743500
C	-2.96023500	2.78684600	-1.46561700
C	-1.86482600	3.82983700	-1.16353500
C	-3.75450600	3.18874000	-2.72351900
C	-4.55948300	-0.03770600	2.51990200
C	-5.90365400	-0.45908700	3.13753800
C	-3.48463000	0.12759500	3.61573400
C	-4.71618400	3.60219100	0.16317200
C	-5.52522300	3.46085400	1.28642400
C	-2.72149700	-0.48533500	-3.87223500
H	-2.45793400	1.83672500	-1.68351400
H	-4.23668100	-0.85479400	1.86543500
H	-5.49655200	-3.96123200	-0.47696200
H	-4.34848700	-3.67320300	0.83183400
H	-5.49332300	-2.41032000	0.35990800
H	-6.07562500	-1.22044700	-2.57268100
H	-5.73224100	-0.54994600	-0.97624000
H	-5.11310600	0.25004500	-2.41808300
H	-3.31033900	0.42246800	-3.72978700
H	-1.67173800	-0.19497000	-3.97750700
H	-3.02682000	-0.92567500	-4.82949800
H	-1.00355500	-3.50648000	-4.04886400
H	-0.24613500	-2.00287200	-3.53320600
H	-0.07369400	-3.46663400	-2.55424800
H	-2.48504600	-5.44680700	-1.47046500
H	-1.02590600	-4.67677700	-0.85239900
H	-2.46311400	-4.80714700	0.17152000
H	-4.74767200	4.52842700	-0.40211200
H	-6.18394300	4.26964000	1.58681000
H	-6.11828800	2.18598200	2.90517100
H	-6.69145900	-0.53729300	2.38149400
H	-5.80120900	-1.43358900	3.62533800
H	-6.24319300	0.24567300	3.90280100
H	-3.37910400	-0.79406700	4.19871800
H	-2.50914000	0.37879800	3.18705000
H	-3.75857400	0.93174600	4.30650700
H	-2.30529300	4.81102900	-0.95974400

H	-1.26983300	3.54629000	-0.29091700
H	-1.19047800	3.93990600	-2.01973600
H	-4.55003300	2.47211800	-2.95186900
H	-4.22569500	4.16900700	-2.60357600
H	-3.08945300	3.25268900	-3.59110900
C	3.36293700	0.92221700	-2.35207400
C	2.06220600	0.16183400	-2.01026100
H	2.19396600	-0.88601900	-2.31850300
H	1.25280100	0.56546000	-2.63861100
C	4.59411700	0.28199900	-1.67670200
H	4.39699000	0.15159400	-0.60425900
H	4.73247000	-0.73102300	-2.08305700
C	5.90326200	1.07164100	-1.82334700
H	6.18050000	1.14949700	-2.88175800
H	5.74782900	2.10224600	-1.47236600
C	7.06943900	0.44368200	-1.04867200
H	6.80856500	0.38117300	0.01748200
H	7.22326400	-0.58989700	-1.38573100
C	8.38972000	1.22203900	-1.20360900
H	8.67320800	1.26042300	-2.26289600
H	8.22188800	2.26253000	-0.88695400
C	9.51601100	0.63109100	-0.39949800
H	9.36296800	0.59975900	0.68065800
C	10.65033400	0.14758300	-0.90598100
H	10.84789000	0.15897000	-1.97560400
H	11.42722800	-0.27058500	-0.27291900
C	3.51935300	0.99218200	-3.88053000
H	3.63043600	-0.01123700	-4.30978900
H	2.64540600	1.46038100	-4.34682600
H	4.39602900	1.57547500	-4.17240000
H	3.26782300	1.95341100	-1.98340400
C	1.57767600	0.19424800	-0.54249500
H	2.36482900	-0.23070200	0.09070400
C	0.36597800	-0.76697000	-0.40193100
H	-0.39106500	-0.27855700	-1.08610100
H	0.61026400	-1.72175500	-0.88008000
C	1.25665000	1.62757400	-0.04276500
H	1.05579100	2.27091100	-0.90976400
H	0.32737200	1.62607300	0.54116900
C	2.35096500	2.27093900	0.82467000
H	3.29973200	2.29511300	0.27476300
H	2.52895400	1.63923700	1.70663000
C	1.99430500	3.69026000	1.28328800
H	1.82864600	4.32659600	0.40275400

H	1.04300900	3.67428900	1.83239200
C	3.07530300	4.32905200	2.17592600
H	4.02856800	4.32707600	1.62648900
H	3.22849900	3.71118600	3.06976600
C	2.73741200	5.73700200	2.58599100
H	2.62344200	6.45460900	1.77191300
C	2.56471800	6.14929400	3.84179300
H	2.67209500	5.47070600	4.68520600
H	2.31975500	7.18075100	4.07648400
C	-1.38940200	-2.01859700	1.04027900
C	-0.17650200	-1.03866800	1.03592300
H	-1.97072000	-1.91465900	1.96082800
H	-1.07724000	-3.05556900	0.92091100
H	-0.50961600	-0.08437100	1.45919600
C	0.94517600	-1.56216900	1.98541400
H	1.66363700	-0.74930500	2.14695900
H	0.47389100	-1.74526600	2.95808700
C	1.70172200	-2.82291600	1.54667900
H	0.99703700	-3.64219800	1.35255700
H	2.23224000	-2.64115700	0.60198200
C	2.71746700	-3.28419500	2.60260000
H	3.42782700	-2.47085200	2.80461200
H	2.19960700	-3.48017400	3.55012400
C	3.49407400	-4.54656700	2.18323300
H	2.79088000	-5.36998100	2.00364300
H	3.99647400	-4.34727100	1.22444700
C	4.51560900	-4.96911800	3.20460100
C	4.51212300	-6.13275000	3.85451800
H	5.30368200	-4.24499000	3.41635500
H	5.27556100	-6.38146700	4.58530100
H	3.74747000	-6.88526200	3.67451100

**3C<sub>cyt</sub>, -1655.798526**

Ti	-1.10118800	-0.51471300	-0.19281800
O	-2.68091400	0.18830600	0.26120800
C	0.14473700	-0.52675400	-2.26951600
C	0.32636100	-1.82692000	-1.72792700
C	-0.95955500	-2.46228100	-1.64962300
C	-1.93516700	-1.55305300	-2.14972500
C	-1.26141100	-0.34120400	-2.50099100
C	-3.97414200	0.65820000	0.28824300
C	-4.20352200	2.02335700	-0.00428200
C	-6.32367300	0.28535300	0.64390500
C	-5.02283400	-0.22850400	0.63041700
C	1.23827800	0.38456100	-2.73881800

C	1.65941600	-2.48315600	-1.49403300
C	-1.21345600	-3.89732200	-1.27432100
C	-3.39225800	-1.83434700	-2.38076600
C	-3.05965600	2.99545300	-0.26261800
C	-2.65338900	3.69740300	1.05114900
C	-3.36790500	4.03177600	-1.35743700
C	-4.75485800	-1.66627900	1.05575000
C	-5.82145700	-2.66524300	0.57417800
C	-4.59475500	-1.74614200	2.58946100
C	-5.52764900	2.47398400	0.02414800
C	-6.58056500	1.61904600	0.33742700
C	-1.89473300	0.84525400	-3.17064500
H	-2.19876600	2.41300100	-0.60143900
H	-3.80472700	-1.96995300	0.60256300
H	-1.10360900	-4.53792300	-2.15775600
H	-0.50993900	-4.27082600	-0.52568600
H	-2.22568200	-4.05313000	-0.89226400
H	-3.56011500	-2.06851700	-3.43918800
H	-3.74276000	-2.69031400	-1.80097700
H	-4.02429000	-0.97896400	-2.13078000
H	-2.93211800	0.98384400	-2.85819300
H	-1.35283400	1.77156200	-2.96591100
H	-1.89535200	0.70280200	-4.25861000
H	1.51602800	0.12084200	-3.76724100
H	0.92951300	1.43215300	-2.74928800
H	2.13814600	0.30215700	-2.12655600
H	2.10294700	-2.76938400	-2.45582000
H	2.37340400	-1.81861600	-1.00033300
H	1.57655000	-3.39799700	-0.90305100
H	-5.73713300	3.51512000	-0.19671300
H	-7.59929300	1.99355000	0.35254900
H	-7.14986400	-0.36789500	0.90299600
H	-5.98849200	-2.59369000	-0.50477300
H	-5.50902300	-3.68879600	0.80586900
H	-6.78290900	-2.50746200	1.07188400
H	-4.31923400	-2.75911100	2.90350000
H	-3.83293800	-1.04909700	2.95283100
H	-5.53521600	-1.48598700	3.08569300
H	-3.47745400	4.30846200	1.43407300
H	-2.39022000	2.97333900	1.82893700
H	-1.79284800	4.35515900	0.88864400
H	-3.69997200	3.55686500	-2.28593300
H	-4.14356200	4.73891500	-1.04789700
H	-2.47115200	4.62000700	-1.57744600



C	3.89577700	2.34735200	0.68743600
C	2.39548800	2.25786500	0.32887100
H	2.30515100	2.37377200	-0.75944200
H	1.88162800	3.12611900	0.76437700
C	4.72351700	1.25002700	-0.01369800
H	4.27225700	0.26780400	0.18642900
H	4.65391000	1.39785100	-1.10215600
C	6.20344000	1.18062200	0.39156300
H	6.71148300	2.11297000	0.11748500
H	6.27872700	1.10378800	1.48609100
C	6.94560900	0.00169900	-0.25144600
H	6.45831300	-0.94035600	0.04014100
H	6.86027500	0.06290300	-1.34454200
C	8.43689800	-0.06009200	0.12986200
H	8.93737700	0.86165000	-0.19178800
H	8.51689000	-0.09250000	1.22689400
C	9.14346500	-1.25148900	-0.45811000
H	8.76504400	-2.22797800	-0.15028000
C	10.16435700	-1.19479000	-1.31345400
H	10.57696200	-0.24517500	-1.64679200
H	10.63230200	-2.09242800	-1.70653800
C	4.40689400	3.75692000	0.34176900
H	4.34580500	3.94251800	-0.73766500
H	3.81126900	4.52550600	0.84532700
H	5.44739700	3.89874700	0.64494600
H	4.00628500	2.21981900	1.77351600
C	1.59443400	0.99601900	0.75673500
H	2.07333900	0.11763000	0.30299400
C	0.14388800	1.12587600	0.22798400
H	-0.48218000	1.61380100	0.98971600
H	0.09820600	1.77295300	-0.65621700
C	1.57695700	0.81613300	2.30035700
H	1.63584100	1.81046700	2.76070700
H	0.59922200	0.42409400	2.60733200
C	2.66370900	-0.07605200	2.92210300
H	3.66049700	0.26609600	2.62738400
H	2.61651300	0.04206200	4.01244100
C	2.55601500	-1.57684000	2.60309500
H	3.35011600	-2.10063600	3.14359400
H	2.74956400	-1.76097700	1.53923800
C	-1.02145900	-1.99281500	1.75044000
C	0.24798300	-2.44675800	1.86740000
H	-1.48657600	-1.39067000	2.52606500
H	-1.69285400	-2.47210600	1.03113700

H	0.62562100	-3.11782400	1.09708400
C	1.18612400	-2.19589900	3.00219200
H	0.69840800	-1.59898900	3.77952000
H	1.36414000	-3.18952100	3.43921800
<b>3TS<sub>cyc</sub>, -1655.7872801, <i>i</i>175.80</b>			
Ti	-1.12403900	-0.80154400	-0.07772300
O	-2.59148000	0.19803800	0.14334400
C	0.39243400	-1.86848200	-1.65027800
C	-0.34832100	-2.92682200	-1.06563900
C	-1.73564900	-2.72769000	-1.36956100
C	-1.84597000	-1.55773000	-2.18258900
C	-0.53542300	-1.01161100	-2.34126700
C	-3.75645600	0.91155900	-0.00240000
C	-3.69644600	2.20295000	-0.57384900
C	-6.13327900	1.09622800	0.30043900
C	-4.96809800	0.33491800	0.44097400
C	1.89210500	-1.77262300	-1.68957900
C	0.24378800	-4.12684100	-0.38276700
C	-2.85291800	-3.67575000	-1.03654700
C	-3.09912900	-1.04529300	-2.83289300
C	-2.37766700	2.83395200	-1.00201100
C	-1.83842900	3.76703700	0.10228300
C	-2.46739900	3.57784200	-2.34662200
C	-5.00720500	-1.03479600	1.10631600
C	-6.21037600	-1.89046600	0.67194800
C	-4.96881100	-0.88914100	2.64251600
C	-4.89643300	2.91291600	-0.68913300
C	-6.10473600	2.37119500	-0.25878300
C	-0.17418700	0.15014100	-3.22690700
H	-1.64989500	2.02533700	-1.13131300
H	-4.10332200	-1.57311100	0.80308600
H	-2.88670900	-4.48980900	-1.77113200
H	-2.73141700	-4.13905700	-0.05312100
H	-3.82634500	-3.18168900	-1.05471500
H	-3.23512300	-1.52180700	-3.81136700
H	-3.98887200	-1.25747300	-2.23649900
H	-3.06485700	0.03414600	-2.99520500
H	-0.96198600	0.90643500	-3.25720400
H	0.75083700	0.64030400	-2.91324600
H	-0.02128700	-0.19974000	-4.25529000
H	2.28581500	-2.38477900	-2.51045300
H	2.24000500	-0.75161500	-1.85711500
H	2.35415600	-2.13622900	-0.76776900
H	0.60637500	-4.83723700	-1.13581900

H	1.09990400	-3.87257300	0.24911100
H	-0.48525100	-4.66465000	0.22809900
H	-4.88445800	3.90862500	-1.12025200
H	-7.02242600	2.94252400	-0.35707300
H	-7.07946500	0.68507500	0.63648600
H	-6.27374200	-1.97738500	-0.41764600
H	-6.12598500	-2.89853800	1.09077600
H	-7.15880100	-1.47585600	1.02679000
H	-4.93837800	-1.87110600	3.12793900
H	-4.09719800	-0.31240900	2.97032500
H	-5.85980800	-0.36545000	3.00401600
H	-2.52208200	4.60595500	0.26863300
H	-1.73024700	3.24030500	1.05637400
H	-0.86271500	4.17968300	-0.17762700
H	-2.87566000	2.93903000	-3.13655600
H	-3.10054800	4.46778500	-2.28111500
H	-1.47334900	3.91476200	-2.65845900
C	3.83897400	2.18159500	0.08838500
C	2.33224300	1.84159000	-0.00021900
H	2.15129800	1.38362100	-0.98264400
H	1.74842200	2.77184500	0.01190800
C	4.72010800	0.96420400	-0.26352000
H	4.37565400	0.08580900	0.30006000
H	4.57473800	0.71831300	-1.32637900
C	6.22020700	1.14290900	0.01325100
H	6.61895100	1.96568300	-0.59259700
H	6.36266600	1.43902400	1.06236800
C	7.03556700	-0.12534600	-0.27115900
H	6.65662000	-0.95042000	0.34925000
H	6.88664400	-0.43474900	-1.31421200
C	8.54403400	0.05152700	-0.01353300
H	8.93577700	0.85149800	-0.65407300
H	8.68507600	0.38541200	1.02541300
C	9.32917600	-1.21142900	-0.24369300
H	9.06328800	-2.05857900	0.39102900
C	10.29282000	-1.36184300	-1.15240500
H	10.59383900	-0.54538700	-1.80507600
H	10.82346000	-2.30147800	-1.27359600
C	4.14174800	3.38926900	-0.81416700
H	3.92450700	3.15823500	-1.86436600
H	3.53616200	4.25648100	-0.53084600
H	5.19108200	3.68812000	-0.75209400
H	4.07007400	2.47426300	1.12277500
C	1.77637800	0.91596000	1.12300300

H	2.45310300	0.05623300	1.20530600
C	0.38010400	0.41549100	0.73132000
H	-0.38782100	1.10088000	1.11089700
H	0.32868700	0.43212100	-0.40096700
C	1.73374600	1.68500800	2.47384800
H	2.38675600	2.56034400	2.40569400
H	0.72555500	2.09742200	2.60529800
C	2.14234800	0.91186200	3.73777000
H	3.23585200	0.84604500	3.78793800
H	1.84188800	1.51357000	4.60401400
C	1.58094000	-0.51220700	3.88779300
H	1.69872500	-0.81194300	4.93388300
H	2.20480600	-1.21351800	3.31984700
C	-1.29401700	-2.04291500	1.78018000
C	-0.07115500	-1.50396300	2.18283800
H	-2.19616300	-1.72412200	2.29727000
H	-1.30901700	-3.04952600	1.38334000
H	0.82736400	-2.00020200	1.82022400
C	0.10670400	-0.72276500	3.47224300
H	-0.46082700	0.21367700	3.45745000
H	-0.39154700	-1.34112600	4.22987300

**3P<sub>eyes</sub> -1655.8202074**

Ti	-1.29464100	-0.91216200	-0.27677300
O	-2.55762500	0.30053700	0.04117400
C	0.19004500	-1.96924700	-1.82901500
C	-0.75635400	-2.96132300	-1.43849900
C	-2.05586300	-2.49931800	-1.82081400
C	-1.90684100	-1.24225700	-2.49684300
C	-0.52097200	-0.90917700	-2.48826700
C	-3.58125000	1.21416100	-0.00701300
C	-3.30034900	2.53206400	-0.42909700
C	-5.89299000	1.75114100	0.35089400
C	-4.87135900	0.79716200	0.39255400
C	1.68576400	-2.08846700	-1.71620600
C	-0.43293300	-4.31073600	-0.87008900
C	-3.34079300	-3.25843100	-1.64838000
C	-3.00885800	-0.46151500	-3.15445500
C	-1.89323900	2.98554300	-0.79661700
C	-1.27335100	3.81763900	0.34523600
C	-1.84316800	3.75901300	-2.12709700
C	-5.13361900	-0.61376300	0.90402800
C	-6.45642100	-1.21006900	0.39159000
C	-5.07873700	-0.64632900	2.44619400

C	-4.36395100	3.44086200	-0.44267800
C	-5.64794300	3.05917700	-0.06210600
C	0.10841500	0.29637800	-3.13069200
H	-1.27350600	2.08930500	-0.92107200
H	-4.32572600	-1.25564400	0.53654100
H	-3.47061100	-3.96775100	-2.47521900
H	-3.35594700	-3.83368400	-0.71916900
H	-4.20946200	-2.59667700	-1.65020100
H	-3.17765800	-0.83626700	-4.17109200
H	-3.95324500	-0.54559400	-2.61199800
H	-2.76838800	0.60073000	-3.23168500
H	-0.58829800	1.13362200	-3.20700400
H	0.99360800	0.64145800	-2.58859500
H	0.43392600	0.05011500	-4.14896700
H	2.08789000	-2.59275700	-2.60342500
H	2.17884600	-1.11512800	-1.65142000
H	1.98733500	-2.67980400	-0.84794000
H	-0.13891900	-4.99237600	-1.67756100
H	0.39774600	-4.27692500	-0.15981700
H	-1.29213900	-4.75914300	-0.36704200
H	-4.18346400	4.46512000	-0.75323200
H	-6.45753300	3.78195500	-0.08326300
H	-6.89650900	1.46821600	0.65087800
H	-6.52505900	-1.16582500	-0.70026200
H	-6.53883500	-2.25806900	0.69699600
H	-7.32740000	-0.68873100	0.80037000
H	-5.21404300	-1.66790200	2.81751000
H	-4.12242900	-0.26731100	2.82144900
H	-5.87082200	-0.02439200	2.87609900
H	-1.84459100	4.73664800	0.51134200
H	-1.26606100	3.26069200	1.28792400
H	-0.24353600	4.10212300	0.10387800
H	-2.29272100	3.18741600	-2.94578500
H	-2.37595900	4.71250400	-2.06232000
H	-0.80640900	3.98687500	-2.39573600
C	3.71469000	1.95921000	0.95918000
C	2.23032000	1.52637800	0.95865700
H	1.92846100	1.37665400	-0.08999000
H	1.61050500	2.35270500	1.33304100
C	4.57696600	1.01043100	0.09893800
H	4.34874700	-0.03213500	0.36182200
H	4.28345800	1.12889100	-0.95564600
C	6.09449200	1.20763000	0.22628400
H	6.37058200	2.21929200	-0.09539800

H	6.38156900	1.13435300	1.28484200
C	6.90016800	0.18808500	-0.58958500
H	6.64459500	-0.82881500	-0.25840800
H	6.60882200	0.24704100	-1.64681700
C	8.42349600	0.38933500	-0.47988500
H	8.68970700	1.39116100	-0.83937600
H	8.70568000	0.35317600	0.58300800
C	9.20690100	-0.64617800	-1.24044200
H	9.06586200	-1.67954200	-0.91879300
C	10.02992700	-0.39237600	-2.25791200
H	10.20429700	0.62151200	-2.61125700
H	10.56754400	-1.18456100	-2.77036700
C	3.82933700	3.41934600	0.49243400
H	3.45849400	3.53243500	-0.53407800
H	3.24455700	4.08648800	1.13444900
H	4.86367800	3.77167100	0.50987500
H	4.08931200	1.90937900	1.99198400
C	1.89797700	0.26285400	1.78664200
H	2.64509500	-0.50945000	1.56411600
C	0.50941300	-0.29281000	1.36325700
H	-0.25056600	0.43603200	1.68261400
H	0.58763900	-0.24318800	0.24018800
C	1.91177700	0.57402800	3.30263800
H	2.61165600	1.39516500	3.48838600
H	0.92546700	0.96935700	3.58024400
C	2.29119200	-0.59055800	4.23356300
H	3.38250600	-0.69364100	4.25864200
H	1.99426000	-0.31409100	5.25202700
C	1.68564100	-1.96189700	3.88114900
H	1.72617300	-2.59493000	4.77430200
H	2.31523100	-2.46992200	3.13876400
C	-1.32846900	-2.12745100	1.37196400
C	0.11145800	-1.73039700	1.82429300
H	-2.07738600	-1.68228800	2.03911400
H	-1.45635900	-3.20830800	1.35598300
H	0.81887100	-2.41974000	1.34617700
C	0.23762800	-1.94307100	3.35822500
H	-0.36634600	-1.19382500	3.88610800
H	-0.22796400	-2.91082900	3.57169700

**Table S5** Optimized Cartesian coordinates (Å) and zero-point energy corrected energy (a.u.) of **4C**, **4TS**, and **4P**, as well as the imaginary frequency (cm<sup>-1</sup>) of **4TS**

Atom	x	y	z
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**4C, -1655.8045789**

O	1.93191900	-0.11415300	-0.46225600
C	0.02963800	-0.09052100	3.14546600
C	1.14290600	0.73780700	2.80823000
C	2.25627500	-0.11794900	2.50537800
C	1.81555700	-1.46727000	2.62625300
C	0.43363600	-1.44971900	3.00382500
C	-1.28692100	0.34414000	3.72368600
C	1.20871800	2.23423700	2.91592400
C	3.66717800	0.32800800	2.24962400
C	2.68678700	-2.68748800	2.52678800
C	-0.39455800	-2.63597700	3.41420900
C	3.08421700	0.14509300	-1.17197500
C	3.41209300	1.48856800	-1.47146100
C	4.58435500	1.72780400	-2.19662500
C	5.40454400	0.68814400	-2.62243700
C	5.05419000	-0.62545500	-2.32756200
C	3.89850900	-0.93115600	-1.60032500
C	2.52802900	2.66217600	-1.07473200
C	3.54367800	-2.39172400	-1.35497900
H	-1.35716400	0.00202600	4.76324000
H	-2.14550300	-0.07592900	3.19107400
H	-1.39272600	1.42897800	3.73390700
H	1.56833900	2.52050700	3.91221800
H	0.23399000	2.70211200	2.77026800
H	1.89933900	2.66578000	2.18814800
H	4.21152300	-0.37085600	1.61109400
H	4.21152900	0.40267900	3.19901200
H	3.70713000	1.30839800	1.77156400
H	3.15927700	-2.88455300	3.49719500
H	3.48952900	-2.56494800	1.79774500
H	2.12146400	-3.58563000	2.26377600
H	-1.45236800	-2.50890100	3.16635800
H	-0.33553500	-2.76923400	4.50163500
H	-0.04578500	-3.56694900	2.96159400
Ti	0.70128000	-0.44774600	0.80298300
C	3.30016700	3.75565600	-0.31130500
H	3.82336700	3.35288800	0.56226600
H	4.04930600	4.24126600	-0.94418100
H	2.61252300	4.53574400	0.03198100
C	1.83459800	3.25769300	-2.31735700
H	1.22486200	2.50929300	-2.83313900
H	1.18622200	4.09362900	-2.03580200
H	2.57179500	3.63588200	-3.03292100

H	4.85478600	2.75117300	-2.43710400
H	6.30758400	0.89944000	-3.18633500
H	5.68966000	-1.43482300	-2.67299900
C	-3.27784500	1.56596500	0.48955800
C	-0.91806800	0.70374200	0.33174000
H	-0.77083400	0.62778100	-0.76077800
H	-1.45689800	-0.22623400	0.64945500
H	-3.41092000	1.01888600	-0.45439100
C	-3.30244700	4.12649200	-1.47019500
C	-1.95294500	3.38877900	-1.51123600
C	-1.32298300	3.17988600	-0.12051800
C	-4.49002000	3.35269400	-0.88057700
C	-1.77797200	1.92670100	0.66723700
C	-4.29273300	2.73345600	0.51903800
H	-3.16154900	5.05716300	-0.90291900
H	-2.05659100	2.43120100	-2.04193200
H	-1.54011500	4.06925100	0.48387700
H	-4.77488000	2.54335800	-1.56935300
H	-3.56979200	4.43483400	-2.48822800
H	-1.26241900	3.98691000	-2.11629900
H	-0.23232200	3.14602900	-0.20843100
H	-5.35096200	4.03170400	-0.84699100
H	-1.63875500	2.15491100	1.72886900
H	-3.53142200	0.84930600	1.28269700
H	1.74705000	2.28283900	-0.40924800
H	2.70863600	-2.41633600	-0.64789200
C	4.70404900	-3.18725900	-0.72586700
H	4.37782900	-4.19977200	-0.46599500
H	5.54464300	-3.28703900	-1.41887100
H	5.08551900	-2.70543900	0.17985200
C	3.07909400	-3.07169800	-2.66076600
H	3.89873200	-3.12059100	-3.38450500
H	2.74225600	-4.09656600	-2.47045000
H	2.26305300	-2.52025800	-3.13954700
C	-5.64304700	2.24252700	1.06729600
H	-6.05875500	1.44886000	0.43425800
H	-5.54184800	1.84086800	2.08137100
H	-6.37621900	3.05433400	1.10110800
H	-3.91948900	3.51172300	1.20151700
C	-0.12324800	-2.76835500	0.08127200
C	-0.38837400	-2.37545100	-1.18734200
H	0.88633700	-3.06544200	0.35803700
H	-0.91968700	-3.03464700	0.76765700
H	0.45586100	-2.20609500	-1.85417300



C	-1.73815400	-2.18387900	-1.80671200
H	-1.80484500	-1.14920300	-2.17541600
H	-1.73532900	-2.79188900	-2.72504000
C	-2.96265300	-2.53278400	-0.95581200
H	-2.88353900	-3.57255800	-0.61215300
H	-2.98311300	-1.90593300	-0.05382900
C	-4.27923700	-2.34977400	-1.72311800
H	-4.35894200	-1.30951400	-2.06825100
H	-4.26865800	-2.97251900	-2.62664700
C	-5.51951600	-2.70495300	-0.88217600
H	-5.51328600	-2.08801300	0.02952400
H	-5.45573700	-3.75010000	-0.55427900
C	-6.80972200	-2.48619900	-1.62611500
H	-7.00545600	-1.46249500	-1.94885000
C	-7.69614600	-3.43857600	-1.91487500
H	-8.61051900	-3.22183100	-2.45855100
H	-7.54348200	-4.47208800	-1.61211600
<b>4TS, -1655.7883053, i197.74</b>			
O	1.93831200	-0.24591200	-0.38126600
C	-0.60990200	-1.65560100	2.40868100
C	0.71317100	-1.14315900	2.66639600
C	1.65137100	-1.98257400	1.99407400
C	0.91292200	-2.97093100	1.27327700
C	-0.47865500	-2.78826500	1.56748400
C	-1.87419800	-1.19269100	3.08071200
C	1.05000500	-0.03675300	3.62911600
C	3.14635300	-1.90195700	2.10000000
C	1.48939600	-4.12636700	0.50559300
C	-1.56589700	-3.75986500	1.21512100
C	3.24937000	0.05592300	-0.66921600
C	3.83917500	1.19587100	-0.07720500
C	5.17000500	1.48098100	-0.40440400
C	5.89289800	0.67600300	-1.27864400
C	5.28624800	-0.43802400	-1.85342200
C	3.95938100	-0.77503900	-1.56853700
C	3.06734400	2.13613100	0.83982900
C	3.29071100	-1.95572500	-2.26033100
H	-2.01265800	-1.72748400	4.02843000
H	-2.76068800	-1.38161800	2.47048600
H	-1.85261700	-0.12624400	3.32027100
H	1.16003800	-0.44323600	4.64215900
H	0.26929600	0.72722200	3.67283900
H	1.98961800	0.45837800	3.37530500
H	3.64461800	-2.22652000	1.18433900

H	3.49469000	-2.54946600	2.91404000
H	3.48956100	-0.88881200	2.31757900
H	1.51277800	-5.02409500	1.13597500
H	2.51357500	-3.93119700	0.18236900
H	0.89648900	-4.37178600	-0.38031300
H	-2.55250600	-3.29477700	1.19467700
H	-1.59691300	-4.55476000	1.97116100
H	-1.39475300	-4.25119200	0.25362700
Ti	0.40304800	-0.79537400	0.37569900
C	3.84572300	2.50915500	2.11544200
H	4.18709900	1.62127500	2.65768200
H	4.72814000	3.11629600	1.89243300
H	3.21215200	3.09787200	2.78696700
C	2.64251400	3.40565700	0.07285700
H	2.03529300	3.16085200	-0.80525500
H	2.06546200	4.07706100	0.71776200
H	3.52000700	3.95634100	-0.28122000
H	5.64680200	2.35284800	0.03191600
H	6.92414400	0.91764700	-1.51595800
H	5.85503300	-1.05606000	-2.53953700
C	-1.75713200	2.85867500	-1.13135200
C	-0.81756600	0.92003500	0.17706700
H	-0.76412900	0.56054300	1.23730600
H	0.13819000	1.37903000	-0.11190100
H	-0.70704500	3.17845100	-1.17817200
C	-1.91885300	5.25406300	1.03846500
C	-1.26368100	3.99529400	1.63181000
C	-2.11301500	2.72421400	1.44657100
C	-2.00480600	5.32499500	-0.49291800
C	-1.94960300	1.94630200	0.10351900
C	-2.64864700	4.12188000	-1.21611800
H	-2.92960400	5.33951500	1.46124800
H	-0.25544900	3.85553900	1.21973500
H	-3.16859600	3.00457100	1.54375500
H	-0.99639800	5.46638300	-0.90865200
H	-1.37270700	6.13760100	1.39003000
H	-1.12792400	4.16113200	2.70704100
H	-1.92627400	2.02783300	2.27364700
H	-2.56439200	6.23106100	-0.75510600
H	-2.88872100	1.39195500	-0.01615800
H	-1.91512800	2.25315700	-2.03171600
H	2.15515600	1.62094200	1.15952000
H	2.49346100	-2.31068700	-1.59948700
C	4.23179900	-3.14802900	-2.50327800

H	3.66163700	-4.00396900	-2.87825200
H	4.99631700	-2.92242000	-3.25295900
H	4.74388300	-3.45515000	-1.58578000
C	2.64043400	-1.50138400	-3.58530900
H	3.40415700	-1.14495000	-4.28404700
H	2.10769400	-2.32986100	-4.06555900
H	1.93348600	-0.67986600	-3.42769300
C	-2.90978700	4.48037900	-2.68864500
H	-1.97049200	4.69244800	-3.21363200
H	-3.41027000	3.66240000	-3.21810600
H	-3.54257600	5.36899200	-2.77306000
H	-3.62096300	3.90546800	-0.74892200
C	-0.46634900	-1.78509200	-1.38224600
C	-1.17395900	-0.59359800	-1.64529200
H	0.46144100	-1.94246400	-1.92549600
H	-1.03638000	-2.68080400	-1.16634300
H	-0.64570300	0.16431400	-2.21922000
C	-2.67552100	-0.54898200	-1.79974400
H	-3.02936400	0.48367000	-1.79338900
H	-2.83593500	-0.89293900	-2.83472200
C	-3.53227200	-1.39860500	-0.85739200
H	-3.25196400	-2.45476500	-0.94053100
H	-3.33129300	-1.10038400	0.18094800
C	-5.03285100	-1.25673300	-1.14951100
H	-5.32490200	-0.20122300	-1.06107000
H	-5.23362300	-1.54319400	-2.18958200
C	-5.91249300	-2.10905100	-0.21584000
H	-5.69024200	-1.83151000	0.82638800
H	-5.64613900	-3.16831500	-0.32315800
C	-7.38424300	-1.93037900	-0.47684200
H	-7.77301200	-0.92070800	-0.33698400
C	-8.21373400	-2.89789500	-0.86664800
H	-9.26788800	-2.70892700	-1.04445300
H	-7.87047500	-3.91903500	-1.01716200
<b>4P, -1655.8181861</b>			
O	1.72360000	-0.51981800	-0.44927000
C	0.09838600	-0.87387600	3.18506700
C	1.49031500	-0.61358200	2.94075800
C	2.04407700	-1.75029900	2.28391900
C	0.98576900	-2.70422200	2.09896400
C	-0.20353600	-2.17406300	2.69173400
C	-0.82798500	0.01444200	3.96943600
C	2.23203000	0.61364200	3.39423400
C	3.48703600	-1.96280500	1.92556400

C	1.13627800	-4.07981000	1.51430000
C	-1.49875400	-2.90768700	2.87520800
C	2.86129800	-0.48366300	-1.21944900
C	3.72763000	0.62673000	-1.11838000
C	4.86362900	0.63254900	-1.93611600
C	5.13548700	-0.41656100	-2.80861700
C	4.26229100	-1.49990800	-2.88693800
C	3.10708400	-1.56238200	-2.10269100
C	3.44393600	1.81411800	-0.20787800
C	2.12760700	-2.72108000	-2.23905500
H	-0.70852300	-0.17719000	5.04293200
H	-1.87754500	-0.16804900	3.72621900
H	-0.62146100	1.07602400	3.80915800
H	2.47666000	0.52972800	4.46036400
H	1.63916900	1.52621000	3.27649700
H	3.17032500	0.74916200	2.85460200
H	3.60269800	-2.55443400	1.01457400
H	3.99695800	-2.50018000	2.73415000
H	4.01524100	-1.01995700	1.77237500
H	1.35774600	-4.80226200	2.30975300
H	1.95644700	-4.13064200	0.79483400
H	0.22491300	-4.41429300	1.01280500
H	-2.36564400	-2.24365900	2.81713100
H	-1.52022100	-3.38023500	3.86484300
H	-1.62868200	-3.70118400	2.13619000
Ti	0.50919100	-0.78136900	0.83042900
C	4.63226500	2.14367000	0.71588500
H	4.95318500	1.27192400	1.29551800
H	5.49928700	2.49185400	0.14641600
H	4.36246200	2.94144500	1.41562900
C	3.04151200	3.05221300	-1.03473900
H	2.17296700	2.84592200	-1.66769300
H	2.79830900	3.89376800	-0.37740200
H	3.85990700	3.36778400	-1.68975400
H	5.54563900	1.47571900	-1.88874900
H	6.02505500	-0.39036600	-3.43010100
H	4.48298500	-2.30996600	-3.57347700
C	-1.28925800	2.83847300	-1.00240600
C	-1.61734500	0.77697500	0.47139800
H	-2.21960800	0.36754300	1.28966600
H	-0.60824700	0.99256400	0.93462800
H	-0.22067200	2.65980100	-0.80873300
C	-0.89587700	5.21730100	1.16894600
C	-1.01697900	3.84346800	1.85001300

C	-2.26426400	3.05357400	1.40763400
C	-0.57890400	5.21034800	-0.33348900
C	-2.12992600	2.19887400	0.12291300
C	-1.48756900	4.35546900	-1.24354000
H	-1.83722300	5.75807000	1.33752600
H	-0.09956300	3.25670400	1.68556300
H	-3.08171400	3.76954300	1.26602800
H	0.45759000	4.87551900	-0.48483300
H	-0.12030300	5.80188700	1.67860900
H	-1.07664800	4.00638200	2.93276600
H	-2.59764300	2.39678900	2.22138400
H	-0.60970000	6.24867600	-0.68544700
H	-3.14835100	2.05585700	-0.25985800
H	-1.51072100	2.30423800	-1.93376700
H	2.59246700	1.55387300	0.43184200
H	1.58333200	-2.80634900	-1.29236800
C	2.80866400	-4.07748200	-2.48993700
H	2.06628300	-4.88091300	-2.45014500
H	3.27715200	-4.12608100	-3.47768900
H	3.58070800	-4.28898100	-1.74315300
C	1.09129500	-2.42002800	-3.34302000
H	1.58187200	-2.33002300	-4.31774800
H	0.35220900	-3.22589300	-3.41301600
H	0.56195900	-1.48093400	-3.15235300
C	-1.20837800	4.69229900	-2.71779800
H	-0.17521000	4.44330400	-2.98984600
H	-1.87221300	4.13586600	-3.38784500
H	-1.35282100	5.75904200	-2.91435300
H	-2.53721200	4.61219300	-1.03798700
C	-1.04901300	-1.65271300	-0.17817200
C	-1.55053400	-0.26806500	-0.68300500
H	-0.72436000	-2.28083100	-1.01198700
H	-1.80994500	-2.17586100	0.40012000
H	-0.84663700	0.10262200	-1.43834000
C	-2.92048200	-0.41522700	-1.41492300
H	-3.14022600	0.53045200	-1.92550300
H	-2.77640600	-1.15879400	-2.20751900
C	-4.12987300	-0.81821300	-0.56064600
H	-3.93042400	-1.76443500	-0.04140500
H	-4.31305800	-0.06870000	0.22148300
C	-5.40497100	-0.97511700	-1.40265900
H	-5.61514600	-0.03206300	-1.92565400
H	-5.23952900	-1.72767600	-2.18413900
C	-6.63423700	-1.37938400	-0.56713100

H	-6.78241500	-0.62920700	0.22455000
H	-6.43949500	-2.33403900	-0.06182000
C	-7.88873700	-1.49114100	-1.39114500
H	-8.21051200	-0.57765900	-1.89344000
C	-8.60386700	-2.60470800	-1.54929400
H	-9.50100600	-2.62578000	-2.16039500
H	-8.32204200	-3.53793700	-1.06657900

**Table S6** Optimized Cartesian coordinates (Å) and zero-point energy corrected energy (a.u.) of **7C<sub>12</sub>**, **7TS<sub>12</sub>**, **7P<sub>12</sub>**, **7C<sub>cyc</sub>**, **7TS<sub>cyc</sub>** and **7P<sub>cyc</sub>**, as well as the imaginary frequency (cm<sup>-1</sup>) of **7TS<sub>12</sub>**, and **7TS<sub>cyc</sub>**.

Atom	x	y	z
<b>7C<sub>12</sub>, -1968.7060065</b>			
O	-2.40607300	-0.37180900	-0.16755300
C	-0.07021200	-0.89241100	-3.49467000
C	-1.48523500	-0.61411500	-3.56406100
C	-2.17390200	-1.65630600	-2.87666900
C	-1.19499000	-2.52115200	-2.30483600
C	0.10686100	-2.07307100	-2.73961400
C	1.00619800	-0.14474000	-4.22952300
C	-2.13267000	0.44068100	-4.41823600
C	-3.65877500	-1.86531100	-2.81859500
C	-1.47595000	-3.80810900	-1.57829100
C	1.37245200	-2.86486000	-2.58027400
C	-3.58248900	-0.52256000	0.53018600
C	-4.70203500	0.26933500	0.18248900
C	-5.86429800	0.11628300	0.94661400
C	-5.92812600	-0.78698900	2.00326300
C	-4.81599300	-1.56376000	2.31530500
C	-3.62252800	-1.45502600	1.59400300
C	-4.66864100	1.28993700	-0.94883400
C	-2.40958700	-2.28520200	1.99482100
H	1.13823200	-0.56966200	-5.23239700
H	1.97073400	-0.20300700	-3.72045200
H	0.76277100	0.91187900	-4.36948800
H	-2.36166500	0.02924600	-5.40880100
H	-1.48444600	1.30534800	-4.57724200
H	-3.07348300	0.79889000	-3.99234900
H	-3.99890500	-2.16812000	-1.82514600
H	-3.94718900	-2.65751400	-3.52039000
H	-4.20704500	-0.96555600	-3.10079000
H	-1.55625200	-4.63525000	-2.29493300
H	-2.41606900	-3.76597100	-1.02361500
H	-0.67993800	-4.06790300	-0.87532700
H	2.25578600	-2.28124300	-2.84019300

H	1.34230200	-3.73286500	-3.25059000
H	1.50799400	-3.25188300	-1.56605900
Ti	-0.95265200	-0.49048600	-1.20771800
C	-5.89983400	1.20195400	-1.87144300
H	-6.06103200	0.18487600	-2.24045200
H	-6.81401200	1.51480100	-1.35813100
H	-5.77466600	1.86559200	-2.73362600
C	-4.52139000	2.72369200	-0.39763300
H	-3.63543600	2.82788900	0.23617900
H	-4.44829000	3.45040100	-1.21444700
H	-5.39014900	2.99396000	0.21116000
H	-6.73614200	0.71703100	0.70844200
H	-6.84169700	-0.88622800	2.58094100
H	-4.87334600	-2.26649700	3.14014800
C	4.45764600	1.62848000	0.20036200
C	3.03255500	-0.32173300	-0.62958400
H	3.09859000	-1.34978000	-0.99966100
H	2.61352000	0.27126900	-1.45558500
H	3.70991400	2.22216200	-0.34951300
C	6.33080000	2.22405100	-2.38581900
C	5.33132000	1.09001500	-2.66678300
C	5.35640700	-0.02450900	-1.60242300
C	6.02319600	3.11966400	-1.17747700
C	4.46900600	0.18285800	-0.34906700
C	5.79028600	2.41562800	0.17708900
H	7.32472900	1.77379200	-2.25577100
H	4.31670100	1.49929400	-2.78166400
H	6.39699000	-0.16162700	-1.28473800
H	5.13535300	3.73266600	-1.39550000
H	6.40607800	2.86398600	-3.27380000
H	5.58623600	0.64898300	-3.63796500
H	5.06947900	-0.97923900	-2.06263800
H	6.85316100	3.82858900	-1.06618500
H	4.89676400	-0.45971500	0.43269600
H	4.09749100	1.59035100	1.23602700
H	-3.78797800	1.07127000	-1.56197300
C	-2.75073300	-3.76255400	2.26303100
H	-1.83380200	-4.33445300	2.43860700
H	-3.37858100	-3.88332000	3.15091800
H	-3.27931100	-4.21561100	1.41849000
C	-1.70293600	-1.65968700	3.21555300
H	-2.36134700	-1.66760200	4.09039200
H	-0.79783600	-2.22113300	3.47183800
H	-1.42183700	-0.61800700	3.02821300

C	5.80483400	3.45632300	1.30917800
H	4.98749800	4.17870700	1.18901700
H	5.68855000	2.98252700	2.28984900
H	6.74278900	4.02033700	1.31946000
H	6.61901900	1.71573300	0.35904500
C	0.59355300	-0.57635900	0.15771600
C	2.04260800	-0.27955100	0.55226700
H	-0.05172100	-0.43271100	1.03453000
H	0.46013700	-1.65016600	-0.15960200
H	2.02209500	0.75101900	0.93167500
C	2.49028300	-1.14407700	1.76604100
H	3.43793100	-0.74151200	2.14436400
H	1.76229800	-0.99908200	2.57524900
C	2.65982100	-2.64867100	1.51387100
H	1.72598100	-3.07201300	1.11472000
H	3.42683700	-2.81871600	0.74697800
C	3.04569100	-3.42074400	2.78335400
H	3.97695800	-3.00486800	3.19140700
H	2.28052800	-3.26798800	3.55586400
C	3.22500500	-4.93180600	2.54468800
H	3.98752000	-5.07466700	1.76414300
H	2.29222400	-5.35816200	2.15249000
C	3.63566800	-5.67606000	3.78651700
H	4.58256800	-5.36867800	4.23273800
C	2.93294300	-6.65012800	4.36446400
H	3.27995400	-7.14945200	5.26393000
H	1.98509400	-6.99150300	3.95371400
C	-0.77280900	1.84555100	-1.75776100
C	0.00622600	1.99611000	-0.64381600
H	-0.30652100	1.83123000	-2.73462900
H	-1.83773600	2.06404300	-1.71936700
H	1.08543200	1.96846700	-0.77480500
C	-0.48550400	2.43466900	0.70162700
H	-1.54689100	2.19718300	0.81958000
H	0.06241200	1.91535400	1.49518700
C	-0.26556600	3.96006600	0.87271900
H	0.79504500	4.19689500	0.71646900
H	-0.82272600	4.49355100	0.09274500
C	-0.70481100	4.45370500	2.25776900
H	-1.76207700	4.20777900	2.41984000
H	-0.14023200	3.91644300	3.03196200
C	-0.50683700	5.97082300	2.43964000
H	-1.08719500	6.51222400	1.68220700
H	0.55106000	6.21111700	2.25692800



C	-0.89954100	6.44472700	3.81331900
H	-0.33552900	6.01703100	4.64349900
C	-1.86966000	7.32170900	4.07076300
H	-2.45495500	7.77620600	3.27447200
H	-2.10971700	7.62652700	5.08477800
H	-1.70190500	-2.26838800	1.15972400
<b>7TS<sub>12</sub>, -1968.7054388, i149.89</b>			
O	2.42961000	-0.16564700	0.14725500
C	0.19441000	-0.71117600	3.53044000
C	1.58241900	-0.33099200	3.56466600
C	2.33433600	-1.34896000	2.89886600
C	1.41389600	-2.30880000	2.38825400
C	0.09212500	-1.93078800	2.81951300
C	-0.92668800	-0.01029700	4.24470900
C	2.16500000	0.80342400	4.35994900
C	3.83003800	-1.45007300	2.82368400
C	1.77290300	-3.60008900	1.70590500
C	-1.12447200	-2.80509200	2.70274100
C	3.61393800	-0.28679300	-0.54079500
C	4.67445200	0.60235500	-0.24901100
C	5.85062000	0.47079500	-0.99512200
C	5.98036400	-0.50007400	-1.98423000
C	4.92237500	-1.36588600	-2.24691200
C	3.71923600	-1.28476900	-1.53788800
C	4.54956700	1.70156300	0.79898200
C	2.55690200	-2.20546300	-1.88798900
H	-1.03486000	-0.41265800	5.25956600
H	-1.88629600	-0.14229800	3.73888500
H	-0.74731100	1.06263600	4.35167900
H	2.42105900	0.46001300	5.36966200
H	1.46455400	1.63389500	4.47436300
H	3.08010200	1.19594300	3.90939600
H	4.17372100	-1.81453500	1.85272400
H	4.19116800	-2.15159600	3.58576100
H	4.31324700	-0.48998400	3.01063700
H	1.90388700	-4.39649800	2.44933500
H	2.70829400	-3.51896100	1.14800600
H	0.99465300	-3.93216200	1.01328400
H	-2.04562800	-2.25590900	2.90065800
H	-1.06065000	-3.61413900	3.44101100
H	-1.21432800	-3.27917800	1.72093600
Ti	1.01491500	-0.31685000	1.23328700
C	5.80029100	1.83583200	1.68768500
H	6.08789000	0.87877700	2.13341200

H	6.66118200	2.21084100	1.12603700
H	5.61267900	2.54922500	2.49703800
C	4.21753200	3.05497200	0.13579800
H	3.30874500	2.99676600	-0.47147100
H	4.07827900	3.83617700	0.89145000
H	5.03142200	3.37100400	-0.52476700
H	6.68014600	1.14202400	-0.79843100
H	6.90342700	-0.58125100	-2.54954800
H	5.03116500	-2.11750800	-3.02188300
C	-4.71366200	1.21557300	-0.33990700
C	-3.04221900	-0.47793900	0.58589700
H	-2.96581900	-1.49128300	0.99402600
H	-2.72781100	0.19684400	1.39560000
H	-4.06271700	1.93020300	0.18802400
C	-6.68627700	1.64822600	2.20439400
C	-5.54199300	0.67831500	2.54166400
C	-5.39642100	-0.47201100	1.52612100
C	-6.49038100	2.52766900	0.96148500
C	-4.53075000	-0.19326200	0.27133400
C	-6.14373100	1.80778400	-0.35996100
H	-7.60578400	1.05819200	2.08625100
H	-4.59635500	1.23027000	2.64723000
H	-6.40281500	-0.76737100	1.20628600
H	-5.69987100	3.26731500	1.15973300
H	-6.86205400	2.30724200	3.06367800
H	-5.74592400	0.24609600	3.52864100
H	-4.98441600	-1.35703200	2.02883500
H	-7.40964600	3.10803000	0.81370500
H	-4.85202900	-0.92244900	-0.48512900
H	-4.33961100	1.18469700	-1.37105600
H	3.71358600	1.43603600	1.45454000
C	2.98388500	-3.66863000	-2.10376000
H	2.10122000	-4.30208000	-2.23911400
H	3.60255800	-3.78672800	-2.99842600
H	3.55338400	-4.05419700	-1.25248600
C	1.80022200	-1.67322900	-3.12326700
H	2.44933600	-1.67581700	-4.00499400
H	0.92882500	-2.29860600	-3.34685100
H	1.45882900	-0.64322600	-2.97440200
C	-6.28864000	2.78831600	-1.53578500
H	-5.58222500	3.62255400	-1.44063300
H	-6.09428900	2.29537900	-2.49444000
H	-7.29619100	3.21380200	-1.57690000
H	-6.86385000	0.99144700	-0.51758400

C	-0.58683200	-0.41410200	-0.15165100
C	-2.05112700	-0.34133700	-0.58866200
H	0.07266200	-0.37139400	-1.02479000
H	-0.41344400	-1.40483400	0.36784600
H	-2.17643700	0.65807700	-1.02415600
C	-2.33454000	-1.32739900	-1.75842600
H	-3.33220900	-1.10450000	-2.15505200
H	-1.63397600	-1.10125600	-2.57304300
C	-2.25442500	-2.82594400	-1.43430200
H	-1.26269500	-3.07153400	-1.02556100
H	-2.98181400	-3.08295000	-0.65326500
C	-2.51138800	-3.70959300	-2.66296800
H	-3.50022000	-3.47290700	-3.07859500
H	-1.78518000	-3.46869600	-3.45049800
C	-2.43657400	-5.21650900	-2.35319200
H	-3.16127400	-5.44669500	-1.55762100
H	-1.44404800	-5.46362000	-1.95354200
C	-2.72344700	-6.07619600	-3.55464700
H	-3.71028100	-5.95165800	-4.00268100
C	-1.87098000	-6.94642500	-4.09550700
H	-2.13398700	-7.53849800	-4.96669500
H	-0.87781400	-7.10611200	-3.68099100
C	0.63697400	1.84105700	1.63213300
C	-0.24865000	1.78944900	0.54534500
H	0.21853800	1.95368600	2.62471000
H	1.62143600	2.27904500	1.48060700
H	-1.30928200	1.77066000	0.77619500
C	0.12529600	2.33615500	-0.81060900
H	1.17984800	2.12898900	-1.02036400
H	-0.46550400	1.86589000	-1.60279500
C	-0.12374900	3.86241900	-0.85501300
H	-1.17348100	4.06871900	-0.60685000
H	0.48048200	4.35169500	-0.08107200
C	0.20703700	4.46200300	-2.22847800
H	1.25362100	4.24945100	-2.48214100
H	-0.40287200	3.96967800	-2.99824400
C	-0.02589900	5.98385000	-2.28839900
H	0.59805200	6.48268700	-1.53633400
H	-1.07180000	6.18966200	-2.01621400
C	0.26170800	6.56054800	-3.64866100
H	-0.35193000	6.17957900	-4.46634200
C	1.19681100	7.47372700	-3.90981000
H	1.82902700	7.88431000	-3.12560700
H	1.36025300	7.85298900	-4.91391600

H	1.85950900	-2.19776600	-1.04330100
<b>7P<sub>12</sub>, -1968.7286435</b>			
O	2.47237800	-0.03478700	0.03792400
C	0.55409100	-0.96751400	3.53594600
C	1.88549900	-0.44910400	3.53824700
C	2.70568200	-1.33432900	2.75687200
C	1.87095400	-2.37361600	2.25046100
C	0.54051600	-2.14550200	2.73366800
C	-0.61215500	-0.42020900	4.30707700
C	2.37919400	0.71914600	4.34239700
C	4.19840000	-1.26189400	2.60707200
C	2.32868100	-3.56629000	1.45786700
C	-0.62131300	-3.08486100	2.55911800
C	3.59099800	-0.02824900	-0.76002300
C	4.59027800	0.94333000	-0.52503400
C	5.70490100	0.93297500	-1.37055700
C	5.82639700	0.00543900	-2.40193600
C	4.82267200	-0.93710500	-2.61199700
C	3.68412600	-0.98035100	-1.80090500
C	4.45288000	1.99980500	0.56456100
C	2.55988700	-1.96695200	-2.09107300
H	-0.71563100	-0.95353100	5.25996600
H	-1.55769600	-0.53598600	3.76962200
H	-0.48642800	0.63812900	4.54522500
H	2.70033000	0.38204600	5.33557700
H	1.60381300	1.47408300	4.48945300
H	3.23640700	1.20697200	3.87232400
H	4.53073000	-1.55891100	1.60951900
H	4.67557700	-1.93584100	3.32895900
H	4.57830900	-0.25735800	2.80003700
H	2.58284500	-4.39170600	2.13456500
H	3.21956400	-3.34458600	0.86633900
H	1.55497400	-3.93580100	0.77917600
H	-1.58218800	-2.58307800	2.69520700
H	-0.56479800	-3.88341300	3.30919300
H	-0.62597500	-3.56727300	1.57843300
Ti	1.22182100	-0.36202600	1.26511300
C	5.75719100	2.23313100	1.34885100
H	6.16807900	1.29853700	1.74325000
H	6.52922400	2.69829000	0.72836700
H	5.57406400	2.90968000	2.19008100
C	3.93476700	3.32677600	-0.02887500
H	2.98211400	3.18969200	-0.54972600
H	3.79204900	4.07423200	0.75925300

H	4.64970500	3.73404200	-0.75127900
H	6.49053800	1.66613700	-1.22066700
H	6.70117300	0.01915500	-3.04446800
H	4.92447300	-1.64902900	-3.42432300
C	-5.13712200	0.88743600	-0.60378000
C	-3.31361400	-0.44199300	0.58509200
H	-3.11872200	-1.39225800	1.10093200
H	-3.15479200	0.34706300	1.33455100
H	-4.62361500	1.73756600	-0.12943900
C	-7.30740100	1.29621800	1.77763500
C	-6.06395900	0.54229000	2.27657600
C	-5.69850800	-0.67653000	1.40668900
C	-7.15611400	2.05974200	0.45448300
C	-4.80388600	-0.40988400	0.16979900
C	-6.63089300	1.26228900	-0.75908400
H	-8.12776800	0.57108300	1.68287000
H	-5.21159800	1.23160000	2.36343800
H	-6.63218200	-1.14645000	1.07533200
H	-6.48898100	2.92165500	0.60573400
H	-7.62599900	2.00951400	2.54785200
H	-6.26739300	0.19187600	3.29551300
H	-5.19953300	-1.43388800	2.02579000
H	-8.13532900	2.48315900	0.19825400
H	-4.97299600	-1.25315800	-0.51423500
H	-4.69732000	0.80203600	-1.60552500
H	3.70193500	1.64425500	1.27800600
C	3.06009400	-3.37516800	-2.45776300
H	2.21380500	-4.06418700	-2.54514100
H	3.58023100	-3.38518600	-3.42029400
H	3.74707800	-3.77082700	-1.70342300
C	1.63409200	-1.41316800	-3.19504900
H	2.18283200	-1.29724900	-4.13526900
H	0.79537700	-2.09367100	-3.37878200
H	1.23254700	-0.42974000	-2.92857300
C	-6.83371700	2.08322900	-2.04362900
H	-6.25483200	3.01459900	-2.00971800
H	-6.51394700	1.52505900	-2.93022600
H	-7.88535700	2.35404000	-2.18032600
H	-7.22100800	0.33921800	-0.85810600
C	-0.83949400	-0.10090000	0.04681900
C	-2.27595500	-0.27040000	-0.54547800
H	-0.11962600	-0.41300000	-0.73014800
H	-0.81777300	-0.84124400	0.88441800
H	-2.48791400	0.67347500	-1.05965100

C	-2.33048100	-1.37461300	-1.62482100
H	-3.32905000	-1.35945700	-2.07692400
H	-1.63765400	-1.09998200	-2.43166400
C	-2.01758800	-2.80722100	-1.16903900
H	-1.00769300	-2.85016100	-0.73266600
H	-2.70909200	-3.11117500	-0.37262300
C	-2.09903700	-3.82432200	-2.31570400
H	-3.10715100	-3.79784400	-2.75047800
H	-1.41358800	-3.53023400	-3.12146700
C	-1.77105600	-5.26356300	-1.87646100
H	-2.46143400	-5.54929800	-1.06846700
H	-0.75868900	-5.29954300	-1.45121200
C	-1.87742800	-6.25824900	-3.00080800
H	-2.86073900	-6.34681700	-3.46458800
C	-0.87450400	-7.00741000	-3.45836400
H	-1.01045500	-7.70706700	-4.27723900
H	0.12180100	-6.95576200	-3.02391500
C	0.52163400	1.52215600	1.65644600
C	-0.54091100	1.38329400	0.52105400
H	0.07285600	1.73313300	2.62547900
H	1.27906500	2.27525800	1.42997900
H	-1.49042300	1.71154500	0.95944900
C	-0.21248100	2.25884500	-0.70586600
H	0.81678300	2.04770200	-1.02553000
H	-0.85707200	1.97120200	-1.54601900
C	-0.38401800	3.76330900	-0.45466900
H	-1.42155900	3.96035000	-0.15000500
H	0.24550500	4.07702400	0.38836300
C	-0.04367700	4.61586600	-1.68403200
H	0.99316300	4.42525300	-1.99120700
H	-0.67429100	4.30653300	-2.52908100
C	-0.22438700	6.12612900	-1.44038400
H	0.41876700	6.44602900	-0.61072800
H	-1.26156400	6.30730700	-1.12079300
C	0.07524800	6.95404700	-2.66086100
H	-0.54921800	6.75735900	-3.53370100
C	1.03212000	7.87829800	-2.74372600
H	1.67615000	8.11065500	-1.89835900
H	1.20290100	8.44439100	-3.65436100
H	1.96161700	-2.06947300	-1.17692500
<b>7C<sub>cyc</sub>, -1655.8212888</b>			
O	-2.28954800	0.13287100	-0.28170400
C	0.53444200	-0.34758900	2.61307900
C	-0.08906000	-1.62561700	2.51636000

C	-1.50875500	-1.43324000	2.53666100
C	-1.76165000	-0.03543900	2.63875900
C	-0.49583800	0.63834600	2.68375800
C	2.00803100	-0.10903400	2.76613100
C	0.61427900	-2.95125200	2.61456300
C	-2.54826700	-2.51706100	2.60404100
C	-3.10655300	0.60441000	2.82740800
C	-0.31446000	2.10467900	2.94960500
C	-3.54728500	0.59159600	-0.60135700
C	-4.57257100	-0.34455400	-0.87428400
C	-5.83205200	0.15566000	-1.22138600
C	-6.07620200	1.52392500	-1.29209900
C	-5.05015700	2.42373500	-1.01787400
C	-3.76769300	1.98821100	-0.66881300
C	-4.32402100	-1.84684400	-0.86914000
C	-2.65597500	3.00126100	-0.42871400
H	2.31345300	-0.30231500	3.80199800
H	2.28019100	0.92177300	2.53564700
H	2.60577400	-0.76289800	2.12505100
H	0.64054800	-3.27622600	3.66210800
H	1.65145800	-2.89438600	2.27524300
H	0.10902100	-3.74436300	2.05566900
H	-3.48774100	-2.21970100	2.13333900
H	-2.77232600	-2.75113300	3.65239000
H	-2.21555500	-3.44946300	2.13908800
H	-3.37045500	0.60652300	3.89226000
H	-3.89627500	0.07235100	2.29278000
H	-3.11759900	1.64131000	2.48625500
H	0.68959100	2.45089100	2.69836500
H	-0.46978500	2.30575500	4.01678900
H	-1.03147400	2.71843300	2.39835000
Ti	-0.78391700	-0.38372200	0.53596500
C	-5.44530900	-2.64707300	-0.18139800
H	-5.64952400	-2.27484400	0.82770900
H	-6.38251100	-2.60485100	-0.74418600
H	-5.16446200	-3.70268800	-0.10636100
C	-4.09447400	-2.36001700	-2.30668600
H	-3.28669500	-1.81394200	-2.80590100
H	-3.84644100	-3.42729200	-2.30722400
H	-4.99628500	-2.22657600	-2.91282200
H	-6.63499500	-0.53928200	-1.44420900
H	-7.06213500	1.88808900	-1.56332200
H	-5.24792900	3.48868600	-1.08001300
C	4.84619300	-0.28928900	-0.69129800

C	3.03104500	1.50109400	-0.54164500
H	2.76728400	2.51105600	-0.88407800
H	3.10504100	1.56363800	0.55127000
H	4.54237900	-0.47899900	0.34967400
C	7.37366400	1.22375700	0.67010800
C	6.11540600	2.10673700	0.68936100
C	5.44468600	2.24693500	-0.69101200
C	7.15094700	-0.27585500	0.42888700
C	4.43170500	1.14414600	-1.09481500
C	6.34024300	-0.67067300	-0.82464100
H	8.05075400	1.61458400	-0.10217900
H	5.40024900	1.73367000	1.43664500
H	6.23757400	2.29629200	-1.44724200
H	6.65116700	-0.71540100	1.30560600
H	7.90733400	1.33874900	1.62174700
H	6.40906200	3.10513100	1.03422100
H	4.92816900	3.21300000	-0.75135000
H	8.13543000	-0.75749200	0.37553800
H	4.37912800	1.17355900	-2.19137500
H	4.25838600	-0.98814000	-1.30171100
H	-3.40735100	-2.02612200	-0.30039800
H	-1.85711300	2.49461300	0.12031200
C	-3.10104000	4.20312600	0.42481800
H	-2.23879600	4.83591800	0.65939500
H	-3.82570000	4.83374200	-0.09900700
H	-3.55930300	3.88642400	1.36750500
C	-2.06492300	3.47908800	-1.77192200
H	-2.82154400	4.00801100	-2.36082600
H	-1.22737300	4.16520200	-1.60598400
H	-1.70746600	2.63838700	-2.37516100
C	6.47780900	-2.18201600	-1.07353100
H	6.05972200	-2.75736000	-0.23736700
H	5.95260800	-2.48750100	-1.98548300
H	7.52697200	-2.47484300	-1.18003000
H	6.76243800	-0.15100800	-1.69712700
C	0.55872200	1.09237400	-0.17625500
C	1.83845900	0.57025500	-0.89852100
H	-0.07473100	1.63421100	-0.88756400
H	0.83495900	1.80702500	0.59928800
H	2.09564100	-0.43659800	-0.53715400
C	1.64019600	0.52817100	-2.43467800
H	1.47951800	1.56529800	-2.75552400
H	2.57550500	0.21322700	-2.91332000
C	0.49213100	-0.33517100	-2.99013000



H	-0.38816900	-0.25006300	-2.33985700
H	0.16932600	0.09030000	-3.94723700
C	0.83360600	-1.81349000	-3.25894300
H	1.55026900	-1.85827200	-4.08703000
C	-0.69928200	-2.56172000	-0.72612600
C	0.63063800	-2.77675800	-0.85600900
H	-1.30991900	-2.25957900	-1.56993100
H	-1.22149400	-2.93750700	0.15200500
H	1.16757000	-3.18437200	-0.00063600
C	1.45118000	-2.59669000	-2.09317400
H	2.42499800	-2.17904800	-1.81219100
H	1.68908400	-3.62050500	-2.42692700
H	-0.06380800	-2.33292200	-3.61766100
<b>7TS<sub>eye</sub>, -1655.8104259, i239.95</b>			
O	-1.90259100	-0.55135700	0.06784600
C	-0.74750300	2.86001500	-1.72905300
C	-1.66935600	3.42293100	-0.80965200
C	-2.87289500	2.64444700	-0.85272200
C	-2.70240300	1.61749100	-1.83155800
C	-1.37712000	1.73027500	-2.35388400
C	0.58569900	3.43476300	-2.11380600
C	-1.47835400	4.69942700	-0.04188800
C	-4.15152400	2.96831100	-0.13347800
C	-3.76202000	0.66068700	-2.29776200
C	-0.79363400	0.92430700	-3.48177200
C	-2.64814800	-1.70778900	0.02608900
C	-3.81421500	-1.79072600	0.82484800
C	-4.53955400	-2.98576400	0.78850300
C	-4.13983800	-4.05642900	-0.00677200
C	-2.99393600	-3.94458500	-0.78720800
C	-2.22160200	-2.77712700	-0.79386200
C	-4.26295900	-0.65405200	1.73490900
C	-0.96781100	-2.71818600	-1.65753700
H	0.46435000	4.13778700	-2.94684400
H	1.28823000	2.66598900	-2.44682600
H	1.05287500	3.98932100	-1.29494300
H	-1.86358800	5.54446600	-0.62578300
H	-0.42510400	4.90946500	0.16223200
H	-2.01841500	4.70708300	0.90881500
H	-4.78359400	2.08753900	-0.00219600
H	-4.73015600	3.70091100	-0.70989800
H	-3.97737700	3.40745600	0.85286200
H	-4.35414800	1.12007300	-3.09854000
H	-4.45087600	0.38618100	-1.49593900

H	-3.33555700	-0.26326500	-2.69278900
H	0.28961400	0.80568000	-3.38899300
H	-0.98140300	1.42747000	-4.43837800
H	-1.23573200	-0.07097200	-3.54687300
Ti	-1.20706500	1.08531500	-0.10585600
C	-5.77612600	-0.37879800	1.65577700
H	-6.10524100	-0.21539600	0.62435500
H	-6.36584900	-1.20557000	2.06291000
H	-6.02774900	0.51212000	2.24046800
C	-3.83555800	-0.92272000	3.19310400
H	-2.75555800	-1.08515800	3.27231800
H	-4.10968100	-0.08297800	3.84142900
H	-4.32862300	-1.81940100	3.58254000
H	-5.43384200	-3.08045200	1.39569200
H	-4.71985100	-4.97384500	-0.01738900
H	-2.68738700	-4.78292400	-1.40515300
C	5.15165100	-0.17017200	0.89403600
C	2.99144100	-0.29056300	-0.45624100
H	2.41580000	-0.93577600	-1.13559300
H	3.24143500	0.61575100	-1.02570100
H	5.10368400	0.89018200	0.60328500
C	7.39726400	-0.35359600	-1.44212200
C	5.97586500	-0.35526000	-2.02805500
C	5.05527500	-1.41629300	-1.39426100
C	7.53691900	0.13411300	0.00695300
C	4.31299600	-1.01229100	-0.09481900
C	6.64317600	-0.54803100	1.06551800
H	7.79634800	-1.37479400	-1.51793500
H	5.53109700	0.64712600	-1.94918900
H	5.65817500	-2.31016100	-1.19372800
H	7.34080500	1.21609300	0.04733400
H	8.04381500	0.26799100	-2.07386300
H	6.05322500	-0.56150500	-3.10215200
H	4.30235700	-1.73514700	-2.12683000
H	8.58634100	0.01085400	0.30258500
H	4.05034500	-1.95159900	0.40994700
H	4.66691700	-0.22713100	1.87735100
H	-3.75542700	0.25698600	1.40388400
H	-0.53007300	-1.71995900	-1.55036500
C	-1.28981500	-2.93092300	-3.15049900
H	-0.38921300	-2.80363600	-3.76038500
H	-1.66969700	-3.94047800	-3.33519300
H	-2.04981500	-2.22935000	-3.50924200
C	0.08456300	-3.74356100	-1.18906600

H	-0.27332400	-4.76819800	-1.33137900
H	1.01136500	-3.63561300	-1.76273200
H	0.31972600	-3.62391600	-0.12760100
C	7.12353100	-0.16103500	2.47424000
H	7.02985500	0.91982500	2.63786200
H	6.53848200	-0.66718600	3.24992000
H	8.17500400	-0.42628200	2.62259800
H	6.74714900	-1.63866400	0.96699600
C	0.94824600	0.99644800	0.18447500
C	2.06936700	0.10554900	0.73335600
H	0.51385000	0.44084000	-0.71288300
H	1.40031100	1.89683500	-0.23273100
H	2.67285500	0.74895900	1.37903700
C	1.63501200	-1.13803700	1.53870300
H	1.37596700	-1.93801600	0.83406500
H	2.51382900	-1.49985000	2.08518500
C	0.46212100	-0.98201400	2.51794300
H	-0.46096100	-0.83710000	1.95045700
H	0.32960100	-1.93904800	3.03668800
C	0.58232900	0.11576600	3.58353000
H	1.39953500	-0.12063000	4.27513700
C	-1.44925200	1.89604800	1.90936000
C	-0.04199700	2.07216000	1.94437800
H	-1.87276600	1.11920700	2.54162500
H	-2.05946700	2.78601000	1.81294800
H	0.31445200	3.01982500	1.54574300
C	0.83142600	1.54100600	3.05993200
H	1.88275300	1.68813100	2.80951000
H	0.63974100	2.25131200	3.87964600
H	-0.33081300	0.10572200	4.19085900
<b>7P<sub>cycs</sub> -1655.8360702</b>			
O	2.21023300	0.41235600	0.14718100
C	0.22741700	-2.17158900	-2.21278900
C	1.23553800	-3.01919300	-1.66866900
C	2.49067900	-2.34337100	-1.79382100
C	2.26486400	-1.09615300	-2.46431000
C	0.86417300	-0.98313100	-2.70766100
C	-1.22309600	-2.53036900	-2.39154900
C	1.03796800	-4.42707800	-1.19176800
C	3.82823500	-2.90280300	-1.40100900
C	3.32671800	-0.12541200	-2.89592900
C	0.17297400	0.13714200	-3.43577800
C	3.07792900	1.46744700	0.28312800
C	4.32699900	1.23469100	0.90219200

C	5.18384800	2.33072400	1.04545900
C	4.81962600	3.59980000	0.60058400
C	3.57891300	3.79808200	-0.00003200
C	2.67916000	2.74165300	-0.17743200
C	4.70755300	-0.13672700	1.44580700
C	1.30433900	2.98939900	-0.78510300
H	-1.36122100	-3.06358100	-3.34012400
H	-1.86859900	-1.64867000	-2.42551000
H	-1.58840300	-3.18870900	-1.59904100
H	1.00363300	-5.10762300	-2.05134800
H	0.10048200	-4.55661900	-0.64363700
H	1.85615600	-4.76042900	-0.55017100
H	4.56845500	-2.11612500	-1.24137200
H	4.21128000	-3.55353100	-2.19689800
H	3.77020600	-3.50183800	-0.48863300
H	3.72711200	-0.41957400	-3.87350900
H	4.16311400	-0.09197000	-2.19433000
H	2.93910000	0.89079100	-2.99194000
H	-0.82478800	0.34113100	-3.03570100
H	0.04485700	-0.12621000	-4.49295300
H	0.74610200	1.06563800	-3.40025900
Ti	1.20886800	-0.95758700	-0.39318200
C	6.17450500	-0.51299100	1.17278300
H	6.42471900	-0.42515000	0.11048600
H	6.87154200	0.11925700	1.73131800
H	6.36095400	-1.54607300	1.48320400
C	4.39149200	-0.22508800	2.95400300
H	3.33811000	-0.00474300	3.15639300
H	4.61429300	-1.22615700	3.33882100
H	4.99268000	0.49428500	3.51980500
H	6.15087500	2.19061900	1.51698700
H	5.50168400	4.43495300	0.72548300
H	3.30307700	4.79300000	-0.33465700
C	-5.28738600	-0.11900600	0.63713300
C	-2.91116700	0.77293800	0.40966700
H	-2.30426600	1.68818800	0.46586800
H	-2.83918800	0.41643300	-0.62959800
H	-4.96961300	-0.76609000	-0.19475700
C	-6.83910400	1.54133600	-1.68296500
C	-5.34050600	1.88367000	-1.65684600
C	-4.82982100	2.28763600	-0.25991600
C	-7.25676500	0.25267600	-0.96062300
C	-4.38904200	1.13951300	0.68304300
C	-6.81464300	0.09861800	0.51084800

H	-7.38756600	2.38988900	-1.25070600
H	-4.75321500	1.04657800	-2.06181900
H	-5.61906400	2.86844700	0.23208400
H	-6.87816000	-0.61678700	-1.51899900
H	-7.17189000	1.47019900	-2.72597900
H	-5.17346500	2.72276500	-2.34277800
H	-3.98468200	2.98068800	-0.36346700
H	-8.35069900	0.18223000	-1.00716100
H	-4.44623500	1.54479400	1.70232600
H	-5.09600000	-0.69896600	1.54891600
H	4.08274400	-0.87946600	0.93873600
H	0.87649400	2.01549900	-1.05216400
C	1.35952800	3.82741800	-2.07541400
H	0.36380400	3.89738400	-2.52545200
H	1.69715300	4.84999600	-1.88176500
H	2.04025500	3.39104200	-2.81370400
C	0.36147800	3.63872700	0.24938900
H	0.73386500	4.62332700	0.55011900
H	-0.64180400	3.77389900	-0.16943900
H	0.27882000	3.02903600	1.15524500
C	-7.56670600	-1.07753400	1.15590700
H	-7.31943600	-2.02288300	0.65688200
H	-7.31008200	-1.18366200	2.21548800
H	-8.65063700	-0.94239400	1.08649500
H	-7.09056200	1.01063100	1.06041400
C	-0.85746800	-0.66001200	0.85702300
C	-2.28361500	-0.28439000	1.34419100
H	-0.18336400	0.14823500	1.17740200
H	-0.93901400	-0.62773900	-0.25868900
H	-2.88079500	-1.19839800	1.26093500
C	-2.28160800	0.19301200	2.83672100
H	-2.51039500	1.26448200	2.85100100
H	-3.11145600	-0.29413800	3.36159900
C	-0.98447100	0.00116700	3.64464700
H	-0.16893000	0.55143100	3.15839600
H	-1.11482900	0.49893600	4.61184900
C	-0.55166400	-1.45794100	3.89636700
H	-1.07018200	-1.84184300	4.78300600
C	1.20005600	-2.23059500	1.21495100
C	-0.33969000	-2.07212700	1.33238200
H	1.72081700	-1.70515800	2.02324400
H	1.50423000	-3.27511900	1.19515400
H	-0.80443100	-2.80272400	0.65926600
C	-0.85443400	-2.43672300	2.75500500

H	-1.93928400	-2.57408300	2.68422100
H	-0.44362500	-3.42127700	3.00324000
H	0.51548100	-1.47846700	4.14703300