

Supporting Information

**Mechanism, Chemoselectivity and Stereoselectivity of NHC-Catalyzed Reaction
of Aldehydes and Hydrazones: A DFT Study**

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1. Computational details

The extent of enantioselectivity, in terms of enantiomeric excess (ee %), was calculated by using the Boltzmann distribution of diastereomeric transition states with the following equations:

$$\frac{[R]}{[S]} = \frac{\exp(-G_{[R]}^\ddagger)}{\exp(-G_{[S]}^\ddagger)} = \exp(\Delta G^\ddagger / RT) \quad (1)$$

$$ee = \frac{[R] - [S]}{[R] + [S]} \times 100\% = \frac{\frac{[R]}{[S]} - 1}{\frac{[R]}{[S]} + 1} \times 100\% \quad (2)$$

Where G^\ddagger is the Gibbs free energy barrier of the competing diastereomeric transition state and ΔG^\ddagger is the Gibbs free energy difference between the two diastereomeric transition states.

In distortion-interaction analysis, the transition state was divided into two fragments, followed by single point energy calculations on each fragment. The activation energy ΔE^\ddagger was divided into $\Delta E_{\text{dist}}^\ddagger$ and $\Delta E_{\text{int}}^\ddagger$, where $\Delta E_{\text{dist}}^\ddagger$ and $\Delta E_{\text{int}}^\ddagger$ are distortion energy and interaction energy, respectively. The distortion energy $\Delta E_{\text{dist}}^\ddagger$ of each fragment is the energy difference between the distorted fragment and the corresponding optimized structure without the other fragment. The interaction energy $\Delta E_{\text{int}}^\ddagger$ can be calculated using $\Delta E_{\text{int}}^\ddagger = \Delta E^\ddagger - \Delta E_{\text{dist}}^\ddagger$.

In global reactivity index (GRI) analysis, the electrophilicity index ω which reflects the molecular global electrophilicity character can be measured with the expression $\omega = (\mu^2/2\eta)$ (eV), where μ is the electronic chemical potential and η is the chemical hardness. The values of μ and η can be determined in terms of the one-electron energy of HOMO and LUMO (E_{HOMO} and E_{LUMO}) using $\mu \approx (E_{\text{HOMO}} - E_{\text{LUMO}})/2$ and $\eta \approx (E_{\text{LUMO}} - E_{\text{HOMO}})$. Within the Kohn–Sham scheme, the molecular nucleophilicity character is reflected by the value of the nucleophilicity index N as defined in $N = E_{\text{HOMO}}(\text{Nu}) - E_{\text{LUMO}}(\text{TCE})$, where $E_{\text{LUMO}}(\text{TCE})$ is the LUMO energy of tetracyanoethylene (TCE).

2. Test calculations of computational methods.

Table S1. Single point calculations at different levels.

Level	Functional	Basis set	Solvent model
L1	M06-2X-D3	6-311++G(2df,2pd)	IEFPCM
L2	M06-2X-D3	6-311++G(2df,2pd)	SMD
L3	ω B97X-D	6-311++G(2df,2pd)	IEFPCM
L4	B3LYP-D3	6-311++G(2df,2pd)	IEFPCM
L5	M06-2X	6-311++G(d, p)	IEFPCM
L6	M06-2X-D3	6-31G(d, p)	IEFPCM
L7	ω B97X-D	6-311++G(2df,2pd)	IEFPCM

It should be noted that the single point energies at L7 level were based on the geometries optimized at (IEF-PCM_{THF}) ω B97X-D/6-31G(d,p) level of theory.

Table S2. Comparison of relative energies for stereoselective transition states at different levels. Energies are given in kcal/mol.

	L1	L2	L3	L4	L5	L6	L7
TS4R	2.1	3.3	0.8	1.6	1.9	3.2	2.8
TS4S	0.0	0.0	0.0	0.0	0.0	0.0	0.0

3. Generation of the active catalyst.

Figure S1. Energy profile for generating the active NHC catalyst. Distances are in Å.

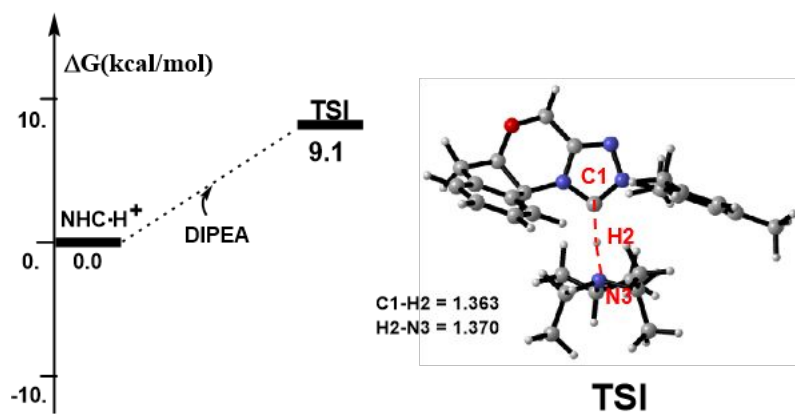


Figure S2a. IRC results of *re*-TS2. Distances are in Å.

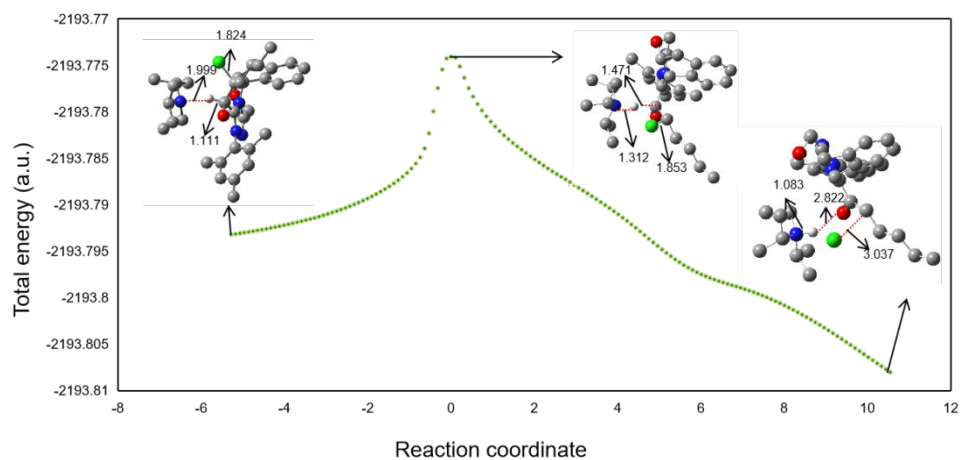


Figure S2b. IRC results of *si*-TS2. Distances are in Å.

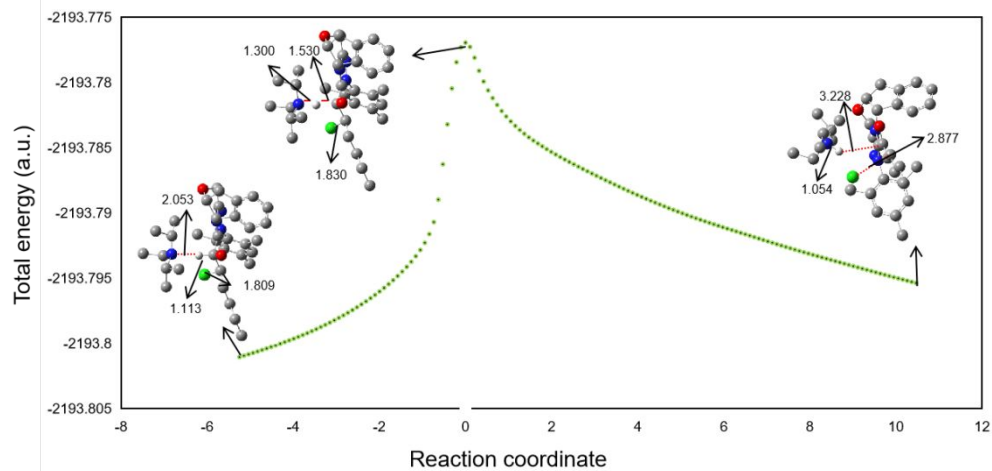


Figure S3. Other possible pathways of steps1-2. Energies are in kcal/mol.

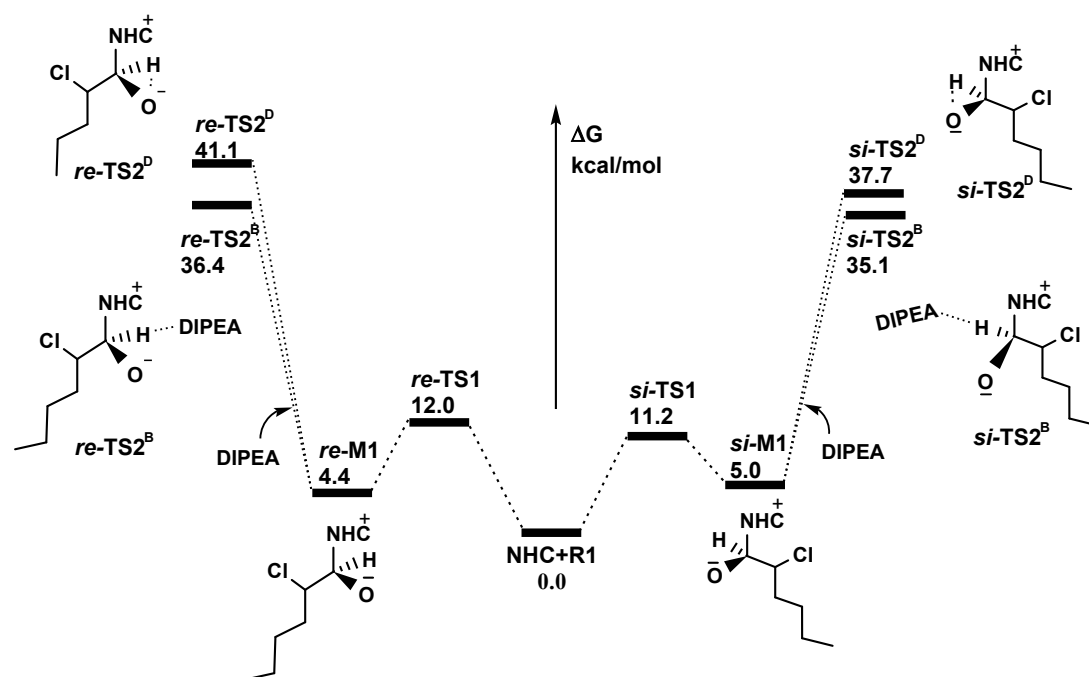
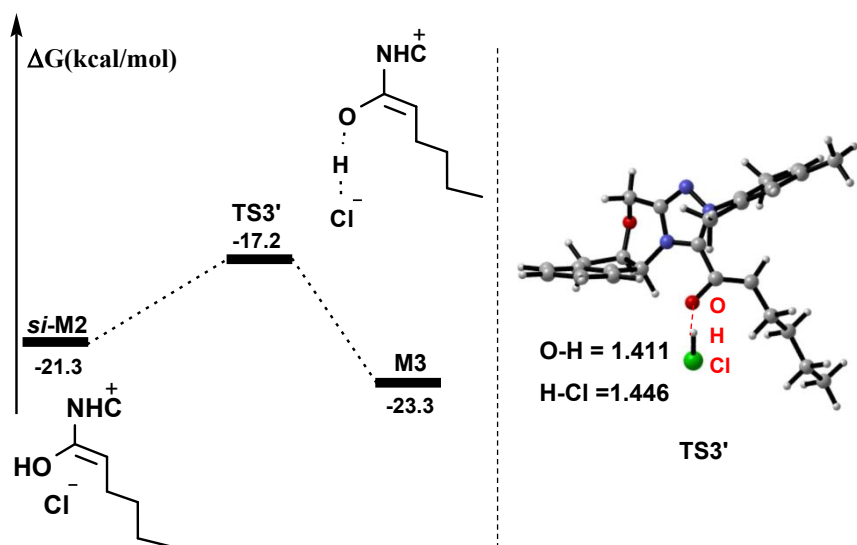


Figure S4. Free energy profile of deprotonation of **M2** by Cl^- . Energies and bond lengths are given in kcal/mol and Å, respectively.



Conformational search for **TS4**.

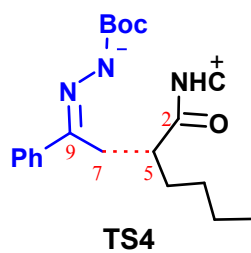


Table S3 Energies of different conformations of the stereoselective transition states.

species	Dihedral angle C2-C5-C7-C9	Free energies (a.u.)	relative energies (kcal/mol)
TS4R	-93.43	-2126.2452627	2.1
TS4R'	24.41	-2126.2364030	7.6
TS4R''	93.88	-2126.2344471	8.9
TS4R'''	167.30	-2126.2394347	5.7
TS4S	-20.65	-2126.2485252	0.0
TS4S'	158.02	-2126.2362982	7.7
TS4S''	-80.61	-2126.2421907	4.0
TS4S'''	92.89	-2126.2466527	1.2

Figure S5. Possible reaction pathways of ring closure step. Energies and bond lengths are given in kcal/mol and Å, respectively.

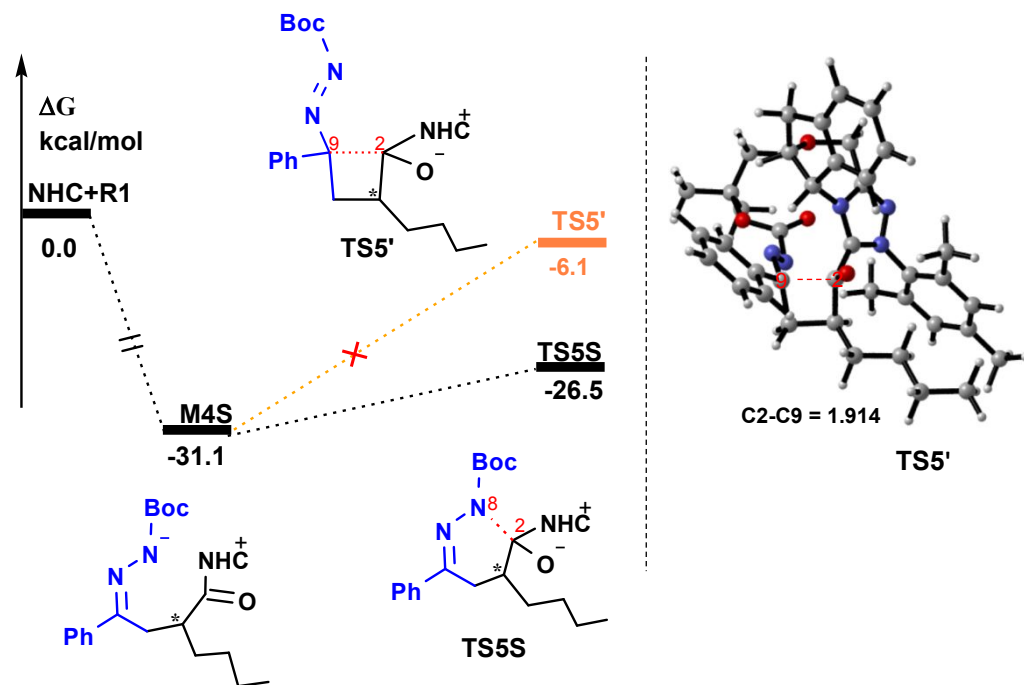


Table S4. The electrophilic and nucleophilic Parr functions (P_k^+ and P_k^-) of the selected atoms in **M4S**.

	M4S		
	C2	C9	N8
P_k^+	0.224	0.014	0.020
P_k^-	0.002	0.248	0.493

Coordinates

NHC

C	2. 93285700	0. 60674800	-0. 54757200
C	4. 26067900	0. 30805700	-0. 24035200
C	5. 14189200	1. 32495500	0. 10618500
C	4. 67090900	2. 63867200	0. 14397000
C	3. 34056700	2. 92931200	-0. 16198300
C	2. 45572700	1. 90946100	-0. 51528600
C	2. 19850000	-0. 66454700	-0. 91726700
C	3. 09109200	-1. 76790200	-0. 29459700
C	4. 50515900	-1. 18009100	-0. 35319700
N	0. 83563100	-0. 74955100	-0. 41439600
C	0. 47253800	-1. 55315400	0. 63490900
C	1. 47727400	-2. 45829000	1. 27688700
O	2. 77292800	-1. 93169400	1. 08065800
C	-0. 23543900	-0. 02184500	-0. 86845500
N	-1. 18941500	-0. 47050500	-0. 02537600
N	-0. 78658700	-1. 40783600	0. 90773300
C	-2. 55695500	-0. 04998300	-0. 02161000
C	-3. 54111200	-0. 96467900	-0. 40902400
C	-4. 86956800	-0. 54227200	-0. 38490200
C	-5. 22068500	0. 75065900	0. 00615300
C	-4. 20724100	1. 63165700	0. 38535300
C	-2. 86471200	1. 25272000	0. 38207600
C	-1. 78337400	2. 21608600	0. 79461200
C	-3. 17024000	-2. 35729200	-0. 84489900
C	-6. 66103100	1. 19486600	-0. 00777400
H	6. 17544300	1. 10290400	0. 35477900
H	5. 34551600	3. 44251600	0. 42099100
H	2. 99150500	3. 95603100	-0. 12186200
H	1. 41648800	2. 11578000	-0. 75448200
H	2. 16185300	-0. 78463000	-2. 00529700
H	2. 98710400	-2. 72817800	-0. 81656800
H	4. 97834200	-1. 42973500	-1. 30931900
H	5. 12373500	-1. 58966200	0. 44879900
H	1. 39928800	-3. 46706300	0. 84579300
H	1. 30157400	-2. 52314300	2. 35122300
H	-5. 64823500	-1. 24029500	-0. 68325900
H	-4. 46712300	2. 63960300	0. 70018200
H	-2. 21731500	3. 10093300	1. 26361300
H	-1. 08775800	1. 75077600	1. 49909400
H	-1. 19654000	2. 53192100	-0. 07261600
H	-2. 81512400	-2. 95147900	0. 00152500
H	-4. 02937700	-2. 86208900	-1. 28991600

H	-2.36014900	-2.32968500	-1.58010700
H	-7.33574400	0.35438500	0.17004800
H	-6.84716500	1.95518100	0.75423500
H	-6.92283500	1.62920700	-0.97811700

R1

C	3.33073700	-0.14921600	-0.04665000
O	3.68505000	-0.04350700	1.09969700
H	4.05483400	-0.21294200	-0.88002600
C	1.86437800	-0.19091400	-0.45138600
C	0.92632600	-0.40792800	0.71986600
H	1.15348400	-1.37542600	1.18229900
H	1.17875600	0.35972900	1.46108400
C	-0.55207300	-0.31668000	0.35718000
C	-1.45592400	-0.47187700	1.57821200
H	-0.80053700	-1.08920500	-0.38049200
H	-0.75005200	0.65103300	-0.12350800
C	-2.93646400	-0.37883600	1.22052200
H	-1.25032800	-1.43702500	2.05750900
H	-1.20279400	0.29974900	2.31575200
H	-3.56975600	-0.49377000	2.10387200
H	-3.16693200	0.58921600	0.76462600
H	-3.21336300	-1.15826000	0.50371500
H	1.63205900	0.73945600	-0.98177200
Cl	1.71347600	-1.49334600	-1.70091400

R2

C	-4.57974400	-1.73966400	-0.16341700
C	-3.37303900	-1.99596600	0.48256100
C	-2.40061400	-1.00438000	0.57537100
C	-2.63193500	0.26332000	0.02826300
C	-3.84025700	0.50832900	-0.63458900
C	-4.80910900	-0.48433100	-0.72427500
H	-5.33469200	-2.51554700	-0.23839700
H	-3.18630200	-2.97241000	0.91790800
H	-1.46169300	-1.20488300	1.07873500
H	-4.01181800	1.47467700	-1.09882000
H	-5.74026200	-0.28115400	-1.24312700
C	-1.61741800	1.33708100	0.14211700
C	-1.87765200	2.64730100	0.19754800
H	-2.89560700	3.01764500	0.17396400
H	-1.06945200	3.36045700	0.30865200
N	-0.27942500	0.85169400	0.31917900
N	0.59418900	1.56536200	-0.19350900

C	1. 93142500	1. 09098900	0. 10385500
O	2. 72939900	1. 83965300	0. 60711000
O	2. 10591500	-0. 14814500	-0. 30867700
C	3. 41704100	-0. 80390800	-0. 17225200
C	4. 45536300	-0. 04238500	-0. 98722700
C	3. 78562600	-0. 90201800	1. 30283100
C	3. 16181200	-2. 18269000	-0. 76454300
H	4. 11438800	0. 06948800	-2. 02007200
H	4. 64958400	0. 94279200	-0. 56250500
H	5. 38786500	-0. 61289900	-0. 99290500
H	2. 97906300	-1. 38666100	1. 85971700
H	4. 68772600	-1. 51163500	1. 40205000
H	3. 97796300	0. 08270400	1. 72925300
H	4. 07747700	-2. 77687700	-0. 71919600
H	2. 37871400	-2. 69946300	-0. 20414400
H	2. 84990700	-2. 09774300	-1. 80853800

DIPEA

N	-0. 07694500	-0. 02214900	-0. 51639700
C	-1. 27348700	-0. 40526300	0. 24803600
C	-1. 48183900	-1. 92154600	0. 20771900
C	-2. 52542200	0. 27698800	-0. 30798000
H	-1. 18503600	-0. 10933800	1. 30967800
H	-0. 70208400	-2. 47239600	0. 73832600
H	-2. 43706500	-2. 17356500	0. 67530400
H	-1. 50161000	-2. 26539900	-0. 83190300
H	-2. 52822300	1. 35612200	-0. 13803800
H	-2. 60720400	0. 09323700	-1. 38454600
H	-3. 41252200	-0. 13385300	0. 18068300
C	1. 14266100	-0. 75143100	-0. 12179700
C	1. 49644900	-0. 72500200	1. 37474100
C	2. 35278700	-0. 32234200	-0. 94885900
H	0. 95458000	-1. 79946800	-0. 38321900
H	0. 66084300	-1. 04791100	2. 00184100
H	2. 33259700	-1. 40575200	1. 56317600
H	1. 79968300	0. 27262800	1. 70260700
H	2. 10755000	-0. 29085800	-2. 01406500
H	2. 72653400	0. 66113500	-0. 64572900
H	3. 16307300	-1. 04141800	-0. 80261300
C	0. 06692500	1. 41888100	-0. 72216900
C	0. 22309900	2. 30691600	0. 51856100
H	-0. 80585700	1. 75688800	-1. 28769700
H	0. 91693400	1. 58299900	-1. 38864700
H	0. 14481800	3. 36045000	0. 23332100

H	-0.55557900	2.10382500	1.26078300
H	1.19357600	2.16651700	1.00089400

DIPEA·H⁺

H	-0.19767700	-0.24852300	-1.47791200
N	-0.03020500	0.01894200	-0.50109300
C	-1.29927600	-0.38929700	0.24246900
C	-1.44323700	-1.90388000	0.31594100
C	-2.49942900	0.23852700	-0.45889100
H	-1.19279200	0.01793100	1.24947500
H	-0.68749300	-2.37515600	0.94577900
H	-2.41773200	-2.12251500	0.75633500
H	-1.41987400	-2.35785600	-0.67962400
H	-2.47683900	1.32896900	-0.45797600
H	-2.57113500	-0.11170200	-1.49401200
H	-3.40633200	-0.07293500	0.06159300
C	1.22212300	-0.77356900	-0.12322100
C	1.64699900	-0.54635300	1.31783100
C	2.34738800	-0.49303300	-1.11170100
H	0.91639100	-1.81154400	-0.25697700
H	0.82765100	-0.67694600	2.02876500
H	2.41483300	-1.28496700	1.55800900
H	2.09066000	0.44256700	1.45344900
H	2.00088800	-0.52694100	-2.14866600
H	2.83682100	0.46594500	-0.92970400
H	3.10179500	-1.27246100	-0.98858200
C	0.16773500	1.52684200	-0.52883100
C	-0.10217600	2.24817400	0.78251700
H	-0.49152100	1.90412700	-1.31121900
H	1.19082700	1.69335600	-0.86105300
H	0.18927800	3.29057200	0.63857600
H	-1.15831600	2.23953300	1.05621200
H	0.47856600	1.85414400	1.61611900

re-TS1

C	0.07307400	0.68907900	0.73356000
C	2.08262100	1.29799100	1.51044000
C	1.82019100	-1.10746400	1.08374500
H	0.97806900	-1.79471500	1.20645600
N	1.44854100	2.42140500	1.37268300
N	0.22149000	2.01507700	0.88540200
N	1.28622700	0.24240100	1.15376500
C	3.43834000	0.97631000	2.04796700
H	3.81788900	1.79125800	2.66379700

H	4. 14642500	0. 78777500	1. 22855700
C	2. 89669800	-1. 35135900	2. 20439200
O	3. 28778100	-0. 16324000	2. 87839400
C	3. 83162000	-1. 86447300	0. 02025600
C	2. 56572500	-1. 33433300	-0. 21433400
C	2. 12289700	-1. 04282500	-1. 50234600
C	2. 97528600	-1. 32026600	-2. 56949100
C	4. 24134100	-1. 86728100	-2. 34390000
C	4. 68007900	-2. 13925000	-1. 04959800
C	4. 08206900	-2. 05052200	1. 49548600
H	1. 14493100	-0. 59498400	-1. 67796000
H	4. 89415500	-2. 07244500	-3. 18631300
H	5. 67092600	-2. 54905500	-0. 87802800
H	5. 02750800	-1. 61121900	1. 82864700
H	4. 10968100	-3. 11249700	1. 75938000
C	-0. 76851500	2. 99662300	0. 55533900
C	-0. 61154900	3. 72310900	-0. 62860700
C	-1. 85852400	3. 16954400	1. 41092400
C	-1. 58647600	4. 66946200	-0. 93812900
C	-2. 81280800	4. 12337400	1. 05524300
C	-2. 68853100	4. 88513200	-0. 10743100
H	-1. 48827700	5. 24515600	-1. 85534300
H	-3. 67210700	4. 27446600	1. 70400200
H	2. 47766700	-1. 97761900	2. 99214000
H	2. 65615700	-1. 10301700	-3. 58349500
C	-1. 47566100	0. 06836400	-0. 83105200
O	-1. 00660300	0. 44426900	-1. 89819000
H	-2. 20003200	0. 67499100	-0. 25728600
C	-1. 49553500	-1. 42956600	-0. 51977400
C	-2. 39958100	-2. 13963100	-1. 52307700
H	-0. 48246900	-1. 83450300	-0. 57749500
H	-3. 41914500	-1. 74351500	-1. 43266600
H	-2. 02755200	-1. 84811000	-2. 51260800
C	-3. 71265700	5. 93575300	-0. 45238600
H	-4. 67855700	5. 71210600	0. 00559400
H	-3. 39363000	6. 91892200	-0. 09146900
H	-3. 85098700	6. 01179000	-1. 53342900
C	-1. 99970100	2. 33675600	2. 65751000
H	-2. 15837900	1. 28275600	2. 40519400
H	-1. 09317500	2. 38850500	3. 26790400
H	-2. 84370400	2. 68167300	3. 25685500
C	0. 55693200	3. 45479400	-1. 53803100
H	1. 50537100	3. 65059800	-1. 03015300
H	0. 54932700	2. 40359000	-1. 84507700

H	0.50198800	4.08109000	-2.43000500
Cl	-2.06706300	-1.71146700	1.17027500
C	-2.40733800	-3.66007500	-1.39998800
C	-3.24612900	-4.32357700	-2.49082400
H	-2.79373200	-3.95085200	-0.41618400
H	-1.37533000	-4.03269200	-1.45488200
C	-3.25946200	-5.84480900	-2.36879900
H	-4.27201500	-3.93853000	-2.43954800
H	-2.85582800	-4.03329400	-3.47393400
H	-3.86251600	-6.30492600	-3.15559800
H	-2.24532200	-6.24992800	-2.44164000
H	-3.67222800	-6.15421200	-1.40357800

si-TS1

C	-0.78385300	-0.98876900	0.25979000
C	-2.76737800	-1.88991600	-0.22877300
C	-2.85816900	0.36871000	0.85533400
H	-2.74738300	0.32826100	1.94026400
N	-1.90719300	-2.78936800	-0.59945600
N	-0.70102400	-2.20926800	-0.28637100
N	-2.13302500	-0.78764900	0.28982900
C	-4.25701300	-1.97276600	-0.35981100
H	-4.60122100	-2.95404800	-0.02921100
H	-4.54235400	-1.84878400	-1.41265600
C	-4.32591100	0.28108600	0.37118800
O	-4.88339400	-1.01100700	0.46122300
C	-3.25206100	2.00085900	-0.83921200
C	-2.43202600	1.68347800	0.24876600
C	-1.44731900	2.55784700	0.68960000
C	-1.24580700	3.74390000	-0.01674300
C	-2.03352100	4.04690700	-1.12848700
C	-3.05132000	3.18465500	-1.53989100
C	-4.31220300	0.94288600	-1.02651900
H	-0.86887400	2.30711000	1.57302200
H	-1.86862200	4.97574300	-1.66538400
H	-3.68416100	3.44406300	-2.38326900
H	-4.01216900	0.23001300	-1.80439600
H	-5.28930200	1.34425300	-1.30340900
C	0.50674100	-2.93202900	-0.55860400
C	1.17085800	-2.68455700	-1.76083300
C	0.96550100	-3.84941700	0.38776700
C	2.35349900	-3.38077100	-1.99908500
C	2.15609100	-4.52042900	0.10845500
C	2.86065400	-4.29794700	-1.07557100

H	2. 89509500	-3. 19824200	-2. 92413400
H	2. 54126200	-5. 23358200	0. 83325600
H	-4. 92303500	0. 90133500	1. 04396000
H	-0. 48261400	4. 44323300	0. 31132000
C	0. 47255500	-0. 12271800	1. 77892900
O	-0. 29245900	0. 36345400	2. 61599300
H	0. 90987000	-1. 13168100	1. 91319500
C	1. 34787700	0. 80882200	0. 91873400
C	2. 04296300	1. 85550900	1. 77905800
H	0. 74464100	1. 28965700	0. 14867500
H	1. 25831700	2. 32738700	2. 38322600
H	2. 72394900	1. 35990900	2. 48236300
C	0. 18694400	-4. 10718400	1. 65084600
H	-0. 78845100	-4. 54630500	1. 41957300
H	0. 72875800	-4. 79142000	2. 30559100
H	-0. 00262400	-3. 18005900	2. 20129000
C	4. 12985300	-5. 05671100	-1. 36699400
H	4. 65661500	-5. 31448100	-0. 44547700
H	3. 90883900	-5. 99060200	-1. 89410600
H	4. 80228400	-4. 47215600	-1. 99883800
C	0. 63323400	-1. 67145100	-2. 73380400
H	-0. 40611500	-1. 89166400	-2. 99598800
H	0. 65565700	-0. 67106400	-2. 28845600
H	1. 22893100	-1. 65814500	-3. 64789500
Cl	2. 56356200	-0. 19029300	0. 02671400
C	2. 78407100	2. 91719100	0. 97233000
C	3. 35214300	4. 02953200	1. 85067300
H	2. 09544200	3. 35107900	0. 23319100
H	3. 59629100	2. 44909200	0. 40336100
C	4. 10181400	5. 08417300	1. 04112800
H	2. 53407200	4. 50245800	2. 40854200
H	4. 02320300	3. 59053200	2. 59933200
H	4. 49952800	5. 87500700	1. 68231400
H	4. 94058600	4. 63510700	0. 50007500
H	3. 44115700	5. 54943900	0. 30258200

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C	0. 06476800	0. 54700800	0. 32887600
C	1. 89827900	1. 17723200	1. 35592900
C	1. 88896500	-1. 21314400	0. 75588500
H	1. 10052700	-1. 96475200	0. 77329300
N	1. 19091600	2. 26125100	1. 26186600
N	0. 05680600	1. 84990900	0. 61734700
N	1. 24287500	0. 10246100	0. 81284400

C	3. 20108000	0. 91910000	2. 03593800
H	3. 43658700	1. 72840500	2. 72606800
H	4. 01239900	0. 82244000	1. 30139900
C	2. 83793300	-1. 43140300	1. 99650700
O	3. 02513600	-0. 26793900	2. 78569500
C	4. 06503800	-1. 75742100	-0. 07876400
C	2. 79288800	-1. 33090500	-0. 44928200
C	2. 45734900	-1. 05534400	-1. 77264500
C	3. 44609600	-1. 23043500	-2. 73931900
C	4. 72565500	-1. 66588800	-2. 38229400
C	5. 04576900	-1. 93142600	-1. 05224700
C	4. 16463100	-1. 97235800	1. 40961700
H	1. 45409700	-0. 69893000	-2. 02242100
H	5. 48208100	-1. 79277400	-3. 15038700
H	6. 04381800	-2. 26090300	-0. 77955600
H	5. 01202400	-1. 44870200	1. 86349600
H	4. 27892700	-3. 03407600	1. 64857300
C	-0. 96894500	2. 80306800	0. 29009900
C	-0. 83070800	3. 53374800	-0. 89180600
C	-2. 03857700	2. 95575600	1. 17347400
C	-1. 82861300	4. 46321000	-1. 18011400
C	-3. 01117300	3. 89613400	0. 83793100
C	-2. 91881400	4. 65793400	-0. 32899000
H	-1. 75437400	5. 04534500	-2. 09515800
H	-3. 85988900	4. 03509300	1. 50261700
H	2. 37985700	-2. 14650300	2. 67963500
H	3. 22226200	-1. 02307500	-3. 78077400
C	-0. 95031800	-0. 07421300	-0. 65984900
O	-0. 49983100	0. 13763000	-1. 89277200
H	-1. 90676800	0. 44025800	-0. 38549400
C	-1. 21087100	-1. 57220500	-0. 39257700
C	-2. 37252500	-2. 06020600	-1. 23717000
H	-0. 31362700	-2. 15266300	-0. 62548300
H	-3. 28628600	-1. 54499300	-0. 91325600
H	-2. 14535900	-1. 71082700	-2. 25096300
C	-3. 96602100	5. 69182900	-0. 65305300
H	-4. 92854700	5. 43279900	-0. 20695700
H	-3. 67198200	6. 67146800	-0. 26270600
H	-4. 09913400	5. 79333200	-1. 73236300
C	-2. 13331600	2. 11758200	2. 42013800
H	-2. 25854300	1. 05760200	2. 17067800
H	-1. 22409700	2. 20500500	3. 02252000
H	-2. 98369400	2. 42814000	3. 02853000
C	0. 33885800	3. 29131800	-1. 80563100

H	1.28300800	3.50756600	-1.29544600
H	0.33992900	2.23617900	-2.10519000
H	0.27193800	3.92492600	-2.69143400
Cl	-1.54777600	-1.85442400	1.38588900
C	-2.57966300	-3.57073200	-1.22807000
C	-3.72087900	-4.00686400	-2.14509400
H	-2.78541400	-3.91196700	-0.20579200
H	-1.65106500	-4.06638900	-1.54255700
C	-3.92538000	-5.51924800	-2.14290800
H	-4.64550100	-3.50727300	-1.83045400
H	-3.51534400	-3.66104600	-3.16554800
H	-4.74560200	-5.81493900	-2.80200500
H	-3.02048400	-6.03458100	-2.48001200
H	-4.15646200	-5.87932900	-1.13545600

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C	-0.42680900	-0.92768600	0.30233700
C	-2.32685300	-1.67281900	-0.48617400
C	-2.55326100	0.35733100	0.98058100
H	-2.43397000	0.07275500	2.02529400
N	-1.45412000	-2.57315900	-0.82565000
N	-0.27744600	-2.09186300	-0.32736400
N	-1.74648100	-0.63848300	0.20969600
C	-3.79345100	-1.71758900	-0.77395300
H	-4.12972600	-2.75452500	-0.74831400
H	-3.99078500	-1.31639800	-1.77591900
C	-4.00932800	0.28946700	0.44827900
O	-4.49850600	-1.01214100	0.22036000
C	-3.07798300	2.32482600	-0.26777300
C	-2.23549400	1.81197400	0.72395100
C	-1.36259900	2.63679200	1.42613300
C	-1.29554300	3.98386500	1.07168800
C	-2.09883900	4.49007900	0.04686100
C	-3.00608200	3.66778400	-0.62134200
C	-4.03498200	1.26458200	-0.74948000
H	-0.74420800	2.19714200	2.20270200
H	-2.03485400	5.54131100	-0.21585300
H	-3.65822900	4.07400600	-1.38837500
H	-3.66349400	0.79198500	-1.66653800
H	-5.03982800	1.64021700	-0.95217500
C	0.89959000	-2.91681900	-0.36688000
C	1.54228400	-3.11660800	-1.58824400
C	1.30258200	-3.52555400	0.82783900
C	2.67653800	-3.92867500	-1.58326900

C	2.44397400	-4.32264600	0.77703100
C	3.14742600	-4.52483800	-0.41319300
H	3.20239900	-4.09877200	-2.51918300
H	2.78568100	-4.80720500	1.68804100
H	-4.64102100	0.69998200	1.23958600
H	-0.61785000	4.64636100	1.60193800
C	0.60702700	-0.17333300	1.15621700
O	0.04462100	0.12071000	2.32486600
H	1.47984800	-0.87033300	1.19184400
C	1.14308400	1.05037600	0.34919200
C	2.06147500	1.90407500	1.19987000
H	0.32785900	1.64971000	-0.05774200
H	1.51734900	2.08076400	2.13458100
H	2.95241800	1.31854400	1.46294400
C	0.50938400	-3.36346200	2.10088200
H	-0.51906600	-3.71034900	1.95111500
H	0.95417500	-3.96210600	2.89713700
H	0.45215600	-2.32312700	2.44241300
C	4.39907300	-5.36324300	-0.42652000
H	4.58334200	-5.78375100	-1.41727400
H	5.26905600	-4.75670600	-0.15527500
H	4.33240800	-6.18281900	0.29260800
C	1.00944700	-2.51554800	-2.86060900
H	0.10389100	-3.03948400	-3.18134700
H	0.75208700	-1.46260000	-2.72220800
H	1.75079400	-2.59081700	-3.65773600
Cl	2.03185500	0.44671200	-1.13195500
C	2.45616200	3.22851000	0.55455100
C	3.24538000	4.12985500	1.50158600
H	1.54598100	3.75213100	0.22894300
H	3.04768900	3.04105300	-0.35020600
C	3.63983100	5.45424600	0.85378800
H	2.64408500	4.32065900	2.39954200
H	4.14421600	3.59957300	1.84003300
H	4.20100500	6.08926700	1.54413500
H	4.26277500	5.28490700	-0.03006900
H	2.75234300	6.00878000	0.53227100

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C	0.30905800	-0.20557400	0.80189400
C	1.35829500	-1.29810100	2.37494600
C	2.44247500	-1.50238100	0.17685300
H	2.10961800	-1.43681900	-0.86390100
N	0.37689700	-0.69853400	2.98112800

N	-0.25710700	-0.00687200	1.98994200
N	1.35754500	-1.01126200	1.03370300
C	2.33269400	-2.33373300	2.83606200
H	2.00160300	-2.76835700	3.77822400
H	3.33601100	-1.90934400	2.96276100
C	2.79495700	-2.98612800	0.56883200
O	2.29486500	-3.34888200	1.84745700
C	4.79270900	-1.62580600	0.59343600
C	3.73086200	-0.74071000	0.41886000
C	3.91798100	0.63588900	0.48471200
C	5.20108000	1.12194500	0.72256500
C	6.27095400	0.23970200	0.88915900
C	6.07529300	-1.13816000	0.82643600
C	4.33337300	-3.05724900	0.49371800
H	3.09052400	1.32686300	0.35633100
H	7.26446800	0.63308700	1.07667800
H	6.90686200	-1.82124700	0.96721200
H	4.71717700	-3.69599400	1.29377800
H	4.64370600	-3.50067300	-0.45786000
C	-1.38654400	0.83478600	2.30364400
C	-1.16043400	2.17397100	2.60889500
C	-2.65568800	0.24120600	2.31385500
C	-2.28499300	2.95681300	2.89520800
C	-3.73519600	1.06040500	2.61129400
C	-3.56933200	2.42301700	2.89478900
H	-2.13954300	4.00749800	3.13288000
H	-4.73393600	0.63166900	2.62198900
H	2.31690000	-3.68604500	-0.11622500
H	5.36872200	2.19175600	0.78023900
C	-0.15933500	0.34552200	-0.52898600
O	-1.54417100	0.32208200	-0.58146400
H	0.20796500	-0.33819900	-1.30926600
C	0.45249100	1.76615500	-0.74359700
C	-0.59871900	2.84386200	-0.94458900
H	1.07551600	2.04312700	0.11121300
H	-1.21475300	2.60893000	-1.81864900
H	-1.26941500	2.77678800	-0.07725500
C	-4.76943600	3.27986500	3.19953600
H	-5.33596100	2.86808200	4.03919400
H	-4.47615500	4.30071700	3.44976100
H	-5.44350000	3.31783700	2.33896100
C	-2.81855600	-1.21951200	2.00073500
H	-2.43537700	-1.42799500	0.99721300
H	-2.26299100	-1.83956400	2.71079900

H	-3.86970300	-1.50758900	2.03921100
C	0.21134900	2.79708200	2.64400700
H	1.01576800	2.05926700	2.60103500
H	0.33674800	3.49928100	1.81243200
H	0.33670500	3.36856200	3.56636900
Cl	1.62649800	1.69820200	-2.12609500
C	-0.01736300	4.25154500	-1.05202000
C	-1.09758000	5.32275800	-0.91400300
H	0.49991900	4.36740900	-2.01137500
H	0.74431500	4.40379600	-0.27376400
C	-0.53769000	6.73490400	-1.05611500
H	-1.87365600	5.15177600	-1.66991400
H	-1.58678100	5.21075900	0.06237100
H	-1.32187400	7.48809700	-0.94826600
H	0.22411100	6.93043400	-0.29498600
H	-0.07132900	6.87203800	-2.03641700
H	-1.71474400	-0.34430600	-1.33684100
N	-1.78406700	-1.42681700	-2.52630700
C	-2.29110500	-0.60143100	-3.66389400
C	-1.20409000	0.35434700	-4.15221000
C	-3.52440500	0.20871500	-3.25885400
H	-2.57790600	-1.25989000	-4.49518300
H	-0.33567500	-0.15390600	-4.57612000
H	-1.61428600	1.00495900	-4.92764200
H	-0.85958000	0.98744700	-3.32815000
H	-4.39735500	-0.41741700	-3.06415400
H	-3.31849100	0.81481600	-2.36988500
H	-3.78424200	0.88513200	-4.07607500
C	-0.55612900	-2.19993300	-2.88664200
C	-0.61359000	-2.97762800	-4.20777100
C	-0.12800300	-3.13239400	-1.75483500
H	0.23551200	-1.44986700	-3.00692700
H	-0.80130100	-2.32800800	-5.06481500
H	0.35470000	-3.45923900	-4.36943700
H	-1.37629700	-3.75779900	-4.19497300
H	-0.13573600	-2.63394700	-0.77721200
H	-0.77447900	-4.01171500	-1.68428100
H	0.88478500	-3.48992700	-1.95842200
C	-2.85591300	-2.23105400	-1.88463700
C	-3.61453100	-3.24218400	-2.74338200
H	-3.56648000	-1.51681200	-1.45967400
H	-2.41437400	-2.74149500	-1.02600000
H	-4.49418800	-3.58410500	-2.19207100
H	-3.96178900	-2.80564300	-3.68387300

H	-3.01105500	-4.12184600	-2.97486500
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C	-0.32018600	0.54507700	-0.29923400
C	-1.95630200	0.61934200	-1.74367700
C	-2.68275400	-0.13915100	0.47935200
H	-2.20671600	-0.66234300	1.31074900
N	-0.93717400	1.13363800	-2.36530600
N	0.07431600	1.09751200	-1.44841600
N	-1.62646900	0.26615900	-0.46568500
C	-3.31632300	0.22653900	-2.22679300
H	-3.31432800	0.12811700	-3.31157600
H	-4.07305700	0.96318300	-1.92951900
C	-3.73262100	-1.05643800	-0.25689600
O	-3.56349400	-1.05198600	-1.66664200
C	-4.85008100	0.84096100	0.74938300
C	-3.48672900	1.06609800	0.92800100
C	-3.01188700	2.27167500	1.43807000
C	-3.93577400	3.25787700	1.77356200
C	-5.30472700	3.03580900	1.60325900
C	-5.77114000	1.82755300	1.09182700
C	-5.11496400	-0.52641400	0.17726700
H	-1.94819300	2.43540000	1.57559600
H	-6.01130500	3.81562300	1.86743100
H	-6.83448600	1.65977800	0.95291800
H	-5.79636900	-0.51523100	-0.67847700
H	-5.55181200	-1.18911400	0.93038900
C	1.29422000	1.80814100	-1.75324000
C	1.49886500	3.02846100	-1.09392100
C	2.14769700	1.31082500	-2.73875000
C	2.66135100	3.72772600	-1.40157700
C	3.29196500	2.06127900	-3.01418600
C	3.57168700	3.25550300	-2.35240100
H	2.85297100	4.67274700	-0.90033700
H	3.98120100	1.69680600	-3.77079000
H	-3.59187400	-2.10004900	0.02785600
H	-3.58922900	4.20613600	2.17013200
C	0.41479900	0.16229200	0.96897600
O	-0.29095800	0.83468400	1.98962000
H	0.29926900	-0.93661300	1.03627300
C	1.92546500	0.44226700	1.03610400
C	2.44303300	0.24413900	2.45600000
H	2.17965300	1.44304000	0.68509500
H	1.94438300	0.99408300	3.08152000

H	2. 14199300	-0. 74821400	2. 81918100
C	1. 88201400	0. 02154800	-3. 46769500
H	2. 47984100	-0. 02182400	-4. 37905900
H	2. 15628800	-0. 83524100	-2. 84386100
H	0. 82939800	-0. 08297200	-3. 73927000
C	4. 81348700	4. 04651700	-2. 66704700
H	4. 55247200	5. 01249500	-3. 10881100
H	5. 38547900	4. 24731400	-1. 75729000
H	5. 45683700	3. 51274500	-3. 36821100
C	0. 50178300	3. 56983300	-0. 10004900
H	-0. 51153300	3. 56490300	-0. 51527400
H	0. 48213100	2. 98854800	0. 82992800
H	0. 75425800	4. 59785300	0. 16113100
Cl	2. 73086000	-0. 70237400	-0. 10137400
C	3. 95275100	0. 42199000	2. 59855000
C	4. 39907900	0. 36157300	4. 05840400
H	4. 24588100	1. 38696400	2. 16368200
H	4. 47385900	-0. 35277800	2. 02617100
C	5. 90937000	0. 52168000	4. 20636300
H	3. 88482600	1. 14506600	4. 62811500
H	4. 08347800	-0. 59553100	4. 49149600
H	6. 21415200	0. 47700300	5. 25463800
H	6. 43944000	-0. 26918900	3. 66709700
H	6. 24071600	1. 48205000	3. 79970300
H	-0. 15940200	0. 37542400	2. 83008200
N	0. 30000000	-3. 33715400	0. 34956300
C	-0. 08061000	-3. 99253000	1. 61371500
C	-1. 13908500	-3. 17670600	2. 35960700
C	1. 12956400	-4. 16893000	2. 53213900
H	-0. 50498900	-4. 99457600	1. 42873100
H	-2. 07375100	-3. 06947400	1. 80286400
H	-1. 38203700	-3. 66493500	3. 30616600
H	-0. 74806800	-2. 17758900	2. 59284000
H	1. 83495600	-4. 91511500	2. 16125800
H	1. 65946200	-3. 21588900	2. 64131400
H	0. 79483000	-4. 49415400	3. 51995600
C	-0. 84128300	-3. 07853700	-0. 55104100
C	-1. 80417700	-4. 24596500	-0. 81427900
C	-0. 39799600	-2. 45974200	-1. 87402700
H	-1. 43050600	-2. 30528100	-0. 04358700
H	-2. 22706200	-4. 65280100	0. 10840600
H	-2. 63446200	-3. 88624800	-1. 43167000
H	-1. 31738600	-5. 06280300	-1. 35196700
H	0. 32087700	-1. 65095500	-1. 70499300

H	0.07162600	-3.19366400	-2.53645700
H	-1.27518100	-2.05893000	-2.39033600
C	1.48968900	-3.91599000	-0.28376900
C	1.40772900	-5.37865700	-0.73209100
H	2.31974200	-3.79795300	0.41650900
H	1.75515300	-3.28912300	-1.13804100
H	2.40118700	-5.73123900	-1.02338700
H	1.04494100	-6.02965200	0.06954700
H	0.74760600	-5.50425600	-1.59386100

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C	-0.05399900	-0.26442100	0.58664600
C	0.93083000	-1.76924400	1.87368200
C	2.37847900	-1.00716100	0.06282500
H	2.25022700	-0.64900200	-0.96054700
N	-0.19235600	-1.53361200	2.46484200
N	-0.80038500	-0.58590300	1.67147300
N	1.07060600	-1.02345100	0.72719000
C	2.00599600	-2.76253800	2.17828100
H	1.61327200	-3.55356500	2.81619300
H	2.85467000	-2.28162200	2.68149600
C	3.00044200	-2.45003700	0.02691400
O	2.37686600	-3.33978900	0.93932900
C	4.58573300	-0.88312700	0.97355200
C	3.38409100	-0.18792200	0.84937000
C	3.21055500	1.06262900	1.43597600
C	4.28143100	1.63179500	2.12213300
C	5.49632200	0.95120600	2.22383300
C	5.65463500	-0.31226600	1.65743500
C	4.50168500	-2.23812100	0.31856200
H	2.25786000	1.58577700	1.38950200
H	6.32011900	1.40451900	2.76493100
H	6.59234000	-0.84924700	1.76075500
H	4.87919900	-3.04757200	0.94972000
H	5.07135300	-2.25866000	-0.61601500
C	-2.00227300	0.03098900	2.16842200
C	-1.92318100	1.36743900	2.59546900
C	-3.16623700	-0.72958500	2.29335900
C	-3.08297800	1.96175300	3.07340900
C	-4.30796300	-0.07947500	2.77644300
C	-4.29133300	1.25856900	3.15408000
H	-3.04482600	2.99646900	3.40385400
H	-5.22767000	-0.65115300	2.87175000
H	2.84143700	-2.90639500	-0.95033100

H	4.16621200	2.60451800	2.58754900
C	-0.45636700	0.51362500	-0.58935200
O	-1.59643600	1.32272600	-0.34354700
H	-0.98985200	-0.43611100	-1.57898400
C	0.65200300	1.39120600	-1.17426400
C	0.28181400	2.86173100	-1.33521800
H	1.56746100	1.33313400	-0.58535100
H	-0.53296100	2.95916500	-2.06022400
H	-0.12685300	3.19808300	-0.37556100
C	-5.53611700	1.94426700	3.65134400
H	-6.32871100	1.22407500	3.86156700
H	-5.33132100	2.51137700	4.56288300
H	-5.90945500	2.65114000	2.90408500
C	-3.23225300	-2.20824700	2.00932400
H	-2.35272000	-2.58094000	1.48517100
H	-3.30193700	-2.75702500	2.95296200
H	-4.12638300	-2.44448000	1.42591100
C	-0.61831400	2.11530500	2.56419700
H	0.17859900	1.53555300	3.04223800
H	-0.31770000	2.32469000	1.53340900
H	-0.71108000	3.06684100	3.08896600
Cl	1.23938300	0.76273700	-2.81521700
C	1.46183900	3.75026100	-1.71951300
C	1.07766600	5.22866600	-1.75218800
H	1.85101900	3.45541800	-2.70029100
H	2.27942100	3.60172300	-0.99985400
C	2.25126200	6.12292400	-2.14195100
H	0.25257600	5.36957800	-2.46099600
H	0.69472100	5.52650700	-0.76840800
H	1.96229100	7.17657800	-2.16072600
H	3.07721200	6.01276400	-1.43240900
H	2.62843100	5.85920500	-3.13474100
H	-2.36132700	0.75989900	-0.17066200
N	-1.70270500	-1.28097000	-2.28608800
C	-2.75911000	-0.58846100	-3.10940800
C	-2.11664000	0.47942700	-3.99002600
C	-3.88041300	0.04704600	-2.28937700
H	-3.21732300	-1.35644900	-3.74045600
H	-1.38157800	0.07923700	-4.69040400
H	-2.89636000	0.97535900	-4.57188100
H	-1.62516500	1.23190700	-3.36482000
H	-4.39477300	-0.65126500	-1.62649100
H	-3.51998400	0.90625900	-1.71944900
H	-4.62475500	0.42376600	-2.99447700

C	-0.71394700	-2.01807500	-3.16278900
C	-1.32265900	-2.86227500	-4.28437700
C	0.25430300	-2.83724500	-2.31714500
H	-0.13195800	-1.22417100	-3.63009000
H	-1.82992100	-2.25412500	-5.03566200
H	-0.50262000	-3.37897400	-4.78945700
H	-2.01865800	-3.61993100	-3.92172800
H	0.62773400	-2.25740900	-1.46843500
H	-0.19656400	-3.75794200	-1.93533900
H	1.10969000	-3.11478200	-2.93731100
C	-2.26056100	-2.09216200	-1.17168200
C	-3.17936200	-3.24909500	-1.54158900
H	-2.78838700	-1.39159600	-0.51741200
H	-1.41101800	-2.46093200	-0.59026000
H	-3.66152700	-3.61913600	-0.63383400
H	-3.96440900	-2.94664300	-2.23926600
H	-2.62573000	-4.08098700	-1.97894900

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C	-0.41242900	0.28715200	-0.40010900
C	-2.02730900	0.69365000	-1.84922300
C	-2.89835600	-0.07178100	0.31003800
H	-2.55826000	-0.76514500	1.07418400
N	-0.95225400	1.06595800	-2.45984100
N	0.05440900	0.83273900	-1.54707100
N	-1.76539400	0.21426800	-0.59038700
C	-3.43152400	0.62514800	-2.35098200
H	-3.43846100	0.62205800	-3.44041300
H	-4.01924400	1.47966700	-1.98913200
C	-4.11472500	-0.67561000	-0.48982900
O	-3.95771800	-0.60741200	-1.89808500
C	-4.81198100	1.30607600	0.72917000
C	-3.43718300	1.20230000	0.92178600
C	-2.71999800	2.18387700	1.59902400
C	-3.40828800	3.29765800	2.07257300
C	-4.78697200	3.41390900	1.87451900
C	-5.49877400	2.41900200	1.20824200
C	-5.35696600	0.10545000	-0.00063500
H	-1.65279200	2.06853500	1.76505800
H	-5.30907500	4.28989400	2.24579700
H	-6.57014000	2.51285600	1.05951700
H	-5.99178800	0.36605800	-0.85318600
H	-5.95753700	-0.51832600	0.66851600
C	1.29974900	1.51164900	-1.80594300

C	1. 47919800	2. 76620800	-1. 20522700
C	2. 19964000	0. 97687000	-2. 72507500
C	2. 65841600	3. 44885900	-1. 48473400
C	3. 35809300	1. 71054400	-2. 98748500
C	3. 61203700	2. 93203700	-2. 36810200
H	2. 82829300	4. 41735300	-1. 02087500
H	4. 07895700	1. 31078500	-3. 69580800
H	-4. 20251800	-1. 74294700	-0. 28020300
H	-2. 87266000	4. 07985200	2. 60009900
C	0. 30232500	-0. 29092600	0. 73528600
O	-0. 56684800	-0. 13497000	1. 85562700
H	0. 45528700	-1. 77114200	0. 37957700
C	1. 70221400	0. 26346400	1. 05429900
C	2. 04711700	0. 15897500	2. 53471800
H	1. 85025400	1. 29707500	0. 73927100
H	1. 28501000	0. 73657200	3. 06852800
H	1. 95038600	-0. 88240200	2. 87073700
C	1. 96688700	-0. 35172700	-3. 38856500
H	2. 50799000	-0. 40631000	-4. 33465000
H	2. 33851400	-1. 15526700	-2. 74404300
H	0. 90688000	-0. 52849600	-3. 58674400
C	4. 87207400	3. 70478800	-2. 65718000
H	4. 63826200	4. 66783500	-3. 12037400
H	5. 41998000	3. 91172400	-1. 73371700
H	5. 53031800	3. 15258200	-3. 33015000
C	0. 42595200	3. 35623100	-0. 30185800
H	-0. 56748600	3. 29343300	-0. 75844900
H	0. 37495400	2. 83733000	0. 66305400
H	0. 64291300	4. 40564800	-0. 09922000
Cl	2. 96260100	-0. 62740300	0. 07037500
C	3. 43022000	0. 69380200	2. 89503800
C	3. 64204800	0. 76262900	4. 40633100
H	3. 55633800	1. 69578600	2. 46179500
H	4. 20515700	0. 06164400	2. 44761700
C	5. 03589600	1. 26398400	4. 77294700
H	2. 88282300	1. 41881900	4. 84934700
H	3. 48108400	-0. 23281800	4. 83874000
H	5. 17013900	1. 31785400	5. 85614600
H	5. 80671600	0. 59976400	4. 37016000
H	5. 21003700	2. 26322800	4. 36169300
H	-0. 51534700	-0. 92046500	2. 41122100
N	0. 37233200	-3. 03946000	0. 10849200
C	0. 57567900	-3. 83152500	1. 37337500
C	-0. 26613600	-3. 28373700	2. 52624800

C	2. 04135600	-3. 87047700	1. 80144500
H	0. 25204200	-4. 85494700	1. 16302500
H	-1. 27457300	-2. 97959600	2. 23505400
H	-0. 37030200	-4. 05647400	3. 29068200
H	0. 25277100	-2. 44758400	3. 00964900
H	2. 65907300	-4. 48689200	1. 14646600
H	2. 46947700	-2. 86363700	1. 83690200
H	2. 09423700	-4. 29929300	2. 80491700
C	-1. 05693000	-3. 10299200	-0. 39351100
C	-1. 75769600	-4. 45174900	-0. 21985400
C	-1. 17748900	-2. 62160800	-1. 83978900
H	-1. 58583000	-2. 37776100	0. 23493100
H	-1. 89714800	-4. 72464300	0. 82786600
H	-2. 75009600	-4. 37337400	-0. 67144400
H	-1. 22841100	-5. 26312800	-0. 72313900
H	-0. 59720600	-1. 71502900	-2. 03346000
H	-0. 85155400	-3. 38714200	-2. 54901200
H	-2. 22641400	-2. 39247700	-2. 04624900
C	1. 39032700	-3. 39067100	-0. 92574000
C	1. 38429600	-4. 83471000	-1. 41354900
H	2. 36040200	-3. 14393000	-0. 49996600
H	1. 24694200	-2. 70594900	-1. 76116800
H	2. 25189600	-4. 97825700	-2. 06213500
H	1. 46577700	-5. 55208400	-0. 59260500
H	0. 49497900	-5. 07762800	-1. 99713400

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C	-0. 00425800	0. 27201000	1. 04733800
C	0. 92672900	-1. 53234400	1. 85954400
C	2. 36991400	-0. 33816900	0. 27841000
H	2. 19041500	0. 32859400	-0. 56961600
N	-0. 24038000	-1. 47388700	2. 43059000
N	-0. 80482200	-0. 34070000	1. 92138700
N	1. 11157200	-0. 48039600	1. 00418600
C	1. 98745500	-2. 58523200	1. 86388900
H	1. 59614700	-3. 51272000	2. 28025200
H	2. 85743300	-2. 26182900	2. 44886600
C	2. 87703200	-1. 73652400	-0. 21697900
O	2. 31192900	-2. 82392000	0. 50447000
C	4. 63806800	-0. 59074900	0. 97514800
C	3. 47919800	0. 15396000	1. 18595800
C	3. 42660300	1. 16294500	2. 14171300
C	4. 58041600	1. 44475400	2. 87101100
C	5. 75267600	0. 72101400	2. 64580600

C	5.78894700	-0.30515900	1.70265500
C	4.41040500	-1.65979800	-0.06453900
H	2.50683000	1.70758700	2.34105900
H	6.64170300	0.95050400	3.22395900
H	6.69648000	-0.88074000	1.54855800
H	4.80966900	-2.63697400	0.21950600
H	4.86806000	-1.37985900	-1.01953300
C	-2.07320800	0.12137200	2.42516700
C	-2.06564600	1.12166700	3.39546900
C	-3.23476800	-0.47841100	1.93633700
C	-3.30280800	1.51827500	3.90260000
C	-4.44245900	-0.04642900	2.47449200
C	-4.49399400	0.94919200	3.45444200
H	-3.33327700	2.29696800	4.66014900
H	-5.36714800	-0.48935100	2.11345800
H	2.57407000	-1.90678800	-1.25050500
H	4.56333800	2.22582000	3.62352700
C	-0.34591500	1.46112400	0.25060000
O	-1.62521100	1.44796500	-0.16399200
C	0.58006200	2.39916900	-0.00806400
C	0.35987700	3.58961600	-0.88476600
H	1.56818100	2.28618100	0.43359300
H	-0.62105600	3.51510300	-1.36357900
H	0.33010000	4.49683000	-0.26780700
C	-5.82010500	1.42469100	3.98688400
H	-6.23161100	2.20116100	3.33432000
H	-6.54492400	0.60838900	4.02886900
H	-5.71590400	1.85136600	4.98661900
C	-3.16299700	-1.51337900	0.84844700
H	-2.70521800	-1.07622300	-0.04500000
H	-2.55695100	-2.37212800	1.15169600
H	-4.16097300	-1.86856200	0.58851000
C	-0.78382200	1.76432900	3.85528900
H	0.00114100	1.02209200	4.03119000
H	-0.41909500	2.47297000	3.10259900
H	-0.94601100	2.31687200	4.78175700
Cl	-2.78863600	3.95485200	0.74278500
C	1.47157500	3.72214900	-1.93165200
C	1.28463300	4.94151200	-2.83106200
H	1.50057500	2.81347700	-2.54748500
H	2.44461500	3.78699900	-1.42547600
C	2.39128000	5.07116100	-3.87376900
H	0.30996800	4.87328000	-3.32909400
H	1.25126200	5.84428200	-2.20904000

H	2. 23938200	5. 94519700	-4. 51226700
H	3. 37002700	5. 17135700	-3. 39393700
H	2. 42493000	4. 18634100	-4. 51727500
H	-2. 06816300	2. 32759800	0. 09014800

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C	-0. 02327400	-0. 37401100	-0. 24221900
C	1. 34589700	-1. 77659400	-1. 20594600
C	2. 39929300	0. 38175200	-0. 62856400
H	2. 02442000	1. 40496500	-0. 55889900
N	0. 22326200	-2. 42640100	-1. 11286900
N	-0. 61871200	-1. 54407900	-0. 49561900
N	1. 23964000	-0. 51834700	-0. 68197000
C	2. 62538800	-2. 11205900	-1. 89933800
H	2. 47959400	-2. 95091400	-2. 57883100
H	3. 41179700	-2. 36273300	-1. 17535100
C	3. 29050300	0. 18588200	-1. 91194000
O	2. 95193800	-0. 96966900	-2. 66878300
C	4. 62417700	-0. 13276600	0. 08792300
C	3. 31025700	0. 01767300	0. 52445200
C	2. 95954200	-0. 16615500	1. 85871500
C	3. 96138800	-0. 51579400	2. 76097100
C	5. 28204100	-0. 67029000	2. 33104100
C	5. 62370000	-0. 47706500	0. 99428900
C	4. 74399200	0. 13468800	-1. 39030300
H	1. 93197900	-0. 02145800	2. 17814800
H	6. 05018100	-0. 94424300	3. 04706900
H	6. 65063700	-0. 59869800	0. 66359200
H	5. 30675700	-0. 63359900	-1. 92884100
H	5. 24345700	1. 09148100	-1. 57218800
C	-1. 94101700	-1. 95910900	-0. 11257400
C	-2. 19667400	-2. 18033200	1. 24478600
C	-2. 89334500	-2. 13646600	-1. 11634500
C	-3. 48347300	-2. 58734400	1. 58632300
C	-4. 16558300	-2. 54891800	-0. 71934300
C	-4. 47715900	-2. 77524200	0. 62122800
H	-3. 71526500	-2. 76801200	2. 63296100
H	-4. 92997200	-2. 69219800	-1. 47820700
H	3. 13289000	1. 01431800	-2. 60191500
H	3. 71554300	-0. 66620900	3. 80691600
C	-0. 56721500	0. 83291600	0. 40359700
O	0. 32428500	1. 44285600	1. 19311600
C	-1. 82719600	1. 22223300	0. 14223000
C	-2. 43575100	2. 46358700	0. 71184100

H	-2.42613400	0.62586000	-0.54234500
H	-3.34736600	2.19750600	1.26422100
H	-1.73542600	2.91371700	1.42222700
C	-2.55784300	-1.88350000	-2.56204700
H	-3.45451300	-1.95188100	-3.17899300
H	-2.12116200	-0.88871400	-2.69954100
H	-1.82771400	-2.61091700	-2.92761600
C	-5.85662200	-3.21779700	1.03409400
H	-5.81634600	-4.18327500	1.54632400
H	-6.30279500	-2.49935600	1.72747700
H	-6.51671200	-3.31582300	0.17058600
C	-1.13235900	-1.97543300	2.29023000
H	-0.95115500	-0.90872900	2.46360600
H	-1.44010600	-2.42170700	3.23666600
H	-0.18305500	-2.42928700	1.98924600
Cl	0.89580100	3.83214100	0.18793200
C	-2.79263800	3.48643800	-0.37410200
C	-3.33858000	4.78539800	0.21275600
H	-3.53054900	3.05069600	-1.06127300
H	-1.89277400	3.70251800	-0.96142600
C	-3.71353500	5.79901400	-0.86475300
H	-4.21363200	4.56426900	0.83720200
H	-2.58048300	5.21561900	0.87876200
H	-4.09491600	6.72638200	-0.42954900
H	-2.84371900	6.04893800	-1.48005100
H	-4.48566200	5.39597000	-1.52792000
H	0.53098100	2.46117700	0.81962200

re-TS2^D

C	0.23962100	-0.01278100	0.94869200
C	0.91960600	-1.98055800	1.67190000
C	2.55248400	-0.79410700	0.26953300
H	2.49680900	-0.27160500	-0.68457300
N	-0.14919300	-1.74141600	2.36152600
N	-0.56820300	-0.51690100	1.90378600
N	1.18881700	-0.97659600	0.77411500
C	1.88782800	-3.11585000	1.76141000
H	1.37406100	-4.04119300	2.02303600
H	2.64040500	-2.90017400	2.53406400
C	3.26360000	-2.18023200	0.06523900
O	2.47802400	-3.28258900	0.49059900
C	4.53629500	-0.79084300	1.60749600
C	3.38646300	-0.06787500	1.30084700
C	3.07874500	1.13176000	1.94168400

C	3.97408200	1.60864600	2.89736700
C	5.13903100	0.89843600	3.20073800
C	5.42703300	-0.30547900	2.56220500
C	4.61767700	-2.06848500	0.80997600
H	2.15744800	1.68195100	1.73276100
H	5.82211400	1.28486000	3.95041000
H	6.32519000	-0.86181700	2.81300300
H	4.77824000	-2.95231900	1.43629400
H	5.44216000	-2.03485200	0.09137100
C	-1.79066300	0.05673900	2.38010100
C	-1.76833100	0.78111500	3.57458600
C	-2.95025800	-0.14988700	1.63137900
C	-2.97931600	1.29583500	4.03064100
C	-4.13646700	0.39525900	2.12354200
C	-4.16818900	1.11473700	3.31866100
H	-2.99463200	1.86025400	4.95989700
H	-5.05619500	0.24683900	1.56321800
H	3.41029500	-2.35691600	-1.00003400
H	3.76101900	2.53815900	3.41515900
C	0.06183900	1.27811600	0.35079000
O	-0.01069200	2.36489100	1.36006300
C	0.80782600	1.68154500	-0.89283800
C	0.36062400	3.04303600	-1.40418300
H	1.89997600	1.69659200	-0.76377000
H	-0.70738900	2.98855600	-1.65128600
H	0.45716800	3.72149000	-0.55042000
C	-5.45576300	1.71230000	3.82490600
H	-6.32216300	1.24515000	3.35217500
H	-5.54587600	1.59365800	4.90761800
H	-5.49370400	2.78472700	3.60849500
C	-2.90064200	-0.92178600	0.34036100
H	-2.28388200	-0.39092500	-0.39390900
H	-2.45644900	-1.91081500	0.48967500
H	-3.90182100	-1.04976200	-0.07365900
C	-0.46977400	1.01737700	4.29214700
H	0.03778900	0.07510300	4.51960100
H	0.18145200	1.60557000	3.63540600
H	-0.63380100	1.55986500	5.22470900
Cl	0.52101700	0.41578800	-2.19407100
C	1.16195400	3.56699600	-2.59073200
C	0.71361500	4.96288600	-3.01900800
H	1.06769500	2.87936400	-3.44004100
H	2.22839300	3.59319400	-2.32682300
C	1.51883500	5.49690900	-4.20023200

H	-0.35162400	4.93341300	-3.27974900
H	0.80362700	5.64909800	-2.16784000
H	1.18278400	6.49321500	-4.49892300
H	2.58223000	5.56172900	-3.94858100
H	1.42317700	4.83542000	-5.06715700
H	-0.93807400	1.86716800	0.67151400

si-TS2^D

C	-0.45367300	0.33913100	-0.64060600
C	-2.12805100	0.90452000	-1.96195500
C	-2.79564600	-0.43902200	0.05831900
H	-2.47826500	-1.47127600	0.19964900
N	-1.10774800	1.52082700	-2.46358500
N	-0.06618500	1.18656000	-1.62974900
N	-1.80051700	0.19125300	-0.83399000
C	-3.51466700	0.85631300	-2.52616700
H	-3.45482500	0.71533200	-3.60653100
H	-4.04086900	1.79929200	-2.33750200
C	-4.21304800	-0.30062600	-0.58262300
O	-4.20121900	-0.25510600	-1.99627900
C	-4.13081400	1.04699800	1.39259900
C	-2.95161900	0.30184200	1.36953200
C	-2.09153600	0.27931900	2.46157000
C	-2.41551900	1.04723000	3.57927900
C	-3.58873800	1.80501800	3.60400700
C	-4.45839300	1.80273400	2.51472500
C	-4.90315300	0.89795500	0.10964500
H	-1.20773800	-0.35400400	2.41825100
H	-3.83219300	2.39298400	4.48351300
H	-5.37784600	2.38004600	2.54186400
H	-4.83488400	1.81215200	-0.48921300
H	-5.96614600	0.70243300	0.26930500
C	1.25783800	1.61960300	-1.95889100
C	1.64495200	2.90873700	-1.58001100
C	2.10157800	0.74806800	-2.65296200
C	2.93685900	3.31670700	-1.90424900
C	3.38600200	1.20021000	-2.95237100
C	3.82041300	2.47415300	-2.58285100
H	3.26226000	4.31336700	-1.61701900
H	4.06176500	0.54065300	-3.49143100
H	-4.75848200	-1.21352300	-0.33575900
H	-1.75568100	1.04696700	4.44196100
C	0.37061200	-0.42780100	0.24233900
O	-0.25853100	-1.47873900	0.99934000

C	1.58881500	0.21320300	0.85134500
C	1.42235600	0.49466100	2.33750600
H	1.87170500	1.12497600	0.32439000
H	0.52114800	1.11858900	2.42222600
H	1.20371300	-0.44796800	2.84974100
C	1.63477100	-0.62514900	-3.05214500
H	2.34027000	-1.08540800	-3.74544900
H	1.54903800	-1.26720500	-2.16915700
H	0.65121000	-0.58311000	-3.52962600
C	5.22564600	2.92081500	-2.89154300
H	5.30205000	4.01005700	-2.90171800
H	5.92203200	2.54415400	-2.13553100
H	5.55664500	2.54007100	-3.86062900
C	0.69665400	3.79565600	-0.81861100
H	-0.24021400	3.93262500	-1.36582600
H	0.44223300	3.35077900	0.15080300
H	1.14359900	4.77439100	-0.63865700
Cl	3.05520600	-0.88780700	0.60725900
C	2.59395500	1.21973100	2.98986100
C	2.30337700	1.58449400	4.44473100
H	2.82118100	2.13411800	2.42316000
H	3.49193400	0.59276100	2.94395300
C	3.47172600	2.30551200	5.11112600
H	1.40526200	2.21400900	4.48737200
H	2.06512000	0.66997400	5.00208100
H	3.24833400	2.55712100	6.15113900
H	4.37051700	1.68107700	5.10131400
H	3.70759100	3.23479400	4.58290400
H	0.43050500	-1.54825600	-0.12437200

re-TS2^B

C	-0.09452700	-0.17759900	0.43386700
C	0.74243600	-1.89693900	1.57921200
C	2.35538600	-0.94450100	0.01487500
H	2.31086700	-0.50817500	-0.98551700
N	-0.39768700	-1.68469400	2.13967400
N	-0.91829300	-0.59537500	1.45350300
N	0.99888600	-1.02784600	0.54864800
C	1.75319000	-2.96488400	1.84118000
H	1.28141600	-3.82416600	2.31752000
H	2.55705800	-2.59374600	2.49253300
C	3.00402400	-2.37669200	-0.08906500
O	2.25294300	-3.37600500	0.58085400
C	4.44740900	-0.89641300	1.18809200

C	3. 28247200	-0. 17632600	0. 93411800
C	3. 06268400	1. 06771000	1. 52035100
C	4. 04375300	1. 59524300	2. 35702800
C	5. 21961300	0. 88306200	2. 60269600
C	5. 42793400	-0. 36718900	2. 02315500
C	4. 43765800	-2. 22345700	0. 47277300
H	2. 13729700	1. 61214200	1. 34744600
H	5. 97334500	1. 30307900	3. 26085300
H	6. 33688900	-0. 92442800	2. 22945500
H	4. 67534800	-3. 06695200	1. 12877300
H	5. 16672700	-2. 23491200	-0. 34370900
C	-2. 05510100	0. 06979000	2. 01345100
C	-1. 90797900	1. 40507700	2. 42924700
C	-3. 24983600	-0. 62720000	2. 22150100
C	-3. 00728600	2. 05394600	2. 97682200
C	-4. 32406300	0. 07013500	2. 78607300
C	-4. 23461000	1. 40815100	3. 14887000
H	-2. 89991200	3. 08852300	3. 29516000
H	-5. 25808300	-0. 46452600	2. 94661800
H	3. 01748500	-2. 70227900	-1. 13000000
H	3. 89008700	2. 56202400	2. 82481500
C	-0. 49153200	0. 68776700	-0. 66054600
O	-1. 62120500	1. 36713800	-0. 53502800
H	-0. 88934900	-0. 41534500	-1. 50274500
C	0. 68889200	1. 47421700	-1. 28336600
C	0. 36462800	2. 94549200	-1. 47667800
H	1. 61807800	1. 38652900	-0. 71730500
H	-0. 42272100	3. 04397800	-2. 23091600
H	-0. 08781100	3. 28895800	-0. 54012900
C	-5. 41608400	2. 14681800	3. 72214100
H	-6. 20307200	1. 45626700	4. 03310600
H	-5. 12324100	2. 74728500	4. 58783200
H	-5. 84311800	2. 83067300	2. 98155600
C	-3. 45932800	-2. 08533500	1. 88661100
H	-2. 52719300	-2. 60970500	1. 68144300
H	-3. 95008900	-2. 58667300	2. 72530000
H	-4. 12187900	-2. 18890800	1. 01972400
C	-0. 58422000	2. 10930300	2. 32771500
H	0. 22458100	1. 48781400	2. 72772100
H	-0. 37375400	2. 32846700	1. 27799300
H	-0. 60597200	3. 04653500	2. 88735200
C1	1. 23705700	0. 80543200	-2. 94736800
C	1. 57190400	3. 81012800	-1. 82587300
C	1. 21701400	5. 29242300	-1. 92725200

H	2. 01000200	3. 47839000	-2. 77494400
H	2. 35093900	3. 67621400	-1. 06084200
C	2. 42385000	6. 15835600	-2. 27876900
H	0. 43408300	5. 42298000	-2. 68456600
H	0. 78412700	5. 62772100	-0. 97643200
H	2. 15522100	7. 21578600	-2. 34765900
H	3. 20762000	6. 05889300	-1. 52092900
H	2. 85210400	5. 85593400	-3. 23967800
N	-1. 60750100	-1. 36931700	-2. 19804000
C	-2. 85256000	-0. 73685900	-2. 75624700
C	-2. 47797700	0. 51704300	-3. 54343400
C	-3. 87039500	-0. 37922200	-1. 67343300
H	-3. 31574600	-1. 46840200	-3. 42990500
H	-1. 77263100	0. 32035200	-4. 35479600
H	-3. 38263700	0. 94155600	-3. 98660100
H	-2. 05001600	1. 24236200	-2. 84339100
H	-4. 32452400	-1. 26359600	-1. 21771000
H	-3. 38674700	0. 24695000	-0. 91507500
H	-4. 67579600	0. 19046200	-2. 14547100
C	-0. 71267100	-1. 90806500	-3. 27663100
C	-1. 39671300	-2. 74945400	-4. 35848900
C	0. 47380500	-2. 64648900	-2. 66785200
H	-0. 31143200	-1. 02082800	-3. 76669100
H	-2. 09150200	-2. 16064700	-4. 96135500
H	-0. 62122500	-3. 12250000	-5. 03348300
H	-1. 93106900	-3. 61234300	-3. 95682200
H	0. 90630700	-2. 06647400	-1. 84855500
H	0. 20120000	-3. 63589600	-2. 28684700
H	1. 24338000	-2. 77850100	-3. 43259000
C	-1. 88704700	-2. 31437200	-1. 09045000
C	-2. 69057000	-3. 56816300	-1. 41981600
H	-2. 40365600	-1. 72138000	-0. 33933100
H	-0. 92808500	-2. 59695900	-0. 64405700
H	-3. 01622000	-4. 03078700	-0. 48333900
H	-3. 58406500	-3. 34391000	-2. 00986600
H	-2. 09697000	-4. 30802200	-1. 96091900

si-TS2^B

C	-0. 31522300	0. 14785800	-0. 31800900
C	-1. 95403300	0. 41732700	-1. 79700400
C	-2. 73921600	-0. 24796500	0. 45801700
H	-2. 34824500	-0. 98469100	1. 15695700
N	-0. 90782600	0. 81076100	-2. 43873500
N	0. 12957000	0. 66486000	-1. 51749100

N	-1.67591000	0.00959900	-0.52017900
C	-3.35927500	0.28822100	-2.28219300
H	-3.37480100	0.14317800	-3.36261200
H	-3.93592200	1.19124800	-2.03818600
C	-4.05324500	-0.72516100	-0.26438800
O	-3.91407800	-0.86145100	-1.67170400
C	-4.47247900	1.33707300	0.96133600
C	-3.13528800	1.01819000	1.17378500
C	-2.30188800	1.80835700	1.95974600
C	-2.83428200	2.97140400	2.51147100
C	-4.17128500	3.31590200	2.28557700
C	-5.00203700	2.49867700	1.52078300
C	-5.16571200	0.28145000	0.13680600
H	-1.28577800	1.46001400	2.14826200
H	-4.57054600	4.22709300	2.72033300
H	-6.04381100	2.76412100	1.36530800
H	-5.65588600	0.68550000	-0.75554400
H	-5.94365000	-0.22421300	0.71652400
C	1.29365500	1.46108400	-1.77146600
C	1.41125000	2.70975800	-1.14806700
C	2.23127600	1.00161800	-2.70009300
C	2.54279700	3.47506700	-1.43039400
C	3.33551300	1.80864000	-2.96609200
C	3.51596700	3.03829100	-2.33034200
H	2.65804100	4.44252600	-0.94723700
H	4.07595700	1.46508800	-3.68454300
H	-4.29871800	-1.73278900	0.07638200
H	-2.21331200	3.61242400	3.12969800
C	0.37566300	-0.40115800	0.81976100
O	-0.32436800	-0.56680300	1.94905100
H	0.36267000	-1.78976500	0.26387900
C	1.81650800	0.12935700	1.01246300
C	2.21839200	0.23531500	2.47250000
H	1.97549000	1.10031200	0.54528300
H	1.37011900	0.71143200	2.97635600
H	2.30812600	-0.76383400	2.91207500
C	2.04653600	-0.32619000	-3.38076700
H	2.82371400	-0.48927800	-4.12960400
H	2.10333900	-1.13281600	-2.64236600
H	1.06832000	-0.38707000	-3.86668100
C	4.74382300	3.86916400	-2.59980700
H	4.54870400	4.93047300	-2.43036900
H	5.56253400	3.57273800	-1.93597000
H	5.09088400	3.73983800	-3.62758900

C	0.35431500	3.19623300	-0.19106100
H	-0.65062500	3.03430900	-0.59456800
H	0.40206000	2.66068500	0.76536500
H	0.48029500	4.26112500	0.01206200
Cl	3.08193200	-0.88675800	0.10969700
C	3.49798700	1.03257000	2.70344000
C	3.82012100	1.19483800	4.18783700
H	3.39733900	2.02626900	2.24223600
H	4.34181800	0.54351700	2.20106600
C	5.09778500	1.99409000	4.42789600
H	2.97614200	1.68492400	4.68917600
H	3.91363700	0.20158200	4.64471400
H	5.31287000	2.10004600	5.49452900
H	5.95682900	1.50492200	3.95789000
H	5.01410100	2.99845200	4.00048500
N	0.15826900	-3.13040900	0.03649700
C	-0.01839400	-3.82657300	1.36082800
C	-1.32774200	-3.45367500	2.05916900
C	1.12626100	-3.47715700	2.31054900
H	-0.01223400	-4.90568600	1.16180800
H	-2.22517400	-3.68960900	1.48400500
H	-1.38213700	-4.02081200	2.99232500
H	-1.29212600	-2.38418200	2.28894200
H	2.11296000	-3.75986700	1.94042900
H	1.08713400	-2.40171300	2.50629200
H	0.96780300	-4.00666900	3.25373900
C	-1.07821400	-3.18504600	-0.81877900
C	-1.74021400	-4.56176300	-0.96699900
C	-0.82879500	-2.58645900	-2.20014600
H	-1.78603100	-2.53281500	-0.30136200
H	-1.85483300	-5.09510400	-0.02242300
H	-2.74063000	-4.40407800	-1.38168800
H	-1.19721200	-5.20702000	-1.65835100
H	-0.24046900	-1.66823300	-2.15242300
H	-0.30736500	-3.28992700	-2.85696800
H	-1.79542100	-2.35120900	-2.65463800
C	1.38562900	-3.59578000	-0.66857200
C	1.41655000	-5.03679200	-1.17319900
H	2.21516000	-3.42725300	0.01305400
H	1.55375200	-2.90879000	-1.50035100
H	2.44964200	-5.28338700	-1.43140500
H	1.08534400	-5.75687500	-0.42098700
H	0.81413700	-5.17655300	-2.07221800

TS3

C	-0.63228100	-0.27777400	-0.25743000
C	0.60293100	-1.86404000	-1.11419700
C	1.73326300	0.32294600	-1.02108100
H	1.37096600	1.35108900	-1.05315500
N	-0.51371200	-2.45079400	-0.79639900
N	-1.26877400	-1.45217900	-0.24883700
N	0.57193800	-0.53587700	-0.79309800
C	1.79480900	-2.33884700	-1.87966400
H	1.56842400	-3.27189300	-2.39439500
H	2.65605100	-2.49005100	-1.21596700
C	2.44740000	-0.07716400	-2.36471400
O	2.04046200	-1.34544000	-2.86013000
C	4.04232400	-0.06657100	-0.53950000
C	2.79087000	0.12290100	0.04098600
C	2.61483600	0.11701300	1.42078400
C	3.73485100	-0.07361800	2.22686400
C	4.99636300	-0.25709200	1.65350100
C	5.15938500	-0.25663800	0.26949500
C	3.95760400	-0.02690500	-2.04426900
H	1.62585400	0.26594900	1.84452500
H	5.85872300	-0.40892100	2.29464000
H	6.13992200	-0.40955300	-0.17063600
H	4.46977900	-0.86151200	-2.53149000
H	4.39606800	0.89674900	-2.43617700
C	-2.54195700	-1.75679100	0.34940000
C	-2.63782500	-1.71752400	1.74258000
C	-3.60514500	-2.09258400	-0.49080400
C	-3.87885100	-2.02267700	2.29834200
C	-4.82236400	-2.39147800	0.11740400
C	-4.97651400	-2.36209000	1.50505000
H	-3.98844100	-1.99953800	3.37938000
H	-5.67163100	-2.65136000	-0.50905700
H	2.17501900	0.62132700	-3.15645400
H	3.62587500	-0.08160400	3.30663800
C	-1.10331400	1.03291100	0.24841500
O	-0.17961800	1.63025800	0.99372400
C	-2.35500100	1.40878300	-0.07034600
C	-3.00519600	2.67837300	0.37500000
H	-2.93349900	0.74690300	-0.70985400
H	-3.97653400	2.44204100	0.82870200
H	-2.40011600	3.14285900	1.16099000
C	-3.43908400	-2.12414600	-1.98690500
H	-4.40447700	-2.26790100	-2.47340900

H	-3.00207700	-1.19217400	-2.36086100
H	-2.77340100	-2.93754900	-2.28902900
C	-6.29724800	-2.71992400	2.13424900
H	-6.40742000	-2.25464000	3.11583700
H	-7.13219100	-2.40589500	1.50398500
H	-6.37498800	-3.80356800	2.26884700
C	-1.45626600	-1.35676600	2.60516700
H	-1.21205000	-0.29077800	2.52818400
H	-1.67128900	-1.57814900	3.65133000
H	-0.56513300	-1.92186000	2.31286900
C	-3.22763400	3.66963500	-0.77463100
C	-3.93110800	4.94950500	-0.33043200
H	-3.82106300	3.18306000	-1.55971100
H	-2.26100300	3.91315300	-1.23564300
C	-4.07309400	5.95979100	-1.46502100
H	-4.91973100	4.69297300	0.06959900
H	-3.37597800	5.40634700	0.49950200
H	-4.60023800	6.85918700	-1.13733500
H	-3.08995200	6.26333900	-1.83936100
H	-4.62987900	5.52942400	-2.30326200
H	-0.05975300	2.80518300	1.15701300
N	0.46948500	3.97799800	1.42199200
C	0.67838000	4.01424700	2.91010500
C	1.44239200	2.78207500	3.39409000
C	-0.65962500	4.08467900	3.64545800
H	1.25970100	4.91216600	3.14976100
H	2.42053100	2.65924200	2.92469000
H	1.60255100	2.87617400	4.47056100
H	0.85237300	1.88005100	3.20840600
H	-1.17024700	5.04135700	3.52100400
H	-1.32156700	3.27787300	3.31084100
H	-0.48047500	3.94724400	4.71394700
C	1.75818100	3.83823900	0.65161200
C	2.89594500	4.75952800	1.09014300
C	1.50211800	3.95672800	-0.84865800
H	2.06886400	2.80450400	0.84335600
H	3.17913700	4.60676900	2.13330300
H	3.77264700	4.53194300	0.47778100
H	2.65551400	5.81441800	0.94888700
H	0.62790500	3.37128400	-1.15489900
H	1.34643600	4.99393400	-1.15950400
H	2.37601400	3.57910600	-1.38731800
C	-0.42917300	5.06438800	0.94587200
C	0.03718500	6.50171200	1.14736300

H	-1.38065300	4.92319000	1.45768500
H	-0.63067200	4.88403200	-0.11140800
H	-0.79877000	7.16780400	0.91780900
H	0.34375900	6.69799400	2.17831400
H	0.86068600	6.76868500	0.48282600

M3

C	-0.05415800	-0.34744000	-0.24240000
C	1.30282200	-1.77192400	-1.21101500
C	2.35424700	0.40069500	-0.69409900
H	1.95965800	1.41410000	-0.63462200
N	0.19319300	-2.43101500	-1.06590900
N	-0.64034900	-1.53536900	-0.44787800
N	1.19703100	-0.50125600	-0.72032700
C	2.56900500	-2.12416300	-1.91933700
H	2.40890300	-2.97053700	-2.58668700
H	3.36485800	-2.37340300	-1.20432100
C	3.25767100	0.16151000	-1.96133200
O	2.89803500	-0.99512100	-2.70745300
C	4.56798000	-0.11922800	0.06289400
C	3.25449800	0.07864200	0.47798000
C	2.88437800	-0.02780600	1.81503900
C	3.86793500	-0.35755400	2.74405700
C	5.18920400	-0.56404800	2.33675000
C	5.55016400	-0.44144900	0.99662000
C	4.70613800	0.07864300	-1.42524400
H	1.85508000	0.17376900	2.09907300
H	5.94370400	-0.82048400	3.07397800
H	6.57841700	-0.60026800	0.68533100
H	5.24250100	-0.73381200	-1.92531600
H	5.24557900	1.00517500	-1.64663600
C	-1.94144900	-1.97613800	-0.02767400
C	-2.16308600	-2.19303700	1.33441200
C	-2.90958100	-2.19758600	-1.00842000
C	-3.42671000	-2.64644200	1.70738000
C	-4.15652200	-2.65300300	-0.58318800
C	-4.43234200	-2.87839600	0.76644600
H	-3.62906800	-2.82717900	2.76016500
H	-4.93069900	-2.83132700	-1.32511100
H	3.13265900	0.98248900	-2.66726500
H	3.60980600	-0.44918600	3.79420300
C	-0.55265400	0.91820000	0.39901700
O	0.36107500	1.59464500	0.98722600
C	-1.88137400	1.18287400	0.22276300

C	-2.50064500	2.44500100	0.73890400
H	-2.50496300	0.48949200	-0.33351100
H	-3.28874800	2.21889500	1.47403100
H	-1.72645400	3.01001400	1.27002800
C	-2.61255000	-1.93727500	-2.46099200
H	-3.51965700	-2.03057300	-3.05967700
H	-2.20720600	-0.92968600	-2.60163400
H	-1.86863100	-2.64253900	-2.84210500
C	-5.79828200	-3.33792200	1.20594900
H	-5.73186800	-4.00089700	2.07169700
H	-6.41658600	-2.48149100	1.49345200
H	-6.31543900	-3.86634600	0.40238500
C	-1.08794800	-1.92672700	2.35315700
H	-0.94853600	-0.84834200	2.48889500
H	-1.35803800	-2.36119600	3.31679900
H	-0.12724300	-2.34780600	2.04023000
C	-3.11372600	3.32050800	-0.36025000
C	-3.77230100	4.58620700	0.18375500
H	-3.85746300	2.73632000	-0.92063200
H	-2.33173900	3.59332000	-1.08097600
C	-4.37639200	5.45728500	-0.91423600
H	-4.55127100	4.30404700	0.90375600
H	-3.02822900	5.16322400	0.74759600
H	-4.84138600	6.35862300	-0.50565900
H	-3.60848600	5.77020900	-1.62899000
H	-5.14205400	4.90706100	-1.47076400

TS3'

C	-0.03327200	-0.36082300	-0.25412600
C	1.27146100	-1.78755700	-1.27462400
C	2.41889900	0.29552100	-0.60640500
H	2.08537400	1.32805300	-0.49367100
N	0.12186700	-2.39049200	-1.20282600
N	-0.67937700	-1.49351600	-0.54986400
N	1.22142100	-0.54737100	-0.70178300
C	2.53505100	-2.15113600	-1.98275900
H	2.35273700	-2.95132400	-2.69906900
H	3.30803500	-2.46962100	-1.27092200
C	3.30989500	0.10965200	-1.89166300
O	2.91684000	-0.99198400	-2.70073700
C	4.61132100	-0.35633600	0.10094800
C	3.30436000	-0.15323600	0.53646400
C	2.93485300	-0.36309500	1.86189800
C	3.91113100	-0.79670600	2.75567600

C	5.22471100	-1.00644700	2.32673600
C	5.58539400	-0.78455600	0.99946700
C	4.75513200	-0.04204500	-1.36592400
H	1.91340900	-0.16929800	2.17595100
H	5.97258800	-1.34561300	3.03633800
H	6.60691200	-0.94808700	0.66993000
H	5.27717400	-0.82072300	-1.93010100
H	5.30936300	0.89063900	-1.51074600
C	-2.01149300	-1.86981500	-0.16273300
C	-2.26044200	-2.11172000	1.19247800
C	-2.97989900	-1.99444200	-1.15854100
C	-3.55588000	-2.48466100	1.53988600
C	-4.26060400	-2.37499500	-0.75643700
C	-4.56547300	-2.61930800	0.58236700
H	-3.78232800	-2.68060600	2.58498900
H	-5.03705000	-2.47804900	-1.50968400
H	3.20210400	0.97450700	-2.54565800
H	3.65149900	-0.96957600	3.79487300
C	-0.51328000	0.85266000	0.44722500
O	0.38449000	1.36118500	1.26798600
C	-1.75043000	1.30773500	0.15413400
C	-2.31407200	2.56080500	0.74726900
H	-2.35518600	0.76187600	-0.56622100
H	-3.23551700	2.32651100	1.29908200
H	-1.59744900	2.96387500	1.47075000
C	-2.65187500	-1.71944000	-2.60189700
H	-3.55745600	-1.73899500	-3.20935700
H	-2.17953300	-0.73851000	-2.71950100
H	-1.95351500	-2.46404000	-2.99397700
C	-5.95654100	-3.01705300	1.00218700
H	-5.93848500	-3.94670000	1.57750200
H	-6.40236700	-2.24784800	1.63956900
H	-6.60608200	-3.16060200	0.13697200
C	-1.17778900	-1.96608100	2.22928800
H	-0.94200300	-0.91114800	2.40899200
H	-1.49699800	-2.40670500	3.17465000
H	-0.25445100	-2.46225700	1.91382000
Cl	1.07336500	3.95596300	0.30143900
C	-2.63089200	3.62515800	-0.31000700
C	-3.13098900	4.92957700	0.30510300
H	-3.38256900	3.23437600	-1.00957300
H	-1.72495400	3.82297300	-0.89549100
C	-3.46634600	5.98200100	-0.74807900
H	-4.01539100	4.72533100	0.92212700

H	-2.36110000	5.31710800	0.98403200
H	-3.81572500	6.91196500	-0.29189800
H	-2.58654900	6.21538400	-1.35585300
H	-4.25031600	5.62281300	-1.42248300
H	0.69696100	2.67291500	0.85126000

TS4R

C	0.03116400	-1.79279900	-0.56023200
C	-1.53291900	-1.90780400	-2.08165600
C	-2.16433300	-2.92167000	0.13587400
H	-1.65330000	-3.83658900	0.42788900
N	-0.54017700	-1.31403700	-2.67579100
N	0.42475300	-1.24118800	-1.71508300
N	-1.23106900	-2.22115400	-0.78725300
C	-2.85047700	-2.26860600	-2.68253900
H	-2.70622200	-2.56321200	-3.72280400
H	-3.51210500	-1.39542400	-2.65088000
C	-3.51443800	-3.17847100	-0.60272600
O	-3.38784900	-3.37838700	-1.99644500
C	-3.88867400	-1.58950600	1.13029000
C	-2.59513200	-2.08077400	1.31912600
C	-1.90039900	-1.82565500	2.49901100
C	-2.49756200	-1.01775200	3.46438500
C	-3.77623700	-0.49446800	3.26353700
C	-4.48663600	-0.79258600	2.10242700
C	-4.47226000	-2.04615600	-0.17802500
H	-0.91567600	-2.25598500	2.64672400
H	-4.23002400	0.12936400	4.02743400
H	-5.49812100	-0.42241900	1.96340100
H	-4.46470300	-1.22175500	-0.89689700
H	-5.49963200	-2.40723700	-0.08825200
C	1.67538300	-0.59283900	-2.00166800
C	1.67377900	0.79231800	-2.18245500
C	2.84242600	-1.36688400	-2.04838400
C	2.91513300	1.42347600	-2.28788700
C	4.05056100	-0.68888400	-2.17653500
C	4.10781100	0.70648500	-2.26064300
H	2.94070800	2.50867100	-2.36576900
H	4.97341600	-1.26425800	-2.19693400
H	-3.89470700	-4.12681100	-0.21663600
H	-1.96674800	-0.80122700	4.38641500
C	0.82598700	-2.15548800	0.67122900
O	0.42259800	-3.21504700	1.23577400
C	1.90868000	-1.38541200	1.05721700

C	2. 77993400	-1. 95036700	2. 14821400
H	2. 29966200	-0. 60939400	0. 41080400
H	2. 24881200	-1. 93875800	3. 11358800
H	2. 94779100	-3. 01853100	1. 94047400
C	5. 43780100	1. 40958800	-2. 33215200
H	6. 06494000	1. 13502200	-1. 47859300
H	5. 98121500	1. 13078800	-3. 24013300
H	5. 30964800	2. 49398800	-2. 32469900
C	2. 80784500	-2. 86699700	-1. 92519100
H	2. 77536700	-3. 17075800	-0. 87298700
H	1. 92999900	-3. 29041200	-2. 42071300
H	3. 70144800	-3. 30128600	-2. 37718300
C	0. 40823000	1. 59531100	-2. 32383300
H	0. 20031900	1. 75460400	-3. 38733800
H	-0. 45959300	1. 09659300	-1. 89455600
H	0. 52463000	2. 57153600	-1. 84840900
C	4. 12976500	-1. 25252000	2. 30131600
C	5. 09633600	-2. 01895500	3. 20140200
H	3. 99105700	-0. 24650000	2. 72060800
H	4. 58442900	-1. 11418900	1. 30907000
C	6. 43129400	-1. 30086400	3. 37767400
H	4. 62662800	-2. 17578300	4. 18067200
H	5. 26383600	-3. 01669600	2. 77721700
H	7. 11231400	-1. 86858400	4. 01708000
H	6. 92287400	-1. 15227000	2. 41078000
H	6. 28745200	-0. 31500000	3. 83128400
C	3. 84292700	4. 31002700	0. 02896000
C	2. 50184000	4. 66204000	-0. 12122200
C	1. 49435700	3. 80072700	0. 30063100
C	1. 80617700	2. 56189400	0. 88163500
C	3. 15689200	2. 21846900	1. 02221400
C	4. 16377100	3. 08461400	0. 60795400
H	4. 62736700	4. 98325100	-0. 30200600
H	2. 23747400	5. 61604900	-0. 56738600
H	0. 45279000	4. 07866600	0. 17930900
H	3. 42543100	1. 25013900	1. 43005600
H	5. 20298900	2. 79121200	0. 72356400
C	0. 74162500	1. 61586800	1. 28481100
C	0. 90937200	0. 58302800	2. 15869000
H	1. 80391100	0. 51297300	2. 76708600
H	0. 04958400	-0. 01033800	2. 44663000
N	-0. 48386500	1. 83323400	0. 65523700
N	-1. 26594800	0. 84656300	0. 61358100
C	-2. 46161600	1. 17388800	-0. 09341600

O	-2.85750100	0.45498000	-0.98880000
O	-3.03633700	2.27948100	0.34865800
C	-4.19658400	2.85436800	-0.33884400
C	-3.83967100	3.14522700	-1.79295600
C	-5.39240800	1.92101600	-0.20138700
C	-4.43183200	4.15032100	0.42574300
H	-2.91611900	3.73020600	-1.83849400
H	-3.70977600	2.22651400	-2.36501800
H	-4.64234500	3.73315700	-2.24618300
H	-5.59655700	1.73034600	0.85526900
H	-6.27183500	2.39743400	-0.64332200
H	-5.21252800	0.97271800	-0.70991400
H	-5.29395800	4.67426700	0.00595500
H	-4.62754300	3.93987600	1.48012700
H	-3.55551900	4.79949900	0.35380400

TS4S

C	-0.54616000	0.75202700	-0.55399200
C	0.70144600	2.19861300	-1.63128500
C	1.73741500	-0.02209900	-1.45349500
H	1.70025300	-0.77441000	-0.66688800
N	-0.35832100	2.87149400	-1.30167200
N	-1.13054900	1.95651100	-0.63910000
N	0.63271500	0.90836000	-1.19682600
C	1.95387000	2.63947200	-2.30973100
H	2.01772500	3.72708000	-2.31292800
H	1.97802300	2.27346200	-3.34581000
C	3.11928900	0.72440200	-1.46572000
O	3.03708800	2.13963800	-1.55297100
C	2.83381900	-0.53693000	-3.51778600
C	1.62748800	-0.63843900	-2.83002600
C	0.51134700	-1.24163300	-3.40064500
C	0.62010900	-1.73591700	-4.69843600
C	1.82551500	-1.63255200	-5.39851800
C	2.94146500	-1.03781200	-4.81270600
C	3.88798000	0.12503200	-2.66696800
H	-0.40548100	-1.33412800	-2.82627900
H	1.89310300	-2.02113900	-6.40970100
H	3.87665700	-0.96137000	-5.35932100
H	4.43868200	0.91445400	-3.18671400
H	4.62150600	-0.61012400	-2.31963800
C	-2.43528100	2.35817800	-0.19624800
C	-3.51883900	2.12689100	-1.04613300
C	-2.55287500	2.95258500	1.05989600

C	-4.77705300	2.51719700	-0.59359000
C	-3.83286100	3.32895100	1.46632600
C	-4.95006300	3.12132000	0.65486700
H	-5.64226900	2.34300700	-1.22830700
H	-3.95956800	3.79004800	2.44250000
H	3.63525800	0.54314900	-0.52150500
H	-0.23562800	-2.20876200	-5.16921500
C	-1.05691700	-0.58375500	-0.08235200
O	-0.29655000	-1.55827100	-0.38119400
C	-2.26317100	-0.65380800	0.58035600
C	-2.96938400	-1.97478800	0.69861900
H	-2.82334200	0.24392300	0.81066300
H	-2.22683500	-2.77775400	0.76793200
H	-3.57841700	-2.00964400	1.61113800
C	-6.31824200	3.56302600	1.10557900
H	-7.09431400	2.89732100	0.72135000
H	-6.38738100	3.58545700	2.19515100
H	-6.53613800	4.57088900	0.73789100
C	-1.34325700	3.13049500	1.93542400
H	-0.88841300	2.15955600	2.16351800
H	-0.57323400	3.71936400	1.42890000
H	-1.61438900	3.62646900	2.86872000
C	-3.32249400	1.42977700	-2.36467900
H	-2.53714700	1.91042700	-2.95556200
H	-3.02307200	0.38822200	-2.19540500
H	-4.24620000	1.43165000	-2.94493800
C	-3.88058300	-2.23508800	-0.50993700
C	-4.65652700	-3.54620900	-0.40630400
H	-3.26097000	-2.24324900	-1.41737400
H	-4.58465800	-1.39788500	-0.62182600
C	-5.54311600	-3.80309600	-1.62198900
H	-3.94654200	-4.37350000	-0.28309900
H	-5.27061100	-3.52953800	0.50315400
H	-6.09278500	-4.74372400	-1.53030000
H	-6.27394200	-2.99774500	-1.74783800
H	-4.94356800	-3.85216100	-2.53646000
C	1.22828900	-5.95783100	1.85007100
C	1.70549400	-5.00416700	0.95147500
C	1.37168700	-3.66339400	1.10565200
C	0.55932600	-3.25003500	2.16842400
C	0.09657000	-4.21266500	3.07302600
C	0.41932600	-5.55713900	2.91009400
H	1.48715600	-7.00442100	1.72537500
H	2.33133100	-5.30934400	0.11859400

H	1. 70619400	-2. 92353500	0. 38793900
H	-0. 50331400	-3. 90339500	3. 92395200
H	0. 05056500	-6. 28884200	3. 62200500
C	0. 21267900	-1. 82125300	2. 35367200
C	-0. 94372700	-1. 38953200	2. 89854500
H	-1. 71384400	-2. 09293300	3. 19163800
H	-1. 09251100	-0. 34097900	3. 11942800
N	1. 22406400	-0. 90728600	1. 96903300
N	0. 87881700	0. 29719100	2. 03042900
C	1. 92440200	1. 23969400	1. 79074600
O	1. 72576700	2. 21633700	1. 10268100
O	3. 01570100	0. 96823100	2. 49504200
C	4. 07651500	1. 97209900	2. 65364600
C	4. 77091100	2. 22133500	1. 32089400
C	3. 49123400	3. 24945700	3. 24825300
C	5. 02256800	1. 30415900	3. 64292300
H	5. 22141300	1. 29485400	0. 95181000
H	4. 07567200	2. 61161000	0. 57540300
H	5. 57467900	2. 94761000	1. 47178100
H	2. 91329600	3. 01382500	4. 14640200
H	4. 31155700	3. 91345900	3. 53313300
H	2. 85188100	3. 76797600	2. 53396700
H	4. 51633900	1. 12137700	4. 59401100
H	5. 37736200	0. 35047600	3. 24443700
H	5. 88422300	1. 95198700	3. 82183800

M4R

C	0. 84593900	1. 18813600	-0. 85679200
C	0. 39737300	3. 28993000	-0. 58206800
C	-1. 18145600	2. 10203500	-2. 15811000
H	-0. 76651500	1. 96021800	-3. 15610400
N	1. 47443700	3. 08660800	0. 11674900
N	1. 74284200	1. 76414400	-0. 06333800
N	-0. 01285100	2. 15441100	-1. 22775400
C	-0. 34105600	4. 58189600	-0. 70417400
H	0. 37342500	5. 40264100	-0. 78039200
H	-0. 95196700	4. 73276100	0. 19477900
C	-1. 94830200	3. 44532800	-2. 00257900
O	-1. 11711800	4. 57838400	-1. 87986700
C	-3. 29270000	1. 74884900	-1. 09774800
C	-2. 27334100	1. 10584700	-1. 81133300
C	-2. 42737700	-0. 21402800	-2. 22476100
C	-3. 58792400	-0. 89837600	-1. 86814800
C	-4. 59270900	-0. 26564100	-1. 13716700

C	-4.45556700	1.06856000	-0.75828800
C	-2.94799900	3.19327900	-0.85892500
H	-1.66071200	-0.70936900	-2.80795400
H	-5.49314800	-0.81235200	-0.87463300
H	-5.25486000	1.57587700	-0.22556400
H	-2.46699600	3.28499500	0.12125400
H	-3.80429600	3.86999100	-0.90041200
C	2.98148200	1.23073600	0.44473100
C	3.03021400	0.76356100	1.75979300
C	4.09680000	1.28703400	-0.39668200
C	4.26462800	0.30155600	2.22006500
C	5.30171200	0.80227200	0.10779400
C	5.40252200	0.30773100	1.41074100
H	4.33479300	-0.07462700	3.23752100
H	6.18429600	0.82237200	-0.52658000
H	-2.50211300	3.59251900	-2.93295200
H	-3.70740000	-1.93637100	-2.16201900
C	0.88216700	-0.18777800	-1.45916100
O	0.50076100	-0.26573400	-2.61025000
C	1.46222700	-1.36071100	-0.71246100
C	2.82088300	-1.74110800	-1.34226900
H	1.60585100	-1.08319200	0.33269700
H	2.64260700	-2.34847100	-2.23884300
H	3.35028200	-0.84297300	-1.68019100
C	6.72770600	-0.17538600	1.93997800
H	7.33053700	-0.61876700	1.14330300
H	7.29781500	0.65802100	2.36338600
H	6.59202200	-0.91917800	2.72832000
C	3.99465700	1.86456900	-1.78462000
H	3.26978000	1.32249300	-2.40248400
H	3.66973500	2.90901300	-1.74560500
H	4.96118600	1.82177800	-2.28824100
C	1.80081700	0.74975800	2.62414400
H	1.26867600	1.70277800	2.56773900
H	1.08909300	-0.00656700	2.27219600
H	2.06568400	0.53675300	3.66108600
C	3.72325200	-2.47745500	-0.35570900
C	5.11589700	-2.75327700	-0.91521800
H	3.25814700	-3.42345000	-0.04764700
H	3.82174300	-1.86550400	0.55124800
C	6.00240100	-3.48622700	0.08741800
H	5.03423900	-3.33745800	-1.84044400
H	5.57963800	-1.79639400	-1.18989500
H	7.01299000	-3.63750000	-0.30101500

H	6.07976900	-2.91731400	1.02021700
H	5.58483800	-4.46778200	0.33304400
C	-3.38540900	-5.95031600	-0.34144100
C	-3.83771300	-4.77308600	0.25909000
C	-3.01702800	-3.65687900	0.32739900
C	-1.71197500	-3.68053800	-0.19742100
C	-1.27415400	-4.86611500	-0.80377300
C	-2.10186200	-5.98720300	-0.87287800
H	-4.02831600	-6.82317700	-0.39443300
H	-4.84047200	-4.72640100	0.67390000
H	-3.36338600	-2.73599100	0.78332900
H	-0.27990900	-4.93211100	-1.23228200
H	-1.73416900	-6.89284100	-1.34603600
C	-0.85756800	-2.46244300	-0.11992600
C	0.48949900	-2.54440000	-0.81196300
H	1.01705000	-3.41951500	-0.41216600
H	0.32971700	-2.75542100	-1.87890500
N	-1.37041400	-1.47035100	0.52061400
N	-0.72603000	-0.28221100	0.56812900
C	-1.35292000	0.65880300	1.31187400
O	-0.93467100	1.82388200	1.39575000
O	-2.46099000	0.25386400	1.98746500
C	-2.98726100	1.03965000	3.07723500
C	-1.93505000	1.17381800	4.17626800
C	-3.49606600	2.40714600	2.62195800
C	-4.16035800	0.19093400	3.56208400
H	-1.58250400	0.18316800	4.47919300
H	-1.08746600	1.76149100	3.81980100
H	-2.36929900	1.66965700	5.04966000
H	-4.11142300	2.29152200	1.72477500
H	-4.11617300	2.84388000	3.41138400
H	-2.66939300	3.08083000	2.40128100
H	-4.64254800	0.66252600	4.42269700
H	-4.89832000	0.07963600	2.76183500
H	-3.81188300	-0.80369600	3.85252600

M4S

C	-0.52447000	0.62281000	-0.57263800
C	0.49955700	2.11113900	-1.79093900
C	1.72353100	-0.00902500	-1.60672500
H	1.77612400	-0.75618200	-0.81155500
N	-0.58003900	2.70999100	-1.38160700
N	-1.21668300	1.76209100	-0.62956400
N	0.55864400	0.82951100	-1.33852100

C	1. 67680000	2. 61661000	-2. 55562000
H	1. 65398600	3. 70474200	-2. 60575800
H	1. 67123000	2. 20752200	-3. 57533100
C	3. 03456900	0. 84860900	-1. 62422300
O	2. 83520700	2. 24024400	-1. 83871600
C	2. 88787600	-0. 48861800	-3. 63305500
C	1. 66304100	-0. 63116800	-2. 98474800
C	0. 58486800	-1. 26179600	-3. 59564200
C	0. 75396200	-1. 75587200	-4. 88777000
C	1. 97988200	-1. 62012900	-5. 54330000
C	3. 05529700	-0. 98783100	-4. 92126100
C	3. 88382500	0. 22212600	-2. 75113900
H	-0. 36201000	-1. 36648200	-3. 07376000
H	2. 09456400	-2. 00873600	-6. 55013700
H	4. 00495700	-0. 87894900	-5. 43646100
H	4. 45255200	0. 99960500	-3. 26810700
H	4. 60244600	-0. 49000700	-2. 33090400
C	-2. 52042200	2. 06121900	-0. 09975800
C	-3. 62077500	1. 91409100	-0. 94577500
C	-2. 61102100	2. 53489600	1. 21246200
C	-4. 87514500	2. 21499000	-0. 41489900
C	-3. 88748200	2. 81829000	1. 69375300
C	-5. 02628900	2. 65623200	0. 90069700
H	-5. 75296400	2. 10188600	-1. 04660800
H	-3. 99367600	3. 18155300	2. 71262300
H	3. 51937700	0. 78473800	-0. 64991100
H	-0. 07220400	-2. 24965300	-5. 38863000
C	-0. 84708100	-0. 72738500	0. 01826300
O	-0. 32799000	-1. 67934100	-0. 53651200
C	-1. 82890100	-0. 93672400	1. 14814000
C	-2. 84307300	-2. 00403200	0. 70584300
H	-2. 36164600	-0. 00692700	1. 36171400
H	-2. 29530200	-2. 92527500	0. 47272900
H	-3. 50031700	-2. 22013700	1. 55656100
C	-6. 39565300	2. 93606600	1. 46227200
H	-6. 82182000	2. 02751900	1. 89978000
H	-6. 35217000	3. 69317200	2. 24810600
H	-7. 07964900	3. 28049800	0. 68364500
C	-1. 37758200	2. 71523000	2. 05198800
H	-0. 85190800	1. 76394900	2. 20243600
H	-0. 65704800	3. 36821800	1. 55178800
H	-1. 63778400	3. 14184100	3. 02206000
C	-3. 46240000	1. 47746400	-2. 37807300
H	-3. 12671700	2. 31519800	-2. 99756100

H	-2.72385100	0.67750000	-2.48559100
H	-4.41322800	1.11667100	-2.77444400
C	-3.68585000	-1.57585800	-0.49124400
C	-4.73734600	-2.60325700	-0.90096300
H	-3.02925900	-1.38397300	-1.35275600
H	-4.18467600	-0.62441200	-0.25969300
C	-5.57006900	-2.12116300	-2.08560400
H	-4.24338900	-3.55029100	-1.15044200
H	-5.39236400	-2.81013300	-0.04554800
H	-6.32692900	-2.85468900	-2.37496000
H	-6.08336000	-1.18472600	-1.84142100
H	-4.93333200	-1.93229900	-2.95631000
C	1.30116400	-6.02105600	3.14436300
C	2.29500200	-5.04165400	3.10117900
C	1.96817600	-3.72125600	2.82538700
C	0.63695900	-3.34308100	2.58675300
C	-0.35069400	-4.33481400	2.63106800
C	-0.02095100	-5.66066400	2.90551500
H	1.55697800	-7.05297500	3.36261400
H	3.33015700	-5.31019700	3.28945200
H	2.73547300	-2.95526900	2.79038700
H	-1.38807300	-4.07994500	2.43591300
H	-0.80349100	-6.41293200	2.93011300
C	0.30954500	-1.93199800	2.28513900
C	-1.08232300	-1.37962600	2.45179000
H	-1.72229400	-2.08121300	2.99012900
H	-0.97053700	-0.48409700	3.07054900
N	1.27587700	-1.14277700	1.93453800
N	0.84865400	0.10070700	1.59032900
C	1.80204000	1.05529500	1.46348000
O	1.56459900	2.14962000	0.94401100
O	3.02666700	0.74339600	1.97576900
C	3.95633500	1.79864100	2.33363100
C	4.54483300	2.47329300	1.09665200
C	3.27958200	2.81040000	3.25740400
C	5.04693900	1.04899500	3.09289300
H	5.12614000	1.75269800	0.51169300
H	3.75617200	2.89331600	0.47154300
H	5.22564000	3.27108400	1.41019200
H	2.79839700	2.28794700	4.09002200
H	4.03198700	3.49043200	3.66704100
H	2.52993500	3.39119900	2.72057200
H	4.63159000	0.57288600	3.98511700
H	5.48490700	0.27499600	2.45673400

H	5.83717100	1.74061300	3.39771100
TS4R'			
C	1.79106100	0.84798800	-0.71800700
C	2.19519200	2.95194900	-0.30614400
C	0.15979500	2.55750600	-1.74026400
H	0.34737000	2.10314900	-2.71223900
N	3.20331000	2.31478100	0.21293400
N	2.94033900	1.00277200	-0.04927400
N	1.30198700	2.09619800	-0.89456600
C	2.02763400	4.43169200	-0.39521300
H	3.00994000	4.90441800	-0.37518100
H	1.44203900	4.80213000	0.45514700
C	0.16040200	4.12310800	-1.79824000
O	1.42493700	4.72986100	-1.63373100
C	-1.87787400	3.43228100	-0.82527800
C	-1.24767400	2.26033800	-1.25671900
C	-1.96466600	1.07011000	-1.35988300
C	-3.31607500	1.07346900	-1.01710700
C	-3.94689600	2.24693900	-0.60387900
C	-3.23082100	3.43655300	-0.50751100
C	-0.93095100	4.59746900	-0.82320900
H	-1.47672900	0.16558500	-1.70638900
H	-5.00430500	2.23342300	-0.35602600
H	-3.71706700	4.35466200	-0.19038600
H	-0.54311600	4.75653500	0.18978400
H	-1.38346400	5.53386400	-1.15684500
C	3.98204600	0.02943200	0.16601000
C	4.34244900	-0.30983200	1.47179500
C	4.61621700	-0.50047300	-0.96533000
C	5.35700500	-1.25546000	1.62728100
C	5.61584900	-1.44550200	-0.75072300
C	5.99077800	-1.84433600	0.53427100
H	5.65731000	-1.53515100	2.63377500
H	6.12412400	-1.87234500	-1.61160700
H	-0.14633000	4.38141700	-2.81415500
H	-3.88225900	0.14923900	-1.06556500
C	1.17732000	-0.41308500	-1.26640900
O	0.53502700	-0.25738400	-2.33681600
C	1.35701200	-1.57637400	-0.52711900
C	0.88540400	-2.88955900	-1.09136800
H	2.15051400	-1.60193800	0.21115500
H	-0.20169000	-2.99062600	-0.95954100
H	1.06036200	-2.90093800	-2.17681800

C	7.05462200	-2.89250700	0.72940700
H	6.62415700	-3.89468500	0.63680300
H	7.83985900	-2.80064100	-0.02448900
H	7.51032100	-2.81456400	1.71851300
C	4.25257700	-0.07072900	-2.36311600
H	3.32695900	-0.54682300	-2.70369800
H	4.11067600	1.01277600	-2.42543900
H	5.04779700	-0.34816600	-3.05653200
C	3.66987000	0.28906400	2.67957000
H	3.44689000	1.34890900	2.53995300
H	2.73049600	-0.22759900	2.90464500
H	4.31219200	0.18530700	3.55569100
C	1.58879200	-4.08094400	-0.44319200
C	1.11210600	-5.42454700	-0.98737700
H	1.42772400	-4.05571000	0.64472600
H	2.67431400	-3.98563400	-0.59065900
C	1.81548700	-6.60856200	-0.32956500
H	0.02823300	-5.50558900	-0.83771100
H	1.27592300	-5.45119400	-2.07206200
H	1.45830300	-7.56187400	-0.72786200
H	2.89695600	-6.55937900	-0.49309700
H	1.64346800	-6.61070100	0.75160000
C	-0.93307300	3.56759400	2.78136200
C	-2.15618800	2.91997300	2.61475000
C	-2.21070400	1.59853500	2.18457500
C	-1.03597600	0.88565700	1.90969200
C	0.18899400	1.54899800	2.07831600
C	0.24330400	2.87028500	2.51020500
H	-0.89651300	4.59852900	3.11931100
H	-3.08169300	3.45193800	2.81479500
H	-3.16701600	1.10840900	2.03913500
H	1.11853100	1.03127900	1.86472700
H	1.21072300	3.34950400	2.64150000
C	-1.08281000	-0.51391600	1.43440100
C	0.01534400	-1.34085100	1.41457100
H	0.90387600	-1.05902900	1.96455200
H	-0.14691900	-2.39786800	1.24042300
N	-2.32717800	-0.98200400	1.05952200
N	-2.33037800	-2.03307200	0.35518300
C	-3.63141700	-2.53837300	0.07311500
O	-3.74697600	-3.65510900	-0.38304000
O	-4.63189100	-1.68901900	0.31279400
C	-6.01137800	-2.05813200	0.00945100
C	-6.16936200	-2.33197400	-1.48292900

C	-6.43492300	-3.24653400	0.86646200
C	-6.78611200	-0.80694800	0.40587900
H	-5.80612500	-1.47752100	-2.06223200
H	-5.62393700	-3.22639600	-1.78250600
H	-7.23023100	-2.47137100	-1.70902300
H	-6.24671100	-3.03138900	1.92209700
H	-7.50678200	-3.41891700	0.73556300
H	-5.89473500	-4.14883200	0.58125800
H	-7.85501500	-0.96250500	0.23967200
H	-6.62233800	-0.57670400	1.46176100
H	-6.46010800	0.04750000	-0.19417400

TS4R"

C	2.27145700	0.94617000	0.14606100
C	4.31232100	0.82983000	-0.64920700
C	3.71493200	-1.11165600	0.71754600
H	3.01130300	-1.27418700	1.53536100
N	3.83274600	1.93398800	-1.14025300
N	2.56189700	1.99112700	-0.64278300
N	3.39702800	0.20100900	0.14596500
C	5.68361900	0.23847200	-0.70328000
H	6.40340100	0.98751800	-1.03244600
H	5.71419200	-0.61816900	-1.38876500
C	5.20213100	-1.14181300	1.21109200
O	6.00973200	-0.12558900	0.62610100
C	4.77523200	-3.02733300	-0.24251900
C	3.65842000	-2.19905400	-0.33324300
C	2.67690700	-2.40943000	-1.29264300
C	2.81344900	-3.48863700	-2.16256200
C	3.92097300	-4.33294000	-2.06628400
C	4.91055900	-4.10729600	-1.10942000
C	5.69978300	-2.55967600	0.85440200
H	1.82139400	-1.74467300	-1.36816100
H	4.01778100	-5.16866200	-2.75167200
H	5.77840100	-4.75711300	-1.05127800
H	6.75098000	-2.52456900	0.55537400
H	5.62792000	-3.21361200	1.73006700
C	1.73945100	3.12566900	-0.96572000
C	1.15377900	3.16529600	-2.23281300
C	1.56512800	4.12053900	-0.00220500
C	0.34339600	4.26053400	-2.52361600
C	0.74389100	5.19381500	-0.34330900
C	0.12337400	5.27706200	-1.59119200
H	-0.12992400	4.31945900	-3.50026500

H	0.58609800	5.98381600	0.38621200
H	5.25290800	-0.94567600	2.28236600
H	2.05604600	-3.67139600	-2.91719400
C	1.04935500	0.64003900	0.98640300
O	1.27417100	-0.13097300	1.95716100
C	-0.17174100	1.17656000	0.58778900
C	-1.32299300	1.06643900	1.54796100
H	-0.19413600	1.95205700	-0.16659400
H	-2.26235200	1.27586600	1.02647100
H	-1.38340300	0.02918200	1.90575800
C	-0.78867500	6.42957500	-1.92040000
H	-1.82610100	6.17535100	-1.68094700
H	-0.52356600	7.31985200	-1.34648200
H	-0.74617500	6.67477400	-2.98393000
C	2.20319200	4.01659100	1.35619000
H	1.68344300	3.26823300	1.96593900
H	3.25357900	3.71997800	1.28464300
H	2.14867200	4.97333500	1.87736600
C	1.38732500	2.06162200	-3.22928600
H	2.42514100	2.05977800	-3.57561800
H	1.19284500	1.07964500	-2.78455400
H	0.73358900	2.18097800	-4.09404400
C	-1.17682300	2.00185400	2.75393800
C	-2.33014400	1.86887500	3.74543300
H	-1.11338900	3.04146600	2.40198600
H	-0.22768500	1.77975000	3.25933600
C	-2.19331800	2.81050400	4.93877500
H	-3.27636900	2.06465000	3.22503700
H	-2.38126600	0.83044000	4.09608200
H	-3.02290200	2.69642800	5.64182700
H	-1.26312500	2.61589200	5.48236500
H	-2.17278300	3.85480100	4.61056200
C	-0.46871800	-5.14716200	0.78951400
C	0.34469300	-4.02839800	0.94625300
C	-0.10777200	-2.76955200	0.55943900
C	-1.37392700	-2.61240300	-0.01631400
C	-2.19384700	-3.74142900	-0.15400300
C	-1.74478100	-4.99493300	0.24667800
H	-0.11876300	-6.12710400	1.09800800
H	1.33365000	-4.12877900	1.38475600
H	0.50548400	-1.89403800	0.75606900
H	-3.18429300	-3.62334300	-0.58140000
H	-2.39126500	-5.85934300	0.12859500
C	-1.83543100	-1.28572200	-0.48289200

C	-0.99702600	-0.34445700	-1.03140400
H	0.00316000	-0.63244400	-1.32788800
H	-1.42758300	0.52993700	-1.50399200
N	-3.20566700	-1.09252800	-0.40427200
N	-3.64017100	0.05634500	-0.70311900
C	-5.06034800	0.16478900	-0.63787100
O	-5.57363700	1.25413400	-0.78012100
O	-5.70913400	-0.98022700	-0.43585500
C	-7.16519400	-1.00310800	-0.33914600
C	-7.62785300	-0.15842500	0.84394900
C	-7.78602200	-0.54705900	-1.65574000
C	-7.46088300	-2.47762000	-0.09090900
H	-7.10328500	-0.46945500	1.75186600
H	-7.44473900	0.90125800	0.66837700
H	-8.69967600	-0.31288600	0.99633700
H	-7.37910600	-1.13428400	-2.48399400
H	-8.86669100	-0.71017300	-1.61750600
H	-7.59534900	0.51028100	-1.83735400
H	-8.53893700	-2.62977900	0.00474300
H	-7.09286700	-3.08455700	-0.92230600
H	-6.97509100	-2.81281400	0.82903700

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C	-2.22132400	0.58348500	0.58109600
C	-3.87344500	-0.19625900	1.79596800
C	-4.49538000	0.15267700	-0.56679400
H	-4.21291400	0.93430500	-1.26795900
N	-2.87606200	-0.10428900	2.62260800
N	-1.85571300	0.38087900	1.85808900
N	-3.52850300	0.22934300	0.54535800
C	-5.29449700	-0.57511100	2.04379200
H	-5.51860500	-0.52337700	3.10883400
H	-5.49501700	-1.59344400	1.68246900
C	-5.97233600	0.32215300	-0.04108400
O	-6.08050600	0.38827400	1.37228900
C	-5.73676500	-1.79072700	-1.22384500
C	-4.46912600	-1.21808700	-1.19904600
C	-3.35934400	-1.88193600	-1.71074900
C	-3.53616900	-3.15540100	-2.24461300
C	-4.80540600	-3.74047400	-2.26846300
C	-5.91293100	-3.06320300	-1.76352200
C	-6.76999100	-0.86502900	-0.63614700
H	-2.38464800	-1.40333500	-1.69657900
H	-4.92907400	-4.73401300	-2.68737500

H	-6.89698700	-3.52186700	-1.78729100
H	-7.37533900	-1.33647000	0.14515200
H	-7.46243700	-0.51001100	-1.40530400
C	-0.59428200	0.61892800	2.50721700
C	0.21873300	-0.48021300	2.77768000
C	-0.27279300	1.93080700	2.87195500
C	1.43025700	-0.22857300	3.42720500
C	0.94220200	2.12672500	3.51890000
C	1.80449600	1.06114700	3.80093400
H	2.08923700	-1.06732700	3.63655700
H	1.22264000	3.13449000	3.81540200
H	-6.36540600	1.27881100	-0.38436200
H	-2.68548700	-3.69516800	-2.64771900
C	-1.46612100	1.12161400	-0.61333600
O	-2.16411000	1.25411000	-1.66068200
C	-0.10400000	1.34577500	-0.48439200
C	0.62396100	2.15847800	-1.51149300
H	0.39207100	1.17757000	0.46270000
H	1.67000600	1.83134600	-1.57053600
H	0.17990800	1.98691400	-2.49978400
C	3.12065100	1.31792700	4.48778400
H	3.84843100	1.73300500	3.78278000
H	3.00447700	2.04073700	5.29935700
H	3.53840400	0.39694700	4.90003000
C	-1.19024300	3.07618000	2.54168600
H	-1.19942500	3.25579300	1.46003400
H	-2.21817400	2.86826900	2.85416100
H	-0.85645800	3.98933900	3.03648300
C	-0.20448500	-1.87940100	2.42159700
H	-0.89248300	-2.27098600	3.17836200
H	-0.72753300	-1.90826000	1.46109400
H	0.66983200	-2.52743000	2.35544100
C	0.58598700	3.65900700	-1.19457400
C	1.35346600	4.49993100	-2.21219300
H	1.00047000	3.82745300	-0.19017000
H	-0.46139700	3.98823700	-1.15821500
C	1.31801000	5.99107600	-1.88854600
H	2.39364100	4.15250900	-2.25387600
H	0.93191700	4.32630500	-3.21026100
H	1.86846400	6.57835900	-2.62846400
H	0.28744600	6.35963100	-1.86590400
H	1.76144300	6.18650400	-0.90679700
C	3.32028700	0.64668600	-5.56657800
C	1.96464300	0.33741000	-5.47447500

C	1. 43341300	-0. 15168400	-4. 28628700
C	2. 24275200	-0. 33193500	-3. 15582800
C	3. 60637800	-0. 02227800	-3. 26215000
C	4. 13748100	0. 45975600	-4. 45447600
H	3. 73381300	1. 02660000	-6. 49516700
H	1. 31632800	0. 46856300	-6. 33533500
H	0. 37836400	-0. 40431500	-4. 24563200
H	4. 24591200	-0. 15951600	-2. 39698600
H	5. 19555100	0. 69671000	-4. 51100500
C	1. 68109700	-0. 82759300	-1. 87584700
C	0. 35356600	-0. 80080300	-1. 55781600
H	-0. 39559300	-0. 46214300	-2. 26652400
H	0. 02118500	-1. 33779900	-0. 67700300
N	2. 63710800	-1. 29379500	-0. 97289500
N	2. 23011000	-1. 53539700	0. 19407900
C	3. 26494300	-2. 02474900	1. 05021400
O	2. 98841700	-2. 76300900	1. 97228600
O	4. 46957500	-1. 54585200	0. 76702900
C	5. 62771200	-1. 91115100	1. 58319400
C	5. 42999500	-1. 41468800	3. 01175500
C	5. 86271100	-3. 41623700	1. 51501900
C	6. 76541200	-1. 15768500	0. 90561400
H	5. 18176200	-0. 34936300	3. 00345900
H	4. 63612700	-1. 96543000	3. 51784900
H	6. 36195100	-1. 54653400	3. 56836800
H	5. 92598200	-3. 73768300	0. 47162600
H	6. 81157900	-3. 65096200	2. 00524900
H	5. 06327400	-3. 96492800	2. 01255200
H	7. 70380800	-1. 35307000	1. 43039700
H	6. 86956800	-1. 48168900	-0. 13305500
H	6. 57145600	-0. 08214700	0. 92021700

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C	-1. 93908900	0. 00901600	-0. 21942500
C	-3. 26289900	1. 01484000	1. 19743400
C	-2. 57335200	2. 42771200	-0. 72492400
H	-1. 66770700	2. 44744100	-1. 33384700
N	-3. 15754000	-0. 19922700	1. 65248500
N	-2. 33899800	-0. 81918200	0. 74773700
N	-2. 54647800	1. 17687800	0. 04318700
C	-3. 86403100	2. 24839400	1. 78635200
H	-4. 03542300	2. 11749400	2. 85421600
H	-4. 81187100	2. 50256500	1. 29384700
C	-2. 67691700	3. 65252800	0. 26315000

O	-2.88727400	3.26210600	1.61433100
C	-4.53128000	3.67731900	-1.30505500
C	-3.82277800	2.50987200	-1.57103700
C	-4.26114200	1.58042500	-2.50973700
C	-5.45601900	1.83776300	-3.17700300
C	-6.18147400	3.00273200	-2.90946500
C	-5.72395600	3.93188800	-1.97810600
C	-3.82753400	4.53062000	-0.28188900
H	-3.66302100	0.69621400	-2.71563300
H	-7.11198200	3.18687000	-3.43693200
H	-6.28861000	4.83745100	-1.77794400
H	-4.47670800	4.84769900	0.54057000
H	-3.42536700	5.43903000	-0.74058000
C	-2.08212700	-2.23295500	0.82275100
C	-2.59814600	-3.04523800	-0.19179200
C	-1.32049000	-2.71985500	1.88761200
C	-2.31064300	-4.40699300	-0.12093800
C	-1.06702700	-4.09023300	1.91055800
C	-1.54359600	-4.94406400	0.91416500
H	-2.69932300	-5.06490900	-0.89400800
H	-0.47323800	-4.49797500	2.72465900
H	-1.72940500	4.19171000	0.28538300
H	-5.82599200	1.13203400	-3.91342300
C	-0.96845000	-0.22919800	-1.34897300
O	-1.28751500	0.26371800	-2.46485600
C	0.20653900	-0.81852200	-0.91396200
C	1.24486600	-1.30085400	-1.88220300
H	0.24642900	-1.19701400	0.10346400
H	1.23278600	-0.66517700	-2.77566500
H	2.24527200	-1.21519200	-1.44511100
C	-1.21501700	-6.41382400	0.93908900
H	-0.30572600	-6.61115900	0.36183400
H	-1.04303500	-6.76420500	1.95898600
H	-2.02028100	-7.00572100	0.49820100
C	-0.77732900	-1.79941900	2.94680400
H	-0.20557300	-0.97514900	2.50503000
H	-1.58407400	-1.34817600	3.53137900
H	-0.11886100	-2.34365300	3.62547800
C	-3.42535200	-2.48374000	-1.31956300
H	-4.17940400	-1.78031600	-0.95164000
H	-2.80215200	-1.94937800	-2.04509400
H	-3.93878600	-3.28957200	-1.84592500
C	0.98651000	-2.75874100	-2.28825300
C	2.04094500	-3.30868500	-3.24587900

H	-0.00804200	-2.82982300	-2.75036600
H	0.94892400	-3.38340400	-1.38412600
C	1.78244400	-4.76354800	-3.62791000
H	2.06618000	-2.68535300	-4.14826800
H	3.03070000	-3.21588100	-2.78132800
H	2.54525900	-5.14397700	-4.31247600
H	1.77788600	-5.40353900	-2.73941200
H	0.80878800	-4.87014500	-4.11691200
C	0.91139900	0.72622900	4.78839000
C	2.08254300	0.16546900	4.28230500
C	2.43423100	0.34737000	2.94850800
C	1.62009300	1.09357800	2.08491900
C	0.45043100	1.66641900	2.61146600
C	0.09976400	1.48219000	3.94460100
H	0.63707100	0.57938200	5.82799100
H	2.72472100	-0.42522400	4.92854100
H	3.34376300	-0.09507000	2.55680500
H	-0.19560100	2.27892100	1.98800700
H	-0.81140800	1.93597900	4.32337700
C	1.96309300	1.21648900	0.64701700
C	0.98501800	1.40592300	-0.29165900
H	-0.00180600	1.70707300	0.02796500
H	1.23347900	1.55124600	-1.33733800
N	3.29731100	1.00691300	0.33373400
N	3.58657900	0.97963900	-0.89468000
C	4.97651600	0.77120400	-1.14036400
O	5.32827900	0.30799900	-2.20308200
O	5.77580500	1.15961900	-0.15024200
C	7.22401400	1.00081200	-0.25800400
C	7.57903600	-0.47592400	-0.39773800
C	7.75829200	1.83921700	-1.41483200
C	7.72230100	1.54633600	1.07488400
H	7.12454500	-1.04732900	0.41669600
H	7.23766300	-0.87612200	-1.35213900
H	8.66469800	-0.59032100	-0.33391800
H	7.42277000	2.87504100	-1.31136100
H	8.85150900	1.82797000	-1.38912600
H	7.42286800	1.44734600	-2.37479100
H	7.43556700	2.59491300	1.18885600
H	7.29497900	0.97476500	1.90289500
H	8.81165900	1.47287100	1.12196600
TS4S"			
C	0.28637200	-1.79238100	-0.17307000

C	1. 92225200	-2. 83641600	-1. 17885600
C	2. 35064600	-0. 43287600	-0. 76898400
H	1. 65990900	0. 40862800	-0. 73943700
N	1. 01379800	-3. 75137600	-0. 99773900
N	0. 00498700	-3. 08718700	-0. 35588800
N	1. 52067900	-1. 63339600	-0. 67502700
C	3. 18515400	-2. 83000100	-1. 97724800
H	3. 24214300	-3. 71483100	-2. 61013500
H	4. 06556200	-2. 79316800	-1. 32156300
C	3. 16167200	-0. 44470300	-2. 11636300
O	3. 09235600	-1. 68843300	-2. 81003300
C	4. 66217100	-0. 13946300	-0. 23384200
C	3. 40006900	-0. 35740500	0. 31483500
C	3. 20837100	-0. 44090600	1. 69097700
C	4. 31860200	-0. 30056600	2. 52100800
C	5. 58733700	-0. 07624600	1. 97993700
C	5. 76756900	0. 00557600	0. 60073400
C	4. 61239700	-0. 07191500	-1. 73717600
H	2. 20801300	-0. 58633100	2. 08729400
H	6. 44131000	0. 03231100	2. 64140300
H	6. 75500800	0. 17713300	0. 18206600
H	5. 31474600	-0. 76029900	-2. 21908800
H	4. 83887800	0. 93858300	-2. 08554600
C	-1. 14101100	-3. 80945500	0. 12502600
C	-1. 26286200	-4. 01202800	1. 50222000
C	-2. 06833700	-4. 27457300	-0. 80841300
C	-2. 38476000	-4. 71144400	1. 94115000
C	-3. 17064800	-4. 97172700	-0. 31655700
C	-3. 34659000	-5. 19387500	1. 05028500
H	-2. 50811000	-4. 88845900	3. 00661700
H	-3. 91063000	-5. 34590100	-1. 01920500
H	2. 72359700	0. 28484800	-2. 79689300
H	4. 19650800	-0. 35944600	3. 59790800
C	-0. 51499500	-0. 73673000	0. 54570600
O	0. 14463900	0. 02478400	1. 30047000
C	-1. 87832500	-0. 71974600	0. 29510000
C	-2. 76771300	0. 08188400	1. 19431400
H	-2. 31625900	-1. 49717400	-0. 32505600
H	-2. 69730900	-0. 31379400	2. 22076600
H	-2. 38277200	1. 10845100	1. 25767100
C	-4. 56323700	-5. 91945100	1. 56260100
H	-5. 32908000	-5. 20513700	1. 88148200
H	-5. 00074300	-6. 55456800	0. 78965100
H	-4. 31513900	-6. 54188200	2. 42546000

C	-1.88743100	-4.00862600	-2.27909900
H	-1.74311000	-2.93905600	-2.46870700
H	-1.00708500	-4.52761400	-2.66835800
H	-2.76306900	-4.34026100	-2.83839300
C	-0.23292600	-3.48921700	2.46926300
H	0.78274000	-3.71553600	2.12952600
H	-0.30800600	-2.40168100	2.58151700
H	-0.37344500	-3.94093500	3.45222000
C	-4.23034300	0.09157300	0.76183300
C	-5.08272100	1.04547200	1.59248400
H	-4.63787500	-0.92774700	0.82379800
H	-4.29997600	0.38772500	-0.29356600
C	-6.53870500	1.07567700	1.13926400
H	-5.02545400	0.75632700	2.65015300
H	-4.65327300	2.05259000	1.51729800
H	-7.13021500	1.78275000	1.72772700
H	-6.60471700	1.37774000	0.08855900
H	-7.00196700	0.08772800	1.23378400
C	-4.89737600	4.55046000	0.20288100
C	-3.68033100	4.66317200	0.87439400
C	-2.59269300	3.88207900	0.49823100
C	-2.69901800	2.96484900	-0.55776400
C	-3.92159800	2.87218500	-1.23480400
C	-5.01089100	3.65206500	-0.85519900
H	-5.74539600	5.16078900	0.49626900
H	-3.57746100	5.36279000	1.69822200
H	-1.64553400	3.97257200	1.01942900
H	-4.01782400	2.19991600	-2.08296800
H	-5.94726600	3.56581800	-1.39823100
C	-1.52985500	2.14974100	-0.97842500
C	-1.63777500	0.91028400	-1.55582500
H	-2.59941600	0.50984900	-1.85178300
H	-0.75566000	0.43178600	-1.96324200
N	-0.30739000	2.73463400	-0.68572500
N	0.71564800	2.23388900	-1.23359100
C	1.93927600	2.84549800	-0.82995500
O	2.97777700	2.44317900	-1.31973700
O	1.83266000	3.79367600	0.08990500
C	3.02659700	4.36356400	0.71331900
C	3.81495200	3.26427000	1.41921600
C	3.85952500	5.11044800	-0.32324200
C	2.43920000	5.33735000	1.72794100
H	3.16082200	2.71276400	2.10082800
H	4.25540600	2.56081700	0.71078800

H	4. 61718200	3. 72255800	2. 00504800
H	3. 23761300	5. 84146800	-0. 84776000
H	4. 66438700	5. 64777700	0. 18626000
H	4. 29698800	4. 42499700	-1. 04817800
H	1. 83215600	6. 09317900	1. 22270300
H	1. 81019200	4. 80489900	2. 44594600
H	3. 24538200	5. 83892500	2. 26908400

TS4S'''

C	0. 34789800	-1. 19957000	-0. 01960200
C	2. 03471500	-0. 48296100	-1. 20919100
C	2. 68904100	-1. 31155000	1. 02321200
H	2. 17325400	-1. 28208700	1. 98079500
N	1. 00275700	-0. 33157000	-1. 98608600
N	-0. 04111400	-0. 79437600	-1. 23807600
N	1. 68218800	-1. 02031900	-0. 00730500
C	3. 45509600	-0. 06877800	-1. 38730000
H	3. 53590900	0. 65476400	-2. 19888000
H	4. 09341500	-0. 93499400	-1. 60875400
C	3. 87034700	-0. 27557400	0. 95807100
O	3. 82900600	0. 57045000	-0. 18384200
C	4. 72807100	-2. 53600700	0. 73284300
C	3. 34092200	-2. 65132600	0. 76082800
C	2. 70681000	-3. 87360700	0. 55742000
C	3. 49667300	-4. 99340300	0. 30908100
C	4. 89006100	-4. 88552900	0. 27467900
C	5. 51529700	-3. 65951100	0. 49050200
C	5. 16522100	-1. 11992400	1. 00568500
H	1. 62416800	-3. 93554100	0. 61406900
H	5. 49139300	-5. 76756700	0. 07868200
H	6. 59795000	-3. 58015200	0. 46486300
H	5. 88633300	-0. 73935100	0. 27564600
H	5. 63324100	-1. 04001200	1. 99182500
C	-1. 34998700	-0. 86939600	-1. 82727400
C	-1. 91779800	-2. 13368300	-2. 02929500
C	-1. 99174800	0. 32220400	-2. 17926600
C	-3. 21482400	-2. 17604700	-2. 53555600
C	-3. 29194900	0. 21890500	-2. 67492800
C	-3. 92427500	-1. 01248900	-2. 84114200
H	-3. 68173700	-3. 14461000	-2. 69528600
H	-3. 82252400	1. 13328000	-2. 92919700
H	3. 79672800	0. 41887900	1. 79481300
H	3. 02838200	-5. 95840400	0. 14503900
C	-0. 41718400	-1. 79024100	1. 13598800

O	0.28653300	-2.44411600	1.95735100
C	-1.76941600	-1.52195700	1.23341000
C	-2.55332800	-2.19744000	2.32226700
H	-2.29813300	-1.03744900	0.42203000
H	-2.40479400	-3.28612100	2.25476000
H	-2.14405400	-1.92073900	3.30631900
C	-5.34736700	-1.08231100	-3.33002300
H	-6.04427000	-0.95164000	-2.49564700
H	-5.55399500	-0.29398900	-4.05733000
H	-5.56066800	-2.04799300	-3.79292700
C	-1.31920900	1.66543600	-2.09153800
H	-0.62588100	1.74051100	-1.25109300
H	-0.74008900	1.84944300	-3.00263100
H	-2.06962500	2.45253600	-1.98956300
C	-1.18495100	-3.40669800	-1.69720800
H	-0.11730400	-3.33272000	-1.92360600
H	-1.28521000	-3.64585100	-0.63276200
H	-1.59917300	-4.23722200	-2.27109500
C	-4.04843100	-1.88919600	2.27759500
C	-4.85302400	-2.68535000	3.30205500
H	-4.43144100	-2.09770100	1.26814400
H	-4.21655000	-0.81668300	2.45194900
C	-6.34288900	-2.35691600	3.26269600
H	-4.70358000	-3.75683900	3.12009600
H	-4.45490100	-2.48492700	4.30456500
H	-6.90293100	-2.93847200	3.99946200
H	-6.51343500	-1.29608000	3.47168300
H	-6.76266900	-2.57191300	2.27483700
C	-4.68301900	3.63097100	-0.33309100
C	-3.52863100	4.36647600	-0.05970000
C	-2.42906400	3.75657200	0.53233200
C	-2.46209000	2.39578200	0.87196300
C	-3.62656700	1.66890700	0.59834000
C	-4.72669200	2.28054000	0.00165700
H	-5.53773400	4.10768200	-0.80195500
H	-3.48529800	5.42153200	-0.31199200
H	-1.52640900	4.32547900	0.72632300
H	-3.66287300	0.60769500	0.82336900
H	-5.61325800	1.69213300	-0.21536100
C	-1.27157700	1.72429200	1.44300600
C	-1.34178600	0.64995900	2.28220600
H	-2.29089200	0.38121200	2.73145100
H	-0.43996000	0.25738500	2.74070400
N	-0.07038900	2.30022600	1.04006500

N	1. 00271300	1. 67746300	1. 26097500
C	2. 11508000	2. 50373100	0. 87169400
O	3. 01074400	2. 73591500	1. 64905200
O	2. 00916000	2. 91786500	-0. 38381900
C	2. 86955500	3. 98516900	-0. 89795300
C	2. 68607700	5. 23070100	-0. 03629400
C	4. 32543300	3. 53851300	-0. 95370400
C	2. 31540400	4. 21012600	-2. 29892900
H	1. 62189600	5. 46606100	0. 05624800
H	3. 10985500	5. 08884600	0. 95860100
H	3. 18764000	6. 07641400	-0. 51397100
H	4. 43505500	2. 65976700	-1. 59296500
H	4. 92302600	4. 35027700	-1. 37853500
H	4. 70000500	3. 29703000	0. 04015900
H	2. 37622000	3. 28685400	-2. 88203500
H	1. 26910600	4. 52295100	-2. 24894800
H	2. 89298700	4. 98584100	-2. 80768300

TS4'

C	1. 94903600	-0. 84780800	-0. 59297400
C	3. 62613500	-2. 25894400	-0. 68656600
C	4. 29519100	0. 17362000	-0. 69987700
H	4. 10695400	0. 74867200	-1. 60450000
N	2. 57393600	-3. 00828200	-0. 55429300
N	1. 53610600	-2. 11950300	-0. 48296800
N	3. 29859100	-0. 93147700	-0. 69164100
C	5. 03719600	-2. 72508800	-0. 88264900
H	5. 05046200	-3. 51061300	-1. 64131800
H	5. 43334000	-3. 14871800	0. 04900600
C	5. 70547500	-0. 47386900	-0. 62367200
O	5. 83046600	-1. 66962600	-1. 36536400
C	5. 25656300	0. 57732700	1. 45418400
C	4. 26267000	1. 00334200	0. 56874800
C	3. 44711900	2. 08893800	0. 87925800
C	3. 62454400	2. 72007800	2. 10947000
C	4. 60195600	2. 28209000	3. 00413300
C	5. 43258200	1. 21222000	2. 67784200
C	6. 04456800	-0. 57007400	0. 87914800
H	2. 71253600	2. 42811200	0. 15633000
H	4. 72738900	2. 78838900	3. 95657800
H	6. 21009700	0. 88584300	3. 36300700
H	5. 71016500	-1. 52086400	1. 31243500
H	7. 12101200	-0. 49666700	1. 05613700
C	0. 20170300	-2. 65905900	-0. 40412100

C	-0.44972000	-2.74563900	0.82378700
C	-0.35605500	-3.13436100	-1.60017000
C	-1.74176700	-3.28085400	0.82251300
C	-1.65031400	-3.63135900	-1.55007700
C	-2.36463400	-3.69446900	-0.34891500
H	-2.28002800	-3.33360300	1.76674300
H	-2.11795800	-3.97530100	-2.46958500
H	6.39779000	0.22700700	-1.09595200
H	2.99786800	3.56886200	2.36818700
C	1.25556600	0.50552900	-0.68317200
O	1.84634600	1.30575900	-1.47622400
C	0.37253100	0.74095100	0.34898800
C	-0.15513300	2.09385400	0.66059100
H	0.02260500	-0.09050300	0.94967400
H	0.48830200	2.85457800	0.19755000
H	-1.15015900	2.23628000	0.20132500
C	-3.79555600	-4.16329900	-0.34003800
H	-4.46576500	-3.30452000	-0.46828200
H	-3.99180400	-4.86657900	-1.15386600
H	-4.04952900	-4.64936200	0.60622900
C	0.41720300	-3.07926200	-2.89116200
H	0.75518500	-2.06033100	-3.11384000
H	1.30616000	-3.71624700	-2.84118500
H	-0.20402400	-3.41607800	-3.72344200
C	0.16154900	-2.29873000	2.12525400
H	0.24610000	-3.14860400	2.81005200
H	1.15569200	-1.86426400	1.99831400
H	-0.49070300	-1.55266800	2.59202000
C	-0.28547000	2.31658500	2.16991900
C	-0.80089800	3.71000300	2.51924600
H	0.69112000	2.15406700	2.64735400
H	-0.96681400	1.55718000	2.57946400
C	-0.93396400	3.92480600	4.02453800
H	-0.12244900	4.46265200	2.09553800
H	-1.77266800	3.86678900	2.03376500
H	0.03351500	3.79968600	4.52351300
H	-1.30583600	4.92681700	4.25885100
H	-1.62716400	3.19760400	4.46070900
C	-2.13976800	4.87047700	-3.67890700
C	-3.26367400	4.14481200	-3.29001600
C	-3.12062100	2.90400200	-2.67821300
C	-1.84760900	2.36951800	-2.45228700
C	-0.71879700	3.11194600	-2.82332400
C	-0.86961200	4.35059200	-3.43876500

H	-2.25371200	5.83950400	-4.15574200
H	-4.25753400	4.54695400	-3.46527700
H	-3.99308000	2.33581300	-2.37030500
H	0.27260100	2.72362000	-2.59085800
H	0.01206900	4.91994400	-3.71881400
C	-1.68652800	1.04073200	-1.82405600
C	-0.60951200	0.23344800	-2.02229800
H	0.13715000	0.48542200	-2.76361300
H	-0.68704800	-0.77930700	-1.65755100
N	-2.64909900	0.70878800	-0.85993900
N	-2.32143000	-0.27592400	-0.14211900
C	-3.21925400	-0.50083900	0.93475000
O	-2.80295100	-0.60442000	2.06784100
O	-4.48473000	-0.64176300	0.54532000
C	-5.55227700	-0.72807800	1.53712900
C	-5.39702000	-1.98028300	2.39536200
C	-5.56685200	0.54544800	2.37747100
C	-6.80438200	-0.81990700	0.67376500
H	-5.32957100	-2.86825900	1.75904200
H	-4.50890900	-1.92047100	3.02515900
H	-6.27967800	-2.08719700	3.03438500
H	-5.61224300	1.42219500	1.72435600
H	-6.45199300	0.54541200	3.02108000
H	-4.67624000	0.61276700	3.00447200
H	-6.87846500	0.05412400	0.02103100
H	-6.77297000	-1.71792700	0.04918500
H	-7.69453600	-0.86538300	1.30774600

TS5R

C	0.77433600	1.12907800	-0.77194100
C	0.51431000	3.28259900	-0.71036100
C	-1.21723100	2.09323000	-2.11538100
H	-0.85581700	1.74189600	-3.08049400
N	1.57521900	3.05368500	0.00406200
N	1.73040400	1.70137900	-0.04254900
N	-0.01193300	2.12751700	-1.22253000
C	-0.04856100	4.63173800	-1.02234000
H	0.77299400	5.32678500	-1.20171900
H	-0.63454500	5.00281500	-0.17309400
C	-1.78805500	3.54075300	-2.16719400
O	-0.81131900	4.55654900	-2.20283500
C	-3.37335500	2.21250600	-1.07868800
C	-2.44485600	1.32595900	-1.63722000
C	-2.79300100	-0.00807100	-1.83903600

C	-4.06002300	-0.44123900	-1.45364300
C	-4.98133900	0.44435900	-0.89725000
C	-4.64443200	1.78370600	-0.71582800
C	-2.81043200	3.60355400	-1.01800100
H	-2.08779100	-0.70389700	-2.27349400
H	-5.96991600	0.09343800	-0.61690500
H	-5.36567700	2.48738800	-0.30964400
H	-2.32300300	3.74639300	-0.04532700
H	-3.54795700	4.39586300	-1.16113100
C	2.93644200	1.16122800	0.54392300
C	2.90831400	0.66581200	1.84879200
C	4.11751000	1.29414400	-0.19823100
C	4.12455900	0.24921800	2.39583800
C	5.30107900	0.85905900	0.39320200
C	5.32370200	0.33893700	1.69058700
H	4.13142800	-0.13449000	3.41266600
H	6.23130000	0.95152200	-0.16282900
H	-2.32572100	3.62324000	-3.11480800
H	-4.32793700	-1.48362700	-1.59528100
C	0.55557500	-0.30933700	-1.15998500
O	-0.00050300	-0.47115200	-2.24681100
C	1.40441100	-1.41870400	-0.58445100
C	2.68987200	-1.54943500	-1.41979100
H	1.66000300	-1.18912800	0.45141600
H	2.45538900	-2.06676900	-2.35838600
H	3.04638100	-0.55318800	-1.70744100
C	6.62472000	-0.08902200	2.31840400
H	7.37701500	0.69899900	2.22645500
H	6.49458700	-0.31993000	3.37721600
H	7.02632900	-0.97930400	1.82526300
C	4.12098400	1.93933400	-1.55953400
H	3.31414300	1.56646100	-2.19813000
H	3.98393900	3.02136300	-1.46632700
H	5.06964600	1.75516800	-2.06651000
C	1.63525100	0.60500900	2.64547200
H	1.07687300	1.54063300	2.56478500
H	0.96537400	-0.17498100	2.26533100
H	1.85689600	0.39898100	3.69403200
C	3.82081300	-2.25797400	-0.68172700
C	5.11744100	-2.26561500	-1.48705400
H	3.53181500	-3.28962100	-0.43997700
H	3.99475900	-1.74540800	0.27543000
C	6.26570200	-2.93345800	-0.73839600
H	4.94939600	-2.77180800	-2.44598000

H	5.38608200	-1.22753800	-1.72612600
H	7.19318300	-2.91383900	-1.31642100
H	6.44815400	-2.42234000	0.21260400
H	6.03077400	-3.97819500	-0.51176900
C	-3.19768100	-6.25377100	-0.35889400
C	-3.74264400	-5.07595100	0.15699500
C	-2.97643500	-3.92202100	0.23626500
C	-1.63893500	-3.91175200	-0.19578900
C	-1.10449600	-5.09907300	-0.71200100
C	-1.87715900	-6.25739800	-0.79269000
H	-3.79872600	-7.15539200	-0.42097000
H	-4.77371100	-5.05952200	0.49747600
H	-3.39442000	-3.00235800	0.63154400
H	-0.07748900	-5.13397000	-1.05924500
H	-1.43930700	-7.16476200	-1.19733700
C	-0.83292500	-2.66169500	-0.10881900
C	0.58106100	-2.71165600	-0.64827300
H	1.13113200	-3.50084200	-0.12104400
H	0.52694900	-3.02596300	-1.69831100
N	-1.42793100	-1.65079100	0.41966400
N	-0.77475100	-0.46696000	0.49175400
C	-1.43406800	0.52576500	1.14976100
O	-0.95340800	1.65441100	1.29490300
O	-2.63725100	0.18902300	1.66730600
C	-3.13439600	0.87745100	2.84115900
C	-2.14547000	0.67508300	3.98708600
C	-3.40785700	2.36215400	2.60080100
C	-4.44729000	0.15282400	3.12279100
H	-1.96409500	-0.39243700	4.14355700
H	-1.19754600	1.16963200	3.76111700
H	-2.54914000	1.09957400	4.91085400
H	-3.99294400	2.48722600	1.68675300
H	-3.98945200	2.75484700	3.44141200
H	-2.48144700	2.92606400	2.50707400
H	-4.91039000	0.54823000	4.03089100
H	-5.13642900	0.29364900	2.28456800
H	-4.27031400	-0.91812400	3.25291500

TS5S

C	-0.88606900	-0.75663800	0.32022300
C	-2.87423300	-0.91182600	1.19701200
C	-2.86653100	0.19848300	-1.00233900
H	-2.14069000	0.88171100	-1.43896000
N	-2.08248600	-1.43858500	2.08362700

N	-0.84528500	-1.34511700	1.51849800
N	-2.18597700	-0.49886700	0.09655200
C	-4.33056200	-0.60141600	1.26902400
H	-4.68434000	-0.69455000	2.29526200
H	-4.90693900	-1.28067900	0.62459500
C	-4.13120900	0.98638300	-0.48391600
O	-4.46857300	0.74602700	0.87084200
C	-4.76331400	-0.55820100	-2.25493000
C	-3.41068800	-0.78416100	-2.01522400
C	-2.72070700	-1.80377600	-2.66613000
C	-3.41510700	-2.60434100	-3.56887600
C	-4.77282100	-2.38180200	-3.81466600
C	-5.45468200	-1.35793200	-3.16186500
C	-5.28243700	0.59990800	-1.44501700
H	-1.66290800	-1.96281700	-2.47848600
H	-5.30104500	-3.01461400	-4.52073300
H	-6.50998300	-1.18810200	-3.35336500
H	-6.17889000	0.35016400	-0.86834800
H	-5.54125100	1.44549500	-2.08960000
C	0.27192500	-1.91892600	2.22202700
C	0.60024500	-3.24997400	1.91911900
C	0.93256800	-1.16850300	3.19091600
C	1.67772500	-3.81217500	2.58861200
C	2.01078800	-1.78647900	3.83779300
C	2.40105900	-3.08878100	3.54704500
H	1.96137200	-4.83768500	2.36511900
H	2.55132000	-1.22300200	4.59445900
H	-3.91351100	2.05266800	-0.51916200
H	-2.89849500	-3.40522000	-4.08750000
C	0.20712200	-0.44783900	-0.68224700
O	-0.16618000	-0.07467100	-1.78635400
C	1.62410500	-0.98260200	-0.48584700
C	2.16630800	-1.44351000	-1.84856700
H	1.58333700	-1.85096400	0.17698400
H	1.36949000	-1.94549200	-2.40896900
H	2.44066300	-0.56233100	-2.44182100
C	3.57337400	-3.72650200	4.24537500
H	4.36559700	-3.96472000	3.52945700
H	3.98964700	-3.06405800	5.00632500
H	3.27708500	-4.66245100	4.72720600
C	0.52846300	0.23429900	3.55961500
H	1.33024600	0.93598900	3.31019100
H	-0.36821700	0.56450700	3.03357200
H	0.35830900	0.29156900	4.63862100

C	-0.16940900	-4.01435800	0.87434900
H	-1.24504600	-3.98202200	1.07131500
H	-0.00763000	-3.59446900	-0.12665400
H	0.14778200	-5.05763900	0.85246200
C	3.35363000	-2.39651900	-1.72591000
C	3.99842600	-2.69709900	-3.07749300
H	3.01753600	-3.33375100	-1.25926000
H	4.12021600	-1.98788000	-1.05384700
C	5.15910800	-3.68167800	-2.96879500
H	3.23717700	-3.09138800	-3.76198900
H	4.34962900	-1.75498000	-3.51858200
H	5.61605100	-3.87305200	-3.94305900
H	5.93646000	-3.29355900	-2.30288700
H	4.82087400	-4.63967700	-2.56126700
C	5.53041900	3.17228000	-2.86461200
C	4.49522400	3.95498900	-2.34977700
C	3.50582900	3.38310400	-1.56230800
C	3.52501500	2.01029900	-1.26484100
C	4.56966800	1.23664500	-1.78642100
C	5.56056200	1.81122500	-2.58034900
H	6.30316400	3.62135300	-3.48030100
H	4.46265400	5.01904900	-2.56358300
H	2.69744600	3.98493300	-1.16109300
H	4.61164600	0.17009600	-1.58752500
H	6.35599300	1.18773600	-2.97700100
C	2.45329400	1.41668400	-0.43224000
C	2.56900900	0.04929500	0.17943100
H	3.59029800	-0.33185500	0.13936900
H	2.28422700	0.13730900	1.23217600
N	1.39068600	2.12225500	-0.21741800
N	0.44988200	1.47297500	0.52027000
C	-0.60940000	2.23206800	0.90175000
O	-1.58164900	1.74710500	1.49340400
O	-0.51526500	3.55762100	0.63399500
C	-1.42805100	4.49602900	1.25353300
C	-2.86639200	4.26540400	0.79352200
C	-1.30005000	4.42954300	2.77378400
C	-0.92693600	5.84302700	0.74011200
H	-2.89690300	4.21212900	-0.30008100
H	-3.26877700	3.34310000	1.21286000
H	-3.48821100	5.10908000	1.10867900
H	-0.25564700	4.57617400	3.06552300
H	-1.89904000	5.22480800	3.22723000
H	-1.64547300	3.46647300	3.15039000

H	0.11855200	5.99089500	1.02334800
H	-1.00058100	5.88412900	-0.35002100
H	-1.52515000	6.65442400	1.16326900

M5R

C	-0.92959100	0.58396400	0.46279000
C	-2.65268800	1.10146100	1.70215600
C	-3.16848300	1.04025500	-0.72213600
H	-2.53164700	1.27857400	-1.57348800
N	-1.66435600	1.02856400	2.54029000
N	-0.58866500	0.70777300	1.75390200
N	-2.24451500	0.86194300	0.41773500
C	-4.03524000	1.62194700	1.89707300
H	-4.14412100	2.05190800	2.89202900
H	-4.78905000	0.83691000	1.75257100
C	-4.20141000	2.19312100	-0.39882900
O	-4.16171100	2.66129700	0.94256000
C	-5.37941200	0.16255600	-1.02580100
C	-4.02684900	-0.16926700	-1.01626800
C	-3.59453700	-1.45283900	-1.34083000
C	-4.55554500	-2.42026600	-1.62334200
C	-5.91694700	-2.10301500	-1.60057600
C	-6.33751500	-0.80708500	-1.31371100
C	-5.59488200	1.62879700	-0.76177300
H	-2.53128900	-1.65882300	-1.37376800
H	-6.65246900	-2.87013600	-1.82269400
H	-7.39378500	-0.55420100	-1.32028000
H	-6.29858300	1.82444700	0.05413600
H	-5.99095000	2.12934000	-1.65074900
C	0.72780000	0.84592900	2.33613900
C	1.42675600	-0.25235200	2.82930100
C	1.21804000	2.16047800	2.44396300
C	2.69784900	-0.01691500	3.36711600
C	2.48519900	2.33860400	2.98305500
C	3.24846400	1.25658700	3.43709600
H	3.26095200	-0.86573900	3.74772500
H	2.88532300	3.34632300	3.06344200
H	-3.95425600	3.07173600	-0.99535800
H	-4.24420100	-3.42938900	-1.87654200
C	-0.07992700	0.20260700	-0.80148300
O	-0.82708100	-0.02747100	-1.83356800
C	0.98638000	1.31105100	-1.00216700
C	0.31597700	2.58005000	-1.52912800
H	1.49354900	1.52321100	-0.05154800

H	-0.05796900	2.38059800	-2.53961300
H	-0.57895100	2.80560700	-0.92775500
C	4.62509200	1.48450700	4.00397200
H	5.05173300	0.55815100	4.39292000
H	5.29964300	1.87432400	3.23595500
H	4.59581200	2.21791700	4.81477300
C	0.38285700	3.34471100	2.03304100
H	-0.05445400	3.21431800	1.03918900
H	-0.44577800	3.48840500	2.73344700
H	0.98660800	4.25386100	2.02236100
C	0.87311500	-1.64861000	2.83692500
H	-0.19081700	-1.66865500	2.59932200
H	1.39992000	-2.26865900	2.10382000
H	1.02330800	-2.10141800	3.82060800
C	1.22953200	3.80499600	-1.52702900
C	0.47918100	5.09749600	-1.84128100
H	2.03692200	3.67196200	-2.25830600
H	1.71712500	3.89968600	-0.54569900
C	1.39586600	6.31722400	-1.86594400
H	-0.02896600	4.99287200	-2.80807600
H	-0.31013600	5.24186900	-1.09181700
H	0.84238700	7.23281200	-2.08980200
H	1.89022000	6.45074700	-0.89830800
H	2.17652000	6.20165700	-2.62432700
C	6.58994600	-1.67021700	-2.59847200
C	5.96030500	-2.28125600	-1.51310800
C	4.67816900	-1.89988300	-1.14087900
C	3.99852100	-0.89735200	-1.84685800
C	4.63735900	-0.29105100	-2.93381400
C	5.92265000	-0.67714500	-3.30814600
H	7.59312600	-1.96760900	-2.88646100
H	6.47469500	-3.05650300	-0.95381500
H	4.18177800	-2.37079800	-0.29940200
H	4.12762800	0.47544600	-3.50856200
H	6.40001500	-0.19971300	-4.15787900
C	2.61599100	-0.50651700	-1.46497900
C	2.02027900	0.77329600	-1.98388200
H	2.80534100	1.51335500	-2.15691600
H	1.51913700	0.57809300	-2.94181000
N	1.98080400	-1.32794700	-0.71215000
N	0.70338500	-1.04593400	-0.30942000
C	-0.08012400	-2.13353300	0.02857500
O	-1.21958900	-1.99755600	0.44804000
O	0.53673900	-3.30546000	-0.12691700

C	-0.17107900	-4.54940600	0.16292600
C	-0.49873800	-4.64423800	1.64935500
C	-1.41850800	-4.67010400	-0.71008500
C	0.85441300	-5.60750000	-0.22723200
H	0.41316100	-4.54718100	2.24609300
H	-1.20882100	-3.87084000	1.94367100
H	-0.93891000	-5.62426700	1.85532500
H	-1.16661300	-4.44979400	-1.75195100
H	-1.79197300	-5.69681900	-0.65667500
H	-2.20345100	-3.98896200	-0.38097500
H	0.45226400	-6.60452900	-0.03066400
H	1.09690600	-5.52875200	-1.29009000
H	1.77263700	-5.47721000	0.35151400

M5S

C	1.08235900	-0.03009000	-0.71161100
C	2.89221000	0.10025800	-1.93982600
C	3.35222200	0.14399400	0.47356800
H	2.75964400	0.51751800	1.30591600
N	1.92127800	0.07652800	-2.80349400
N	0.80157600	-0.01256000	-2.02050900
N	2.42567600	0.03795000	-0.66035200
C	4.35048500	0.34758800	-2.13214400
H	4.54723300	0.67451700	-3.15286800
H	4.93769300	-0.55608800	-1.91991900
C	4.55606400	1.09194300	0.12602500
O	4.67694600	1.40951400	-1.25574700
C	5.37618200	-1.06871700	0.87431400
C	3.99265800	-1.18818800	0.78002000
C	3.35165700	-2.40830200	0.96606800
C	4.13152400	-3.52942500	1.23991500
C	5.52181000	-3.41915600	1.33358300
C	6.15354200	-2.18959300	1.15569600
C	5.81184600	0.35884000	0.65695100
H	2.26801800	-2.45963400	0.90898800
H	6.11583600	-4.30177800	1.54898100
H	7.23407900	-2.10906500	1.23027600
H	6.63262100	0.46016400	-0.05975300
H	6.14509800	0.80979600	1.59745800
C	-0.47616200	-0.07883500	-2.67257200
C	-0.86964600	-1.31704200	-3.19944300
C	-1.24354300	1.07990100	-2.79734500
C	-2.12597000	-1.39089200	-3.79122400
C	-2.49172400	0.95243200	-3.41437300

C	-2.95586800	-0.26938000	-3.89458400
H	-2.46325900	-2.34310200	-4.19321900
H	-3.11351700	1.83874000	-3.51606700
H	4.40955300	2.05776300	0.60996300
H	3.65815700	-4.49490400	1.38717900
C	0.17688400	-0.22808100	0.57670100
O	0.92012500	-0.40436700	1.61107000
C	-0.87390200	-1.38512600	0.28672500
C	-0.90849400	-2.38380800	1.44850300
H	-0.54438300	-1.93189800	-0.60391000
H	0.10657300	-2.51262200	1.83207400
H	-1.48673600	-1.95644600	2.28077600
C	-4.32471100	-0.39032200	-4.51122900
H	-5.03328300	-0.80921400	-3.78977600
H	-4.70447600	0.58356000	-4.82613800
H	-4.30838400	-1.05419000	-5.37889500
C	-0.79352200	2.42675500	-2.29748200
H	-1.38526100	2.72209400	-1.42498000
H	0.25825600	2.43608400	-2.00475500
H	-0.94397000	3.17988100	-3.07531900
C	0.05032100	-2.51027000	-3.17700900
H	0.78902600	-2.42976000	-3.98079200
H	0.60806500	-2.59087100	-2.23944900
H	-0.51460300	-3.43245300	-3.32287000
C	-1.49108900	-3.73867100	1.05120500
C	-1.59221000	-4.70684400	2.22796700
H	-0.86169600	-4.18443000	0.26678800
H	-2.48919100	-3.62346100	0.60473900
C	-2.12762900	-6.07619100	1.81899200
H	-0.60264400	-4.81683800	2.68881500
H	-2.24195900	-4.26810600	2.99598700
H	-2.19572900	-6.75383800	2.67402000
H	-3.12625400	-5.98869600	1.37890000
H	-1.47619800	-6.54162500	1.07230300
C	-6.24242000	-0.05969600	3.39597800
C	-5.57854500	1.15670400	3.22942700
C	-4.40953900	1.21897500	2.48320200
C	-3.88589000	0.06576100	1.88229900
C	-4.55582400	-1.14959200	2.05649100
C	-5.72534500	-1.21148500	2.81152700
H	-7.15637000	-0.10634000	3.97930000
H	-5.97734100	2.05937000	3.68143200
H	-3.88428900	2.15899600	2.35078800
H	-4.15641600	-2.06144700	1.62193700

H	-6.22852700	-2.16386600	2.94400200
C	-2.62905900	0.14499600	1.09874500
C	-2.27942800	-0.83486600	0.01933000
H	-3.00889800	-1.64209100	-0.06087300
H	-2.30941100	-0.28370500	-0.92669800
N	-1.82543600	1.10679900	1.37183600
N	-0.65377600	1.11395100	0.62826600
C	0.08745700	2.27505000	0.73347900
O	1.25877500	2.34724700	0.38921800
O	-0.64574300	3.31168100	1.14906700
C	-0.05094600	4.63751500	1.27233100
C	1.08623500	4.61866000	2.28906500
C	0.39913000	5.14649600	-0.09381400
C	-1.21419700	5.47367800	1.79402300
H	0.73988200	4.17358300	3.22613400
H	1.94060800	4.05316300	1.91848700
H	1.40108000	5.64618600	2.49240300
H	-0.43728500	5.11993900	-0.79913300
H	0.73085800	6.18442400	0.00218800
H	1.22077900	4.54685900	-0.48547500
H	-2.04829000	5.44529400	1.08788900
H	-1.55795100	5.08794000	2.75730600
H	-0.89777600	6.51184500	1.92269800

TS5'

C	0.50994200	-0.02348800	-0.34607200
C	-0.62307700	-0.66140400	-2.10156400
C	-1.73937400	1.09336900	-0.78913500
H	-1.69952900	1.42943300	0.24672700
N	0.49266100	-1.31935100	-2.18333900
N	1.19655600	-0.89827000	-1.08503000
N	-0.63446700	0.16609500	-1.01555500
C	-1.90394300	-0.77784300	-2.85934600
H	-1.93626100	-1.72875400	-3.39218900
H	-2.02663100	0.04949400	-3.57191400
C	-3.09360400	0.37782200	-1.10765800
O	-2.93213700	-0.80084300	-1.88858500
C	-2.92584800	2.43456900	-2.37101800
C	-1.68968300	2.25436000	-1.75591700
C	-0.60828200	3.08682100	-2.02100100
C	-0.78070000	4.10301000	-2.95830000
C	-2.01055500	4.28026400	-3.59695700
C	-3.09415400	3.45493300	-3.30214900
C	-3.93509600	1.43971300	-1.84909400

H	0.32523200	2.95017100	-1.48014900
H	-2.12616600	5.07541800	-4.32728400
H	-4.05221100	3.60555000	-3.79196600
H	-4.53771200	0.96398400	-2.62937400
H	-4.62626700	1.92673700	-1.15088900
C	2.60207500	-1.20603400	-1.02833100
C	3.46683300	-0.28825200	-1.62586600
C	3.01857300	-2.41961000	-0.47799200
C	4.82445400	-0.60484800	-1.63598500
C	4.38746700	-2.67856500	-0.49756500
C	5.29996700	-1.78598300	-1.06766500
H	5.52627100	0.09540200	-2.08298100
H	4.74972200	-3.60936400	-0.06660400
H	-3.55528300	0.02176300	-0.18438200
H	0.04531700	4.76837100	-3.18944800
C	0.89886500	0.76935100	0.90787000
O	1.00892200	1.99831700	0.64932200
C	1.82265100	0.05208200	1.94094400
C	3.01255400	0.89420300	2.38153600
H	2.16993500	-0.91524800	1.56212500
H	2.66541800	1.91223600	2.59957400
H	3.39209100	0.47413400	3.32373800
C	6.77543300	-2.09261300	-1.04494100
H	7.18097600	-1.96565700	-0.03501300
H	6.96949100	-3.12592400	-1.34756900
H	7.33001000	-1.42899900	-1.71315300
C	2.01961700	-3.38929200	0.08867400
H	1.37492700	-2.91543300	0.83772600
H	1.34323100	-3.75138200	-0.69191500
H	2.52932200	-4.24299300	0.54095500
C	2.94448400	1.00051800	-2.20538800
H	2.18599700	0.81062500	-2.97380400
H	2.48110300	1.62016100	-1.42624700
H	3.75621300	1.57270200	-2.66024800
C	4.13511100	0.94803000	1.35534100
C	5.36325900	1.72353400	1.82200800
H	3.75058600	1.41075000	0.43753200
H	4.43282900	-0.07703200	1.08991200
C	6.45597100	1.75398100	0.75633200
H	5.06995500	2.74869400	2.08211100
H	5.75520600	1.27098500	2.74250400
H	7.33805400	2.30869900	1.08985000
H	6.77293300	0.73668800	0.49755200
H	6.08712600	2.22634000	-0.16161800

C	-2.60613700	3.87763000	3.37938100
C	-3.30555700	2.73524800	2.99489600
C	-2.62041600	1.58652700	2.61552500
C	-1.21662800	1.55346400	2.60873800
C	-0.52653600	2.70839300	2.99766600
C	-1.21529600	3.85597500	3.38084400
H	-3.14177700	4.77358200	3.67842800
H	-4.39199300	2.73329800	3.00495300
H	-3.16620100	0.68934200	2.33901200
H	0.55770000	2.71530700	2.97967200
H	-0.65745000	4.74021900	3.67465200
C	-0.46757900	0.33760300	2.17711200
C	0.73323200	-0.12024200	3.00133200
H	0.88587700	0.54378100	3.85764400
H	0.60725100	-1.14623800	3.35782300
N	-1.28697400	-0.60842400	1.60429100
N	-0.77681900	-1.75173900	1.39425200
C	-1.64150900	-2.60635700	0.65798400
O	-1.20349400	-3.33165000	-0.20794600
O	-2.91083900	-2.55584300	1.07097500
C	-3.86804700	-3.57037100	0.64492200
C	-4.13206300	-3.49133600	-0.85454600
C	-3.36713800	-4.95082100	1.06269400
C	-5.12065400	-3.19577500	1.42877100
H	-4.48452900	-2.49507000	-1.13172600
H	-3.22674700	-3.71058300	-1.42214800
H	-4.90417600	-4.22328500	-1.11510600
H	-3.12606000	-4.95538300	2.13037400
H	-4.15416300	-5.69006700	0.88443100
H	-2.48089200	-5.23664300	0.49425500
H	-4.92419400	-3.23235900	2.50394600
H	-5.44037000	-2.18232800	1.16810300
H	-5.93215000	-3.89053400	1.19319200

TS6R

C	-1.12951400	-0.12738400	0.27489800
C	-1.53100500	-0.11687800	2.46123100
C	0.77200600	0.45502400	1.86602600
H	1.45597000	0.19229700	1.05497600
N	-2.69529200	-0.32074700	1.92439300
N	-2.41942700	-0.31169200	0.57271000
N	-0.56620400	0.01475800	1.50025200
C	-1.07599500	-0.08360000	3.88465500
H	-1.78269600	-0.60775600	4.52776700

H	-0.97157800	0.95197700	4.23650300
C	1.23250700	-0.21227800	3.20601200
O	0.15803600	-0.78297700	3.94209500
C	1.46553100	2.19353500	3.35971000
C	0.79783200	1.93917100	2.16472800
C	0.23599800	2.96433800	1.41314900
C	0.36876500	4.27375500	1.86995600
C	1.04911000	4.53822100	3.06125000
C	1.59898600	3.50245300	3.81498400
C	1.95155600	0.91048400	3.98796500
H	-0.30964800	2.74430800	0.49812800
H	1.14108400	5.56207100	3.40911900
H	2.11313600	3.71349900	4.74783700
H	1.72110600	0.83284900	5.05441000
H	3.03676400	0.81023700	3.87905900
C	-3.51044800	-0.30481400	-0.36238200
C	-4.01117300	0.93972600	-0.75259700
C	-4.04129000	-1.51383800	-0.81785600
C	-5.06788300	0.95689500	-1.66393500
C	-5.09936800	-1.44484200	-1.72180200
C	-5.61833100	-0.22425700	-2.16084900
H	-5.47176100	1.91410200	-1.98496400
H	-5.52912600	-2.37131700	-2.09580700
H	1.89526700	-1.05356600	2.99280400
H	-0.06395700	5.09098000	1.30231300
C	-0.21580600	-0.77591300	-1.39496600
O	-1.00319100	-1.49419600	-2.00807300
C	0.25508300	0.56027000	-1.96838900
C	-0.87547700	1.19959300	-2.76813400
H	0.54296900	1.21747500	-1.13687000
H	-0.94782800	0.70597500	-3.74519400
H	-1.82400000	0.98117600	-2.26276900
C	-6.74887600	-0.19493100	-3.15683100
H	-6.40823000	-0.54038600	-4.13773500
H	-7.56348400	-0.85408100	-2.84449200
H	-7.14885600	0.81415300	-3.27446500
C	-3.46878200	-2.82433800	-0.36044500
H	-2.44028300	-2.91745500	-0.71966700
H	-3.43130900	-2.87529900	0.73197800
H	-4.07202200	-3.65572700	-0.73060700
C	-3.41784400	2.21847900	-0.21989100
H	-3.28218200	2.17531900	0.86513400
H	-2.43338400	2.40520600	-0.66596200
H	-4.05921300	3.06915400	-0.45788200

C	-0.72934600	2.70748200	-2.94907700
C	-1.93441800	3.32294800	-3.65725100
H	0.18534600	2.94365100	-3.50978500
H	-0.61095200	3.18378500	-1.96358300
C	-1.83197100	4.83965100	-3.78527700
H	-2.03783100	2.86937300	-4.65065300
H	-2.84486300	3.05448800	-3.10346900
H	-2.70314800	5.26102100	-4.29344000
H	-1.75860900	5.30833800	-2.79844000
H	-0.94086100	5.12361200	-4.35405600
C	6.73371500	0.37872200	-2.50484000
C	6.27685000	-0.10423100	-1.27769600
C	4.92192000	-0.32929500	-1.07456400
C	3.99674000	-0.07130700	-2.09569700
C	4.46302100	0.41295300	-3.32241700
C	5.82360100	0.63253700	-3.52596900
H	7.79284300	0.55590300	-2.66146200
H	6.98158200	-0.30163600	-0.47610100
H	4.55892400	-0.70660400	-0.12458100
H	3.76773100	0.60358200	-4.13374400
H	6.17026400	1.00144000	-4.48582800
C	2.54935600	-0.33225400	-1.88792200
C	1.51438600	0.28623700	-2.79119100
H	1.89088500	1.21289700	-3.23200700
H	1.28094100	-0.40115800	-3.61588000
N	2.24499400	-1.10499400	-0.90800700
N	0.93285700	-1.42596400	-0.67152900
C	0.68277500	-2.44899300	0.23260700
O	-0.44130800	-2.84036500	0.47412200
O	1.79836400	-2.89422100	0.81932400
C	1.75777200	-4.12142300	1.61507700
C	0.85399100	-3.97176100	2.83577800
C	1.32695300	-5.28395200	0.72664200
C	3.21108200	-4.28053900	2.04486200
H	1.11181300	-3.07589600	3.40676300
H	-0.19500500	-3.91100700	2.54955400
H	0.99822600	-4.84127000	3.48417600
H	1.97888700	-5.34877800	-0.14900400
H	1.40916100	-6.21795800	1.28917800
H	0.29382000	-5.16236500	0.39822400
H	3.32653800	-5.19515600	2.63167900
H	3.86274100	-4.33754100	1.16933900
H	3.52175900	-3.42996500	2.65836000

TS6S

C	1. 12368500	-0. 11809200	-0. 78463000
C	2. 73862500	0. 40230800	-2. 22014500
C	3. 53357600	0. 09257200	0. 08355200
H	3. 06986600	0. 33835800	1. 03658300
N	1. 66379300	0. 40201700	-2. 94655600
N	0. 68400500	0. 07548900	-2. 04054100
N	2. 45668300	0. 11222700	-0. 91365600
C	4. 13211900	0. 80059000	-2. 56949600
H	4. 15083700	1. 31792300	-3. 52869100
H	4. 79419200	-0. 07536100	-2. 62014000
C	4. 66877500	1. 12092000	-0. 27923300
O	4. 54192500	1. 71009200	-1. 56613200
C	5. 60630200	-1. 11005400	-0. 02571500
C	4. 22817100	-1. 24734900	0. 11255300
C	3. 63551200	-2. 49700800	0. 26198100
C	4. 45172400	-3. 62541900	0. 25135200
C	5. 83533600	-3. 49592300	0. 10118500
C	6. 42240900	-2. 23923700	-0. 03212300
C	6. 00004100	0. 34148800	-0. 13227800
H	2. 56053300	-2. 57324100	0. 40134100
H	6. 45905900	-4. 38421100	0. 09239300
H	7. 49861700	-2. 14299500	-0. 14315100
H	6. 65133400	0. 55197300	-0. 98693000
H	6. 53507700	0. 66619500	0. 76582200
C	-0. 67179200	0. 02967800	-2. 49830100
C	-1. 08281700	-1. 10850000	-3. 20650100
C	-1. 52792200	1. 09151500	-2. 20787500
C	-2. 41966400	-1. 18976700	-3. 57841700
C	-2. 86801900	0. 95087200	-2. 58418800
C	-3. 33030000	-0. 17516700	-3. 25810500
H	-2. 76738000	-2. 07248100	-4. 10997700
H	-3. 56654300	1. 74588000	-2. 33165600
H	4. 61799100	1. 96674300	0. 40691300
H	4. 01303800	-4. 61160900	0. 36476600
C	0. 40071000	-0. 48545000	1. 04741800
O	1. 41128200	-0. 59298800	1. 76076800
C	-0. 49775200	-1. 72894800	0. 90676500
C	-0. 71865900	-2. 29297800	2. 32315500
H	0. 08524900	-2. 46130200	0. 33638800
H	0. 24914800	-2. 29888000	2. 83164500
H	-1. 36919100	-1. 60862000	2. 88742900
C	-4. 77910000	-0. 29995600	-3. 65095900
H	-5. 40413600	0. 37538900	-3. 06288800

H	-4.91563800	-0.06017200	-4.71044200
H	-5.13971500	-1.32082000	-3.49567600
C	-1.07036000	2.35837000	-1.53219600
H	-1.66459600	2.54705700	-0.63229000
H	-0.01691800	2.32562300	-1.24450900
H	-1.20776100	3.20668100	-2.20997400
C	-0.11265300	-2.22545700	-3.48430900
H	0.72696900	-1.87587500	-4.09132500
H	0.30643500	-2.61582300	-2.54985900
H	-0.60772200	-3.04414000	-4.00843700
C	-1.30619000	-3.70299700	2.35351600
C	-1.37247700	-4.26921500	3.77126000
H	-0.69090300	-4.36534100	1.72816400
H	-2.31594700	-3.72236000	1.92434700
C	-1.95386000	-5.67977600	3.81267300
H	-0.36492500	-4.26963500	4.20498100
H	-1.97688600	-3.60064200	4.39682000
H	-1.98922600	-6.07056600	4.83289500
H	-2.97249100	-5.69388000	3.41211600
H	-1.35089300	-6.36653700	3.21002100
C	-6.67542000	0.46175000	0.30326300
C	-5.90041500	1.31339800	1.09182500
C	-4.53573200	1.09457500	1.22670600
C	-3.91873300	0.01734700	0.57533700
C	-4.70244100	-0.83064800	-0.21475200
C	-6.07148300	-0.60862800	-0.34947500
H	-7.74211900	0.63300800	0.19996200
H	-6.36504400	2.14914300	1.60554300
H	-3.92478900	1.75257400	1.83534400
H	-4.24303500	-1.65399600	-0.75372400
H	-6.66373800	-1.27158600	-0.97269700
C	-2.45054700	-0.18940600	0.68416200
C	-1.82864100	-1.47146200	0.20684700
H	-2.51002700	-2.30346800	0.40244000
H	-1.72113300	-1.41973800	-0.87951400
N	-1.77892800	0.80010300	1.14495900
N	-0.41269800	0.74340100	1.21091500
C	0.24482100	1.95532300	1.39419800
O	1.42520100	2.10445900	1.14299800
O	-0.57849200	2.90819500	1.83496000
C	-0.09267200	4.27236300	2.01763700
C	0.99126700	4.30561900	3.09029200
C	0.38688100	4.85077300	0.68979000
C	-1.34150000	5.00398100	2.49568800

H	0.62862000	3.82190500	4.00174700
H	1.89539900	3.80027700	2.75181500
H	1.23069300	5.34647700	3.32558200
H	-0.40609400	4.77734100	-0.06061300
H	0.62745400	5.90855400	0.82915500
H	1.27452300	4.33118100	0.32863900
H	-2.13194300	4.93428700	1.74340400
H	-1.70600000	4.56558900	3.42829900
H	-1.11219800	6.05833500	2.66927600

PR

C	-0.00335400	-0.20138000	2.52493300
O	0.97458300	-0.54033800	3.14714400
C	-0.92648700	-1.17073600	1.81273500
C	-0.62814000	-2.60746000	2.23488000
H	-0.70783100	-1.05246000	0.73992700
H	0.43938300	-2.79721400	2.08536500
H	-0.80982000	-2.70550000	3.31296900
C	-1.44588700	-3.64726600	1.47240600
C	-1.04062100	-5.07710000	1.82631800
H	-1.32235000	-3.49092000	0.39151800
H	-2.51564400	-3.52186600	1.68395800
C	-1.85870400	-6.11999300	1.07027500
H	0.02607200	-5.21248400	1.60970200
H	-1.15740900	-5.22541300	2.90711300
H	-1.56041500	-7.13641900	1.33943100
H	-2.92559500	-6.01319500	1.29064000
H	-1.73000800	-6.00663000	-0.01081500
C	-6.26101600	2.22831700	0.22962100
C	-5.09133700	2.97574900	0.08809300
C	-3.88384400	2.48174000	0.56283800
C	-3.82625500	1.22675600	1.18348600
C	-5.00216300	0.48254700	1.32038300
C	-6.21358300	0.98406000	0.85005400
H	-7.20341700	2.61534400	-0.14408600
H	-5.12225300	3.94554500	-0.39807800
H	-2.96988400	3.05604600	0.45795800
H	-4.98558500	-0.48568900	1.81068500
H	-7.11961400	0.39898100	0.96914700
C	-2.53864900	0.70761000	1.71124400
C	-2.37816200	-0.75221200	2.03768600
H	-2.67310500	-0.93441700	3.08126000
H	-3.03711300	-1.35075700	1.40666400
N	-1.59869900	1.56396500	1.86612900

N	-0.38566200	1.15149000	2.39073100
C	0.51900900	2.19807700	2.72280800
O	1.70844000	2.02859400	2.81722200
O	-0.13948400	3.33347300	2.90241400
C	0.59395100	4.57289500	3.17480800
C	1.32982900	4.45851600	4.50507400
C	1.52925100	4.89273900	2.01362700
C	-0.52439100	5.60348800	3.26264700
H	0.63089000	4.17218800	5.29593500
H	2.13276200	3.72362800	4.45047000
H	1.75673100	5.43239100	4.75999300
H	0.97270600	4.88414900	1.07216500
H	1.94405600	5.89394500	2.15798200
H	2.35033500	4.17868300	1.95294100
H	-1.07835400	5.64505400	2.32131700
H	-1.21744100	5.34545500	4.06722200
H	-0.10099400	6.59014300	3.46569900

PS

C	3.68615200	-1.32318300	-2.91627800
O	2.48741000	-1.17920000	-2.92855100
C	4.67317600	-0.18825600	-3.10382300
C	3.95990400	1.07193300	-3.58731000
H	5.10471100	-0.00501000	-2.10751700
H	3.49593500	0.86618400	-4.56062100
H	3.13964700	1.29117700	-2.89651100
C	4.87817500	2.28720500	-3.69475600
C	4.11409400	3.56247300	-4.04670800
H	5.64930900	2.11750900	-4.45720700
H	5.40844100	2.43201900	-2.74298400
C	5.02871600	4.77877400	-4.15866000
H	3.58027400	3.41058900	-4.99310000
H	3.34626200	3.74283900	-3.28458600
H	4.46719400	5.68059900	-4.41528600
H	5.54810800	4.96330800	-3.21300900
H	5.78931000	4.62521800	-4.93075700
C	10.45373800	-3.00121900	-4.23319000
C	9.69668100	-3.71426100	-3.30256800
C	8.37041900	-3.37490900	-3.07213400
C	7.77993000	-2.31014700	-3.76628100
C	8.54495400	-1.60052700	-4.69733700
C	9.87328100	-1.94755200	-4.93155100
H	11.49079900	-3.26684700	-4.41087300
H	10.14515900	-4.53611100	-2.75372600

H	7.77423100	-3.92570200	-2.35287400
H	8.10628500	-0.78225400	-5.25918500
H	10.45234700	-1.39135400	-5.66133900
C	6.35479700	-1.95851100	-3.53756900
C	5.80611200	-0.64368400	-4.02120600
H	6.59532500	0.10999400	-4.03180300
H	5.44486500	-0.75074900	-5.05426200
N	5.64309000	-2.82823400	-2.92233800
N	4.29726800	-2.58079800	-2.71549400
C	3.54825300	-3.67511100	-2.20078400
O	2.50353200	-3.53320200	-1.61671000
O	4.16569000	-4.81776700	-2.46165200
C	3.61602000	-6.08099400	-1.96067900
C	3.56205700	-6.05958200	-0.43714900
C	2.25293500	-6.34147400	-2.59182300
C	4.63850200	-7.09939300	-2.44886400
H	4.54401500	-5.79997600	-0.03148600
H	2.82246600	-5.34603400	-0.07468200
H	3.29463900	-7.05680900	-0.07739900
H	2.32569200	-6.27167000	-3.68075900
H	1.93018200	-7.35366400	-2.33322200
H	1.50805800	-5.63134500	-2.23424000
H	4.34030800	-8.10187500	-2.13269700
H	4.70474700	-7.07968700	-3.53956500
H	5.62472400	-6.87792000	-2.03306800

R¹=CH(CH₃)₂

TS4R

C	-0.53657000	0.75655500	-0.52435300
C	0.69189400	2.20757600	-1.61722800
C	1.73356400	-0.01212800	-1.45851300
H	1.70832300	-0.76874400	-0.67528600
N	-0.36551100	2.87701800	-1.27315700
N	-1.12582600	1.95896700	-0.60080300
N	0.63278400	0.91661400	-1.18285900
C	1.93369200	2.65019300	-2.31411800
H	1.99716500	3.73782700	-2.31600200
H	1.94075000	2.28656100	-3.35127000
C	3.11440800	0.73487700	-1.48599000
O	3.02996600	2.14981200	-1.57669800
C	2.80547500	-0.52276700	-3.53614700
C	1.60567200	-0.62160200	-2.83665300
C	0.48046200	-1.21503500	-3.39927200
C	0.57343500	-1.70415300	-4.70028400

C	1. 77264400	-1. 60491500	-5. 41139200
C	2. 89751500	-1. 01851400	-4. 83418800
C	3. 87051600	0. 13205200	-2. 69324600
H	-0. 43311400	-1. 30158600	-2. 81868400
H	1. 82806300	-1. 98930400	-6. 42490400
H	3. 82738900	-0. 94400900	-5. 39003100
H	4. 42206700	0. 91839800	-3. 21659500
H	4. 60179800	-0. 60809300	-2. 35170800
C	-2. 42928400	2. 34643100	-0. 14282600
C	-3. 51780700	2. 10743800	-0. 98440000
C	-2. 54292700	2. 92347700	1. 12160500
C	-4. 77813500	2. 46487000	-0. 51169600
C	-3. 82553800	3. 26725600	1. 54845200
C	-4. 94830400	3. 04553800	0. 74846300
H	-5. 64721500	2. 28286400	-1. 13885500
H	-3. 94982600	3. 71309000	2. 53199200
H	3. 64006200	0. 55661800	-0. 54662500
H	-0. 28988000	-2. 16915000	-5. 16497600
C	-1. 04443400	-0. 58204500	-0. 05768700
O	-0. 29137500	-1. 55729100	-0. 36351000
C	-2. 25212300	-0. 66858800	0. 60485000
H	-2. 81930500	0. 22172700	0. 85070300
C	-6. 32008500	3. 44964600	1. 22287800
H	-7. 08532200	2. 76921300	0. 84271900
H	-6. 37411600	3. 45948500	2. 31346700
H	-6. 56731900	4. 45552500	0. 86859800
C	-1. 32607400	3. 11882900	1. 98312300
H	-0. 84496000	2. 15673100	2. 19317800
H	-0. 57696400	3. 73106300	1. 47281200
H	-1. 59564300	3. 59849400	2. 92534800
C	-3. 32083000	1. 43842700	-2. 31736300
H	-2. 56466600	1. 95767400	-2. 91369700
H	-2. 97975600	0. 40600600	-2. 17280500
H	-4. 25448400	1. 41571500	-2. 88100300
C	1. 16207100	-5. 92591900	1. 99160800
C	1. 66735100	-5. 00284700	1. 07650500
C	1. 35347800	-3. 65355900	1. 19266500
C	0. 53454900	-3. 19999100	2. 23397900
C	0. 04270700	-4. 13228800	3. 15500400
C	0. 34514100	-5. 48560500	3. 02964500
H	1. 40466400	-6. 97945000	1. 89621400
H	2. 29892100	-5. 33901000	0. 26001500
H	1. 70940500	-2. 93742000	0. 46108000
H	-0. 56423200	-3. 79251900	3. 98921600

H	-0.04613600	-6.19329200	3.75372700
C	0.21086200	-1.76098100	2.37613300
C	-0.95207300	-1.29495300	2.88799500
H	-1.72909900	-1.98162500	3.20146200
H	-1.07849900	-0.24234000	3.10350800
N	1.23624600	-0.87530300	1.98707500
N	0.89882900	0.33624600	1.99623900
C	1.95578700	1.26424800	1.76392200
O	1.76273400	2.25571100	1.09435800
O	3.05495800	0.96863500	2.44814300
C	4.12781800	1.95795900	2.60910100
C	4.81027800	2.22112600	1.27265500
C	3.56459800	3.23260300	3.23071000
C	5.07842000	1.26486600	3.57667300
H	5.25324100	1.29758800	0.88740500
H	4.10919500	2.62342900	0.53912900
H	5.61872100	2.94205500	1.42440300
H	2.99342700	2.98900600	4.13109400
H	4.39591600	3.88192200	3.51764800
H	2.92377500	3.77031000	2.53210800
H	4.58186700	1.07384100	4.53125000
H	5.41689300	0.31306700	3.15987500
H	5.94983900	1.89988700	3.75426400
C	-2.96835100	-1.99634600	0.67661400
C	-3.43893400	-2.41083900	-0.72611600
C	-4.15988500	-1.92944200	1.63155400
H	-2.26005900	-2.76077600	1.01953000
H	-2.58426300	-2.46485800	-1.40628200
H	-3.93026100	-3.38993000	-0.70491000
H	-4.15479200	-1.67903400	-1.11859100
H	-3.85746100	-1.64585400	2.64417900
H	-4.87826400	-1.17833900	1.28122700
H	-4.67916000	-2.89088000	1.68482000

TS4S

C	0.02254900	-1.75915600	-0.51724500
C	-1.53973900	-1.92084200	-2.03764800
C	-2.18210900	-2.88148400	0.19544500
H	-1.66239900	-3.77904800	0.52210200
N	-0.54802500	-1.34248200	-2.64759200
N	0.41447800	-1.24024400	-1.68907000
N	-1.24083800	-2.19630800	-0.73355100
C	-2.84834300	-2.30807200	-2.64022700
H	-2.69274200	-2.61351500	-3.67547200

H	-3.52355600	-1.44512600	-2.62390000
C	-3.51634300	-3.18930300	-0.55503700
O	-3.37072700	-3.41665200	-1.94191300
C	-3.96058300	-1.57886200	1.13819500
C	-2.65387500	-2.02361200	1.35258900
C	-1.98774800	-1.72381700	2.53883800
C	-2.62556400	-0.91869400	3.48035700
C	-3.91846400	-0.44301700	3.25244200
C	-4.60024900	-0.78608200	2.08689700
C	-4.51200900	-2.07702600	-0.16814600
H	-0.99331800	-2.12038900	2.71093600
H	-4.40445700	0.17814500	3.99832200
H	-5.62119200	-0.45306900	1.92488200
H	-4.51946500	-1.26659100	-0.90268900
H	-5.52954400	-2.46617800	-0.08489200
C	1.66395500	-0.59842600	-1.99541700
C	1.67811600	0.78811800	-2.14968700
C	2.81586000	-1.39089600	-2.08795400
C	2.92936500	1.40291000	-2.24948400
C	4.03394700	-0.73045500	-2.20513500
C	4.11069900	0.66764600	-2.24555600
H	2.97151800	2.48918800	-2.30238500
H	4.94751900	-1.31840200	-2.25418700
H	-3.87478800	-4.13867100	-0.15091800
H	-2.11578800	-0.66853100	4.40556600
C	0.82664600	-2.10280300	0.72039200
O	0.36660800	-3.10347700	1.34508100
C	1.97279100	-1.39078600	1.04310900
H	2.37610200	-0.64728400	0.36616900
C	5.44809300	1.35761200	-2.31186700
H	6.12990400	0.95710500	-1.55634200
H	5.91799600	1.20867500	-3.28909200
H	5.34082400	2.43115300	-2.14202400
C	2.73142700	-2.89284500	-2.04231900
H	2.49244600	-3.24491800	-1.03372200
H	1.95398000	-3.26139300	-2.71806700
H	3.68451900	-3.33472100	-2.33808400
C	0.42383600	1.61056600	-2.28293700
H	0.27242200	1.85367700	-3.34004000
H	-0.46650300	1.08600300	-1.93849100
H	0.51840600	2.54713400	-1.72926800
C	3.83337300	4.35033400	0.10225000
C	2.49085000	4.70480600	-0.03122000
C	1.48623100	3.82881700	0.36692400

C	1. 80300600	2. 57255900	0. 90680600
C	3. 15467500	2. 22771400	1. 03298600
C	4. 15864900	3. 10768300	0. 64119900
H	4. 61520400	5. 03503000	-0. 21041500
H	2. 22342700	5. 67206300	-0. 44544200
H	0. 44337600	4. 10739400	0. 25777600
H	3. 42364500	1. 24754700	1. 40935800
H	5. 19875400	2. 81203600	0. 74216300
C	0. 74374000	1. 60859200	1. 27840400
C	0. 91129200	0. 56101000	2. 13750600
H	1. 79039900	0. 49730400	2. 76563400
H	0. 05105200	-0. 03834400	2. 40967500
N	-0. 47728400	1. 83039900	0. 64752600
N	-1. 25140100	0. 83802400	0. 57782100
C	-2. 45252500	1. 16272000	-0. 11831400
O	-2. 87515000	0. 41935000	-0. 98147000
O	-3. 00591800	2. 29151400	0. 29366700
C	-4. 18320900	2. 84507700	-0. 38081100
C	-3. 88003500	3. 06438300	-1. 85965600
C	-5. 38067400	1. 93080700	-0. 15418800
C	-4. 37949200	4. 17832700	0. 32959800
H	-2. 94687700	3. 62525800	-1. 96807000
H	-3. 79398700	2. 11965900	-2. 39589000
H	-4. 68778300	3. 65173000	-2. 30441500
H	-5. 54788000	1. 79581900	0. 91750900
H	-6. 27169400	2. 39120500	-0. 58971900
H	-5. 22540300	0. 95551300	-0. 61846900
H	-5. 25634500	4. 68794400	-0. 07691300
H	-4. 52965900	4. 02002300	1. 40038300
H	-3. 50394000	4. 81699700	0. 18835700
C	2. 87918900	-1. 98063600	2. 10364100
C	4. 04997100	-1. 06725400	2. 47108400
C	3. 43717100	-3. 33592800	1. 63696000
H	2. 27486900	-2. 16907200	3. 00272400
H	3. 73953700	-0. 15386500	2. 98572600
H	4. 74657700	-1. 58885600	3. 13424200
H	4. 60353800	-0. 77869800	1. 56852500
H	2. 62266800	-4. 00145700	1. 34399300
H	4. 10403000	-3. 18933700	0. 77891100
H	4. 01481500	-3. 81602400	2. 43430300

R¹=Ph

TS4R

C	-0. 55497100	0. 72818700	-0. 60049500
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C	0.66126500	2.20381000	-1.66782100
C	1.74710200	0.00603400	-1.48989500
H	1.72298500	-0.74982700	-0.70480800
N	-0.41382300	2.85177700	-1.33465200
N	-1.16845100	1.91715700	-0.68105300
N	0.61875700	0.90979500	-1.24218000
C	1.90466000	2.67114000	-2.34539700
H	1.94488200	3.75992800	-2.34882600
H	1.93549400	2.30527800	-3.38136100
C	3.11070700	0.78532400	-1.47942600
O	2.99898300	2.19675500	-1.58852000
C	2.89285300	-0.48462100	-3.53058700
C	1.67251400	-0.60673500	-2.87113800
C	0.57899000	-1.22112700	-3.47272600
C	0.72599800	-1.70739700	-4.77011100
C	1.94573200	-1.58370300	-5.44042300
C	3.03841200	-0.97623000	-4.82499200
C	3.91799100	0.18848200	-2.65445700
H	-0.35434900	-1.32724200	-2.92833000
H	2.04299300	-1.96639400	-6.45144100
H	3.98542500	-0.88245100	-5.34817000
H	4.47638400	0.98049700	-3.16165000
H	4.64681100	-0.53980500	-2.28299400
C	-2.47266000	2.29231300	-0.20927400
C	-3.57870800	1.99717600	-1.00900500
C	-2.56241100	2.91767200	1.03461200
C	-4.83169800	2.34919500	-0.51325000
C	-3.83913900	3.25286700	1.48478400
C	-4.97880500	2.97700100	0.72721300
H	-5.71425800	2.12346800	-1.10660900
H	-3.94515600	3.73412000	2.45364300
H	3.60642200	0.62657000	-0.52077800
H	-0.11204000	-2.18883800	-5.26337900
C	-1.03894400	-0.62325800	-0.13325700
O	-0.28761400	-1.57695000	-0.46007100
C	-2.23171000	-0.70064400	0.58678600
H	-2.73044300	0.22100900	0.85900200
C	-6.34639600	3.36852300	1.22338300
H	-7.08923800	2.60802600	0.97088500
H	-6.34885200	3.51086000	2.30587100
H	-6.66768800	4.30780000	0.76188600
C	-1.32632200	3.17001200	1.85269500
H	-0.80518800	2.22930900	2.06487700
H	-0.61612100	3.79811400	1.30711200

H	-1.58222100	3.65922100	2.79382700
C	-3.41428100	1.27180700	-2.31667900
H	-2.61975500	1.71672600	-2.92281600
H	-3.14996700	0.22290500	-2.13544300
H	-4.34248500	1.29378900	-2.88911500
C	0.98955200	-5.97300200	1.84577800
C	1.64304100	-5.03593100	1.04683700
C	1.37515200	-3.67928600	1.19278500
C	0.45456100	-3.23200400	2.14818100
C	-0.18282900	-4.17975600	2.95737200
C	0.07399500	-5.53850400	2.80122600
H	1.19341100	-7.03217800	1.72496500
H	2.35432100	-5.36579100	0.29574900
H	1.85516700	-2.95083300	0.54872400
H	-0.87906500	-3.85089000	3.72343900
H	-0.43407900	-6.25764500	3.43620900
C	0.15635600	-1.78848400	2.29383000
C	-1.04191600	-1.29979400	2.72156300
H	-1.84849500	-1.96896600	2.99372800
H	-1.13687900	-0.25216500	2.97734300
N	1.19695000	-0.91762000	1.96266900
N	0.85475200	0.29849600	1.90021500
C	1.92015200	1.22131200	1.71851800
O	1.73978100	2.23599200	1.07798200
O	3.01897400	0.90032000	2.39530100
C	4.08531000	1.88502300	2.60773400
C	4.77769500	2.22040700	1.29240800
C	3.51327800	3.12474300	3.28841200
C	5.03397200	1.15037900	3.54620000
H	5.23511500	1.32180600	0.86690500
H	4.07983900	2.65171200	0.57223400
H	5.57728700	2.94083900	1.48811000
H	2.94541400	2.83613200	4.17755700
H	4.33986900	3.76742000	3.60308300
H	2.86742100	3.68910500	2.61601100
H	4.52834400	0.90189800	4.48272900
H	5.38757400	0.22601000	3.08247500
H	5.89648300	1.78327200	3.76952400
C	-3.05993700	-1.90445500	0.67282800
C	-4.40918100	-1.75477700	1.04120800
C	-2.58761400	-3.20489900	0.41125900
C	-5.25619900	-2.85213300	1.14369500
H	-4.79097500	-0.75573100	1.24177600
C	-3.44100400	-4.29835800	0.51572800

H	-1.54729300	-3.33854300	0.14074200
C	-4.77689300	-4.13442700	0.88074200
H	-6.29403500	-2.70520100	1.42804400
H	-3.05249900	-5.29340000	0.31706200
H	-5.43452500	-4.99401700	0.96249000

TS4S

C	-0.01413100	-1.77634200	-0.46948000
C	-1.54827200	-1.96451000	-2.00897200
C	-2.20627700	-2.92936000	0.22281500
H	-1.69694600	-3.84038700	0.53047000
N	-0.55450100	-1.37276400	-2.60510600
N	0.39140700	-1.25651300	-1.63387900
N	-1.26377000	-2.23572900	-0.70088200
C	-2.85079600	-2.35355600	-2.62403800
H	-2.68362600	-2.67811900	-3.65186100
H	-3.51742900	-1.48337300	-2.63210100
C	-3.54422600	-3.20284900	-0.53137100
O	-3.39515900	-3.44471900	-1.91544900
C	-3.95225300	-1.58507000	1.16206900
C	-2.66591400	-2.07987800	1.38925700
C	-2.01072200	-1.82883700	2.59207500
C	-2.63229000	-1.01654100	3.53776800
C	-3.89880300	-0.48300400	3.29416300
C	-4.57431200	-0.78013000	2.11202100
C	-4.50267500	-2.05434600	-0.15572400
H	-1.03478500	-2.26247200	2.77792800
H	-4.37170000	0.14644600	4.04156100
H	-5.57851600	-0.40371300	1.94015100
H	-4.46280000	-1.24072700	-0.88526400
H	-5.53596400	-2.40332400	-0.09108000
C	1.64867200	-0.61625500	-1.91520400
C	1.66409400	0.77318800	-2.05928100
C	2.80808900	-1.40153300	-1.93991700
C	2.91441500	1.39372400	-2.10229800
C	4.02632500	-0.73370100	-2.01640900
C	4.09893600	0.66297800	-2.05530100
H	2.95442000	2.48016200	-2.14520700
H	4.94391600	-1.31783100	-2.01544000
H	-3.93433900	-4.13745700	-0.12209800
H	-2.12964700	-0.80451400	4.47632900
C	0.78713100	-2.09876900	0.77931100
O	0.38725800	-3.13323200	1.36353700
C	1.88126500	-1.28604300	1.10330300

H	2. 17998800	-0. 52013300	0. 40003900
C	5. 43673900	1. 35454100	-2. 05286600
H	6. 02238100	1. 05686500	-1. 17756500
H	6. 01775200	1. 08890200	-2. 94118200
H	5. 31723300	2. 43948400	-2. 02705800
C	2. 75809600	-2. 90117800	-1. 81446800
H	2. 76578600	-3. 20057500	-0. 75997700
H	1. 85908300	-3. 31726000	-2. 27635800
H	3. 63038800	-3. 34741300	-2. 29559200
C	0. 40932300	1. 59044100	-2. 21068100
H	0. 24784200	1. 80749700	-3. 27206400
H	-0. 47747800	1. 07345500	-1. 84556500
H	0. 50803400	2. 53950700	-1. 67941000
C	3. 90367100	4. 17164000	0. 32516400
C	2. 57771500	4. 53519900	0. 09068700
C	1. 53678500	3. 70137800	0. 48525100
C	1. 79802900	2. 48015500	1. 12600700
C	3. 13417600	2. 13309500	1. 36934600
C	4. 17409900	2. 96876100	0. 97380400
H	4. 71520900	4. 81991600	0. 01011300
H	2. 35201600	5. 47525000	-0. 40379000
H	0. 50723400	3. 98480300	0. 29375900
H	3. 36727800	1. 18983700	1. 85348600
H	5. 20107500	2. 67104400	1. 16520800
C	0. 70425500	1. 54570500	1. 46904300
C	0. 84656300	0. 46829800	2. 30593200
H	1. 70173000	0. 39028200	2. 96690800
H	-0. 03218100	-0. 11456300	2. 55736200
N	-0. 47853700	1. 77265500	0. 78760100
N	-1. 26658800	0. 78669700	0. 69211400
C	-2. 42504900	1. 12540300	-0. 05812000
O	-2. 81898400	0. 39305000	-0. 94605000
O	-2. 98789700	2. 25910200	0. 33089300
C	-4. 10487800	2. 83996600	-0. 41674400
C	-3. 68203700	3. 08860500	-1. 86103500
C	-5. 32880800	1. 93834200	-0. 30971000
C	-4. 34320300	4. 15872600	0. 30782300
H	-2. 74865200	3. 65932900	-1. 88157400
H	-3. 54113200	2. 15298900	-2. 40240300
H	-4. 45563100	3. 67490600	-2. 36413800
H	-5. 56840200	1. 75864200	0. 74164500
H	-6. 18215300	2. 43576400	-0. 77901700
H	-5. 16034500	0. 98280100	-0. 80796600
H	-5. 17156700	4. 69441300	-0. 16209400

H	-4.59173200	3.97632600	1.35633900
H	-3.44802000	4.78419400	0.26351200
C	2.92817700	-1.72416900	2.02845400
C	2.68953100	-2.56482300	3.13139800
C	4.24528900	-1.27233500	1.82003400
C	3.72777000	-2.92659500	3.98450200
H	1.68617200	-2.93647200	3.30049200
C	5.27845000	-1.63659000	2.67567300
H	4.45044100	-0.63647900	0.96003000
C	5.02541700	-2.46676200	3.76670700
H	3.51917600	-3.57474500	4.83081600
H	6.28520100	-1.27546000	2.48738000
H	5.82961900	-2.75237000	4.43706300

R¹=4-OMeC₆H₄

TS4R

C	-0.53457000	0.76512700	-0.59787300
C	0.68201400	2.24269800	-1.66407800
C	1.76930800	0.04589300	-1.48626600
H	1.74463600	-0.71063000	-0.70188300
N	-0.39309200	2.89032800	-1.33139000
N	-1.14823600	1.95478900	-0.67864200
N	0.64005600	0.94844300	-1.23886900
C	1.92512000	2.71080400	-2.34151700
H	1.96452600	3.79964000	-2.34507900
H	1.95623500	2.34490900	-3.37748500
C	3.13231700	0.82609200	-1.47439100
O	3.02014400	2.23746600	-1.58500200
C	2.91770500	-0.44369800	-3.52588900
C	1.69677500	-0.56658900	-2.86770100
C	0.60447900	-1.18232300	-3.47005900
C	0.75308900	-1.66842800	-4.76734800
C	1.97324400	-1.54341200	-5.43667000
C	3.06489600	-0.93509100	-4.82018700
C	3.94157500	0.22920500	-2.64805500
H	-0.32873200	-1.28989300	-2.92571000
H	2.07175700	-1.92600900	-6.44761200
H	4.01237500	-0.84068200	-5.34243600
H	4.50107200	1.02115300	-3.15413900
H	4.66952100	-0.49939800	-2.27544400
C	-2.45283200	2.33013200	-0.20919100
C	-3.55614000	2.04156200	-1.01263100
C	-2.54534200	2.95206300	1.03784400
C	-4.81115300	2.39644900	-0.51973200

C	-3.82125800	3.28873500	1.48468600
C	-4.96034200	3.01971700	0.72108300
H	-5.69181300	2.17623800	-1.11765500
H	-3.92966500	3.76702700	2.45501300
H	3.62710100	0.66839000	-0.51503200
H	-0.08393200	-2.15097700	-5.26128400
C	-1.01866100	-0.58631900	-0.13657200
O	-0.26147200	-1.54019500	-0.45638100
C	-2.21729800	-0.66783300	0.57134600
H	-2.72345600	0.25151400	0.83809500
C	-6.32354500	3.42067100	1.22171100
H	-7.11178800	2.85274200	0.72344000
H	-6.40929000	3.26305900	2.29949200
H	-6.50486100	4.48299500	1.02950500
C	-1.31018000	3.20019400	1.85852600
H	-0.78845200	2.25882200	2.06598400
H	-0.59995900	3.83147500	1.31658000
H	-1.56706600	3.68450000	2.80195500
C	-3.39036100	1.31978700	-2.32209300
H	-2.59403800	1.76546000	-2.92528200
H	-3.12718400	0.27020600	-2.14306700
H	-4.31740700	1.34445900	-2.89632800
C	1.01378100	-5.92693500	1.81565900
C	1.68003900	-4.98445800	1.03371800
C	1.41378700	-3.62848900	1.18809700
C	0.48223600	-3.18671300	2.13554700
C	-0.16777400	-4.14006300	2.92787100
C	0.08714200	-5.49818900	2.76287500
H	1.21591800	-6.98559200	1.68767600
H	2.39997800	-5.30956400	0.28880400
H	1.90409200	-2.89604200	0.55655600
H	-0.87395200	-3.81662600	3.68710400
H	-0.43209300	-6.22139000	3.38404400
C	0.18322200	-1.74380900	2.28694100
C	-1.01464100	-1.25618700	2.71578400
H	-1.82254200	-1.92482200	2.98486900
H	-1.11057000	-0.20845500	2.97046900
N	1.22358600	-0.87180700	1.95625500
N	0.88146600	0.34458400	1.90051400
C	1.94557700	1.26828800	1.71844100
O	1.76349800	2.28450600	1.08089100
O	3.04622400	0.94638200	2.39241200
C	4.11176000	1.93155100	2.60553100
C	4.80239200	2.27003700	1.29005400

C	3. 53969900	3. 16958300	3. 28933100
C	5. 06220900	1. 19607000	3. 54157500
H	5. 26142300	1. 37296500	0. 86304700
H	4. 10291800	2. 70039500	0. 57090600
H	5. 60054500	2. 99204900	1. 48586000
H	2. 97266100	2. 87876100	4. 17829700
H	4. 36625600	3. 81193200	3. 60478200
H	2. 89303000	3. 73509300	2. 61870500
H	4. 55800200	0. 94573700	4. 47838900
H	5. 41575900	0. 27266500	3. 07589200
H	5. 92462100	1. 82915800	3. 76476300
C	-3. 03905800	-1. 87622800	0. 65702800
C	-4. 39149800	-1. 74302000	0. 99725000
C	-2. 55388200	-3. 18055300	0. 42537400
C	-5. 24249300	-2. 84147400	1. 10603100
H	-4. 79389200	-0. 74815500	1. 17660900
C	-3. 39087500	-4. 27843200	0. 53253200
H	-1. 50860600	-3. 31307100	0. 17322800
C	-4. 73987100	-4. 12171000	0. 87233400
H	-6. 28190600	-2. 68448900	1. 36857900
H	-3. 01448800	-5. 28283000	0. 36419000
O	-5. 47457200	-5. 26745700	0. 95471600
C	-6. 83829500	-5. 13786000	1. 30308200
H	-7. 24829200	-6. 14722800	1. 31595800
H	-6. 95629000	-4. 68525500	2. 29443800
H	-7. 38255900	-4. 53432600	0. 56736600

TS4S

C	0. 03268000	-1. 83027500	-0. 40361200
C	-1. 49008600	-1. 99122400	-1. 95899200
C	-2. 17639800	-2. 96730200	0. 25873600
H	-1. 67723500	-3. 88421500	0. 56524900
N	-0. 48562200	-1. 40458500	-2. 54161800
N	0. 45327900	-1. 30524200	-1. 56115800
N	-1. 21980500	-2. 27503000	-0. 65053700
C	-2. 79019000	-2. 36508800	-2. 58891800
H	-2. 61607300	-2. 68286100	-3. 61770800
H	-3. 45013400	-1. 48992300	-2. 59596100
C	-3. 50932300	-3. 22514800	-0. 50946500
O	-3. 34924400	-3. 45773400	-1. 89392400
C	-3. 91920600	-1. 61326900	1. 18993800
C	-2. 63969600	-2. 12131200	1. 42601500
C	-1. 99227800	-1. 88273700	2. 63545800
C	-2. 61385900	-1. 06836900	3. 57939300

C	-3.87253500	-0.52049300	3.32701200
C	-4.54103700	-0.80578300	2.13793900
C	-4.46311600	-2.07238400	-0.13422000
H	-1.02201400	-2.32720500	2.82594100
H	-4.34526400	0.11083800	4.07294400
H	-5.53988900	-0.41834800	1.95932200
H	-4.41365200	-1.25549400	-0.85939800
H	-5.49896100	-2.41536800	-0.07825500
C	1.71762600	-0.67336900	-1.82850100
C	1.74362800	0.71690400	-1.96958500
C	2.87207600	-1.46543800	-1.84451000
C	2.99764200	1.32919200	-1.99985800
C	4.09578900	-0.80476600	-1.90668300
C	4.17766200	0.59080100	-1.94359200
H	3.04531200	2.41555800	-2.03903700
H	5.00934700	-1.39504000	-1.89648100
H	-3.90975400	-4.15994000	-0.11074000
H	-2.11744900	-0.86558500	4.52333500
C	0.81926100	-2.17185800	0.84808100
O	0.40334300	-3.20750500	1.42363700
C	1.91747300	-1.37429100	1.18638100
H	2.23024700	-0.60366600	0.49429300
C	5.51749000	1.27883600	-1.94408700
H	6.18720200	0.82758800	-1.20654200
H	6.00049900	1.19260100	-2.92271000
H	5.40927700	2.33935200	-1.70601700
C	2.81356900	-2.96502900	-1.72259000
H	2.82169800	-3.26648500	-0.66875900
H	1.91106100	-3.37478400	-2.18319100
H	3.68202900	-3.41507400	-2.20723100
C	0.49569000	1.54279200	-2.13117300
H	0.34484100	1.76126000	-3.19384400
H	-0.39782700	1.03201200	-1.77415800
H	0.59610900	2.49091700	-1.59858200
C	3.97825700	4.07592000	0.45201100
C	2.65883700	4.45704000	0.20849100
C	1.60482300	3.63155600	0.58557900
C	1.84622300	2.40145000	1.21696600
C	3.17588100	2.03602300	1.46863500
C	4.22888700	2.86349800	1.09091900
H	4.80027100	4.71780000	0.15118100
H	2.44875400	5.40445900	-0.27871800
H	0.58026900	3.92833900	0.38748900
H	3.39299600	1.08482800	1.94475000

H	5.25085900	2.55149300	1.28693300
C	0.73872800	1.47731300	1.54323900
C	0.85929800	0.39678200	2.37759200
H	1.70805600	0.30319800	3.04462900
H	-0.02734500	-0.18034200	2.61321800
N	-0.43547200	1.72215000	0.85124700
N	-1.23338400	0.74600800	0.74357800
C	-2.38136300	1.09975700	-0.01607700
O	-2.77336400	0.37498800	-0.91084900
O	-2.93729900	2.23680900	0.37315000
C	-4.04794200	2.82657900	-0.37705600
C	-3.61890700	3.07701300	-1.81919700
C	-5.27752400	1.93175300	-0.27685600
C	-4.28127400	4.14459200	0.35046900
H	-2.68190200	3.64189100	-1.83512600
H	-3.48231500	2.14229800	-2.36313500
H	-4.38726000	3.66987400	-2.32265700
H	-5.52240300	1.75103200	0.77312800
H	-6.12604200	2.43523100	-0.74844500
H	-5.11283800	0.97633100	-0.77664900
H	-5.10538200	4.68594500	-0.12044900
H	-4.53392500	3.96063800	1.39772800
H	-3.38265100	4.76539300	0.31053600
C	2.94461300	-1.81948100	2.13060400
C	2.68194900	-2.65624400	3.23455200
C	4.26687800	-1.38605500	1.95491400
C	3.69260000	-3.02526300	4.10684500
H	1.67413900	-3.02274800	3.38814400
C	5.29183400	-1.75062600	2.82617000
H	4.50232100	-0.75379100	1.10010600
C	5.00372000	-2.57581900	3.91395600
H	3.48909700	-3.66830100	4.95733700
H	6.29790700	-1.39176900	2.64379800
O	5.91970000	-2.99366300	4.83205400
C	7.25814200	-2.57589600	4.64975200
H	7.82880300	-3.01465600	5.46751900
H	7.65997400	-2.93235000	3.69439900
H	7.34518800	-1.48404200	4.69105200

R²=4-CH₃C₆H₄

TS4R

C	-0.77397300	-0.82733300	0.48799000
C	0.09520300	-2.54102700	1.54447600
C	1.53214500	-0.54706700	1.59391700

H	1. 69990700	0. 23415900	0. 85334500
N	-1. 03708100	-2. 98423500	1. 09046300
N	-1. 57264500	-1. 90423400	0. 44278000
N	0. 29850700	-1. 23756800	1. 20101000
C	1. 18396100	-3. 24589000	2. 27963200
H	1. 04646400	-4. 32472900	2. 21371900
H	1. 18883800	-2. 94659700	3. 33737500
C	2. 74663900	-1. 54266900	1. 65619800
O	2. 39959700	-2. 91937300	1. 63840000
C	2. 53247400	-0. 35493600	3. 75940200
C	1. 42837100	0. 01283100	2. 99509200
C	0. 40507900	0. 79329600	3. 52379600
C	0. 49975300	1. 19189100	4. 85545200
C	1. 60132400	0. 82069900	5. 63115100
C	2. 62729600	0. 04983900	5. 08840700
C	3. 50933300	-1. 16629900	2. 94779400
H	-0. 42778200	1. 09101800	2. 89386000
H	1. 65923200	1. 13839100	6. 66747100
H	3. 48356200	-0. 23433800	5. 69297500
H	3. 85205200	-2. 07351500	3. 45407100
H	4. 39736600	-0. 57301500	2. 70527000
C	-2. 88239500	-2. 03368500	-0. 13009900
C	-3. 98211600	-1. 67467900	0. 65268100
C	-2. 98702500	-2. 50876600	-1. 43619100
C	-5. 24228900	-1. 80477800	0. 07606400
C	-4. 27191800	-2. 62540400	-1. 96814500
C	-5. 40399100	-2. 28133900	-1. 22915900
H	-6. 11864200	-1. 52585800	0. 65631700
H	-4. 38780600	-2. 98904600	-2. 98590800
H	3. 36343600	-1. 40906100	0. 76628800
H	-0. 28584000	1. 79855000	5. 29413700
C	-0. 99495000	0. 60495300	0. 07962400
O	-0. 09693700	1. 40339100	0. 49455600
C	-2. 11061800	0. 93753900	-0. 65986600
C	-2. 56124100	2. 37022900	-0. 71945800
H	-2. 80449900	0. 17417200	-0. 98965600
H	-1. 68529300	3. 02767700	-0. 67971200
H	-3. 08325800	2. 57363200	-1. 66332100
C	-6. 78450200	-2. 43227700	-1. 81375200
H	-7. 39544000	-1. 54912700	-1. 61009600
H	-6. 74329700	-2. 58275000	-2. 89421300
H	-7. 29668200	-3. 29319300	-1. 37281200
C	-1. 75232700	-2. 83229000	-2. 23047800
H	-1. 13024900	-1. 93750800	-2. 35065300

H	-1.13212100	-3.57034300	-1.71384900
H	-2.01852100	-3.21802000	-3.21588300
C	-3.78547100	-1.11988900	2.03706800
H	-3.16613200	-1.78454200	2.64683100
H	-3.27801100	-0.14895700	1.98240300
H	-4.74409100	-0.97882600	2.53811700
C	-3.50071500	2.71351500	0.44530200
C	-4.01502400	4.15042900	0.39691000
H	-2.96208200	2.54614600	1.38822300
H	-4.35156500	2.01682400	0.44508900
C	-4.93235500	4.48765100	1.56904600
H	-3.15837700	4.83601800	0.38674800
H	-4.54817300	4.30993900	-0.54904900
H	-5.28767800	5.52048300	1.51982400
H	-5.80836500	3.83108700	1.57996000
H	-4.40917900	4.35754800	2.52173700
C	2.22951100	5.59336900	-1.29309800
C	2.48815400	4.54977200	-0.41613100
C	1.95934000	3.29602300	-0.69671100
C	1.18853300	3.08060800	-1.84603200
C	0.96186400	4.15609300	-2.71243200
C	1.46985200	5.42240900	-2.43837000
H	3.08087000	4.73227200	0.47324200
H	2.10999000	2.47354000	-0.00782100
H	0.39669800	4.00056500	-3.62620200
H	1.30011500	6.26168400	-3.10315500
C	0.63957900	1.74036400	-2.15720400
C	-0.52648100	1.53475200	-2.80692400
H	-1.15108100	2.36879600	-3.10376900
H	-0.81382000	0.53989400	-3.12034500
N	1.45848800	0.65427900	-1.76925900
N	0.93000700	-0.47176400	-1.93978400
C	1.78209500	-1.58933200	-1.69404900
O	1.35959600	-2.56428800	-1.11247600
O	2.96898400	-1.45938600	-2.27393500
C	3.85349700	-2.62001500	-2.44520100
C	4.36342600	-3.10584500	-1.09447700
C	3.11909700	-3.71562100	-3.21166600
C	4.99098600	-2.05046100	-3.28245100
H	4.93430300	-2.31409500	-0.59977600
H	3.54296300	-3.42413000	-0.44854100
H	5.03687600	-3.95249100	-1.25615500
H	2.68158600	-3.30507700	-4.12617500
H	3.83695300	-4.49061500	-3.49319700

H	2.33296800	-4.16913600	-2.60807300
H	4.61591300	-1.69298100	-4.24471800
H	5.46865900	-1.21787100	-2.75990600
H	5.73900500	-2.82641600	-3.46330800
F	2.73651700	6.81131200	-1.02313000

TS4S

C	0.05621500	-1.75778000	-0.52647000
C	-1.48849000	-1.84669800	-2.07066100
C	-2.14962600	-2.90689500	0.11329500
H	-1.63514300	-3.81833400	0.40813400
N	-0.49272000	-1.23434000	-2.63759900
N	0.46132500	-1.17350100	-1.66366800
N	-1.20162900	-2.18729900	-0.78019800
C	-2.79229100	-2.20742600	-2.70056400
H	-2.62873200	-2.47113500	-3.74602600
H	-3.46621800	-1.34449700	-2.65490500
C	-3.47957300	-3.17694500	-0.65760900
O	-3.32307700	-3.34251500	-2.05262700
C	-3.92120500	-1.62515900	1.09402200
C	-2.61816400	-2.08522900	1.29701700
C	-1.94631300	-1.81770800	2.48788200
C	-2.57718000	-1.03043700	3.44889000
C	-3.86735000	-0.54093700	3.23481300
C	-4.55374700	-0.85092400	2.06268100
C	-4.47466400	-2.07942900	-0.22790200
H	-0.95397300	-2.22454800	2.64892400
H	-4.34759700	0.06577800	3.99617100
H	-5.57216300	-0.50589200	1.91035600
H	-4.48544300	-1.24394900	-0.93388100
H	-5.49174100	-2.47207600	-0.15575400
C	1.69691600	-0.49433300	-1.95392000
C	1.63589600	0.87707300	-2.23352800
C	2.89663800	-1.21669500	-1.97207700
C	2.84308900	1.54424100	-2.43670100
C	4.07305000	-0.49624800	-2.17704600
C	4.06886100	0.88366900	-2.38868900
H	2.81887300	2.61641000	-2.61801200
H	5.01842900	-1.03397000	-2.17289700
H	-3.84362300	-4.14274000	-0.30039000
H	-2.06441000	-0.80531200	4.37896200
C	0.82526000	-2.15174900	0.71274700
O	0.39447100	-3.20967800	1.25907100
C	1.91189500	-1.40440300	1.12646700

C	2. 75225700	-1. 98728600	2. 23189500
H	2. 32462700	-0. 63023400	0. 49173200
H	2. 20582200	-1. 96279100	3. 18829500
H	2. 90037100	-3. 05883500	2. 02745100
C	5. 35657700	1. 63758400	-2. 59817900
H	6. 16702800	1. 20161200	-2. 00877600
H	5. 65862300	1. 60403400	-3. 65005500
H	5. 24944200	2. 68717500	-2. 31326300
C	2. 95472500	-2. 70601900	-1. 75790200
H	3. 14256900	-2. 93844400	-0. 70462000
H	2. 02155800	-3. 19718000	-2. 04361000
H	3. 76414600	-3. 13473400	-2. 35229600
C	0. 33930100	1. 63030000	-2. 37899100
H	0. 06778900	1. 68744400	-3. 43827500
H	-0. 48915800	1. 15261600	-1. 85939400
H	0. 45362300	2. 64757800	-1. 99835500
C	4. 11406600	-1. 31861400	2. 40995300
C	5. 03940000	-2. 09711100	3. 34276500
H	3. 98919300	-0. 30468300	2. 81510200
H	4. 59658900	-1. 20253700	1. 42799300
C	6. 38243900	-1. 40352000	3. 55288900
H	4. 53819200	-2. 23696300	4. 30878100
H	5. 19929300	-3. 10114900	2. 93102200
H	7. 03298300	-1. 97847000	4. 21689900
H	6. 90573200	-1. 27246200	2. 60033400
H	6. 24404600	-0. 41142700	3. 99429000
C	3. 91742400	4. 04775200	-0. 14257900
C	2. 60982000	4. 49185500	-0. 27446500
C	1. 58244400	3. 70086700	0. 22765500
C	1. 85241800	2. 47515100	0. 85571700
C	3. 18893000	2. 07311300	0. 97858300
C	4. 22843600	2. 85447300	0. 48714200
H	2. 41133400	5. 43737800	-0. 76671900
H	0. 55304100	4. 02548100	0. 12370000
H	3. 42580000	1. 11808400	1. 43238500
H	5. 26292100	2. 53746800	0. 56206600
C	0. 75894000	1. 58908400	1. 30932600
C	0. 90393700	0. 57888700	2. 21060700
H	1. 79728500	0. 50255600	2. 81980100
H	0. 03441800	0. 00600500	2. 51074800
N	-0. 46019300	1. 82018700	0. 66945800
N	-1. 26408100	0. 85168700	0. 65481500
C	-2. 45675200	1. 18184600	-0. 05621500
O	-2. 86115600	0. 45329400	-0. 93933200

O	-3.01828900	2.29876100	0.37309800
C	-4.19808400	2.85642900	-0.29631700
C	-3.88870600	3.10739200	-1.76870100
C	-5.38770500	1.92665200	-0.09370000
C	-4.40914000	4.17316300	0.43984900
H	-2.95967900	3.67787700	-1.86087600
H	-3.79233900	2.17435100	-2.32336400
H	-4.69887500	3.69702500	-2.20587400
H	-5.56177800	1.77212700	0.97426200
H	-6.27994100	2.38567300	-0.52810300
H	-5.21972800	0.96088600	-0.57334900
H	-5.28909500	4.68241100	0.03970900
H	-4.56237400	3.99223500	1.50657400
H	-3.53925700	4.82279300	0.31483000
F	4.91575900	4.78800900	-0.66479900

R²=4-ClC₆H₄

TS4R

C	-0.54147100	0.75805000	-0.55628700
C	0.70709600	2.20557400	-1.63134100
C	1.74376100	-0.01555200	-1.45453400
H	1.71154900	-0.76233800	-0.66279200
N	-0.35334700	2.87774800	-1.30265400
N	-1.12600700	1.96267100	-0.64149000
N	0.63863200	0.91511900	-1.19715500
C	1.95952300	2.64939300	-2.30775100
H	2.02211000	3.73706100	-2.30843700
H	1.98560800	2.28569500	-3.34466100
C	3.12571200	0.73249600	-1.47853700
O	3.04149400	2.14801700	-1.55047400
C	2.82361100	-0.53136700	-3.52807400
C	1.62575400	-0.63983900	-2.82682100
C	0.50878500	-1.25547100	-3.38287000
C	0.60813400	-1.75553000	-4.67910800
C	1.80517900	-1.64546400	-5.39248300
C	2.92182200	-1.03793500	-4.82164500
C	3.88173600	0.14456600	-2.69379600
H	-0.40129200	-1.35279100	-2.79866700
H	1.86550100	-2.03886900	-6.40225300
H	3.85052100	-0.95620100	-5.37845600
H	4.41178600	0.94238800	-3.22236300
H	4.63247700	-0.57942700	-2.36037400
C	-2.43116600	2.36567900	-0.20074500
C	-3.51227800	2.14162100	-1.05575100

C	-2.55149400	2.95444800	1.05767600
C	-4.77086600	2.53372900	-0.60603900
C	-3.83183100	3.33285700	1.46119800
C	-4.94661300	3.13258100	0.64465300
H	-5.63430300	2.36506300	-1.24464500
H	-3.96068600	3.78978200	2.43903300
H	3.65278100	0.54308000	-0.54225100
H	-0.24838000	-2.23818900	-5.13835300
C	-1.05113800	-0.57637600	-0.08002300
O	-0.28133400	-1.55098000	-0.36018100
C	-2.26611500	-0.64637300	0.56411700
C	-2.96301200	-1.97067900	0.69628000
H	-2.83496200	0.24969600	0.77840100
H	-2.21478400	-2.76769700	0.77253400
H	-3.57135800	-2.00095000	1.60945900
C	-6.31521100	3.57621100	1.09212800
H	-7.09099400	2.90978700	0.70851700
H	-6.38603200	3.60173600	2.18149800
H	-6.53209200	4.58305000	0.72107400
C	-1.34475900	3.12393200	1.93884200
H	-0.89850300	2.14955400	2.16914400
H	-0.56824000	3.70769600	1.43635100
H	-1.61677900	3.62126800	2.87113300
C	-3.31287100	1.44968600	-2.37657600
H	-2.52747300	1.93386900	-2.96449400
H	-3.01174800	0.40805600	-2.21087200
H	-4.23567700	1.45221800	-2.95820800
C	-3.87329200	-2.24898700	-0.50901900
C	-4.63915500	-3.56492900	-0.39240700
H	-3.25444300	-2.26082900	-1.41686900
H	-4.58374000	-1.41827500	-0.62814200
C	-5.52460500	-3.83986300	-1.60496400
H	-3.92285900	-4.38568100	-0.26208700
H	-5.25269700	-3.54436000	0.51732600
H	-6.06680100	-4.78386000	-1.50411700
H	-6.26176600	-3.04142300	-1.73761000
H	-4.92537000	-3.89272700	-2.51942000
C	1.20453400	-5.93583000	1.82030400
C	1.66695900	-4.99592900	0.90472000
C	1.33174600	-3.65925100	1.08002200
C	0.54592300	-3.25077100	2.16404600
C	0.10671200	-4.21796000	3.07424500
C	0.42204600	-5.56255500	2.90523300
H	2.26924200	-5.31114100	0.06007000

H	1.64545600	-2.91947400	0.35377000
H	-0.47290000	-3.91787100	3.94165000
H	0.08001800	-6.30735500	3.61479300
C	0.20369600	-1.82403600	2.36480400
C	-0.94507100	-1.39816800	2.92537800
H	-1.71366400	-2.10341300	3.21830700
H	-1.09660000	-0.34973400	3.14531800
N	1.21725300	-0.90996500	1.97528500
N	0.87954000	0.29341600	2.05821200
C	1.92631800	1.23419800	1.80891200
O	1.73047100	2.20085800	1.10700000
O	3.01159600	0.96967400	2.52307400
C	4.07678800	1.97163500	2.67091700
C	4.77477000	2.19812500	1.33612900
C	3.49456800	3.25924000	3.24567300
C	5.01706300	1.31335100	3.67193700
H	5.21586700	1.26259000	0.97874600
H	4.08443300	2.58726800	0.58542600
H	5.58583200	2.91774000	1.47936900
H	2.91494700	3.03889000	4.14658300
H	4.31658800	3.92492200	3.52148300
H	2.85774500	3.76910200	2.52292900
H	4.50692000	1.14457200	4.62350900
H	5.37046900	0.35359400	3.28705700
H	5.87998700	1.96087600	3.84555500
Cl	1.62114400	-7.62274600	1.60303900

TS4S

C	0.04862900	-1.78172500	-0.54114000
C	-1.50573400	-1.87380900	-2.07532600
C	-2.15741200	-2.91402400	0.12199800
H	-1.64586500	-3.82644900	0.41924000
N	-0.50996000	-1.27075100	-2.65315200
N	0.44926900	-1.20918000	-1.68516100
N	-1.21282600	-2.20583900	-0.78370400
C	-2.81588200	-2.23209200	-2.69342700
H	-2.66093600	-2.50671500	-3.73738800
H	-3.48404100	-1.36443900	-2.65187200
C	-3.49500500	-3.17950100	-0.63677500
O	-3.34980700	-3.35765500	-2.03150200
C	-3.90968000	-1.60752200	1.10403000
C	-2.61017900	-2.07940900	1.30252800
C	-1.92681100	-1.80811600	2.48590900
C	-2.54204900	-1.00414300	3.44331500

C	-3.82785500	-0.50174200	3.23286300
C	-4.52643200	-0.81632100	2.06913600
C	-4.47713700	-2.06933200	-0.20936500
H	-0.93761800	-2.22425000	2.64319900
H	-4.29564900	0.11836500	3.99115900
H	-5.54226800	-0.46215800	1.92106800
H	-4.48623200	-1.24066600	-0.92334300
H	-5.49708400	-2.45210900	-0.12583900
C	1.69012800	-0.54032200	-1.97282700
C	1.65120900	0.83834800	-2.20650300
C	2.87760100	-1.28336400	-2.00907100
C	2.87248100	1.49449400	-2.36806700
C	4.06606000	-0.57744800	-2.18006900
C	4.08542100	0.81197600	-2.33160600
H	2.86833300	2.57411600	-2.50380600
H	5.00307900	-1.12957300	-2.19114600
H	-3.86486300	-4.13910900	-0.26908100
H	-2.02035300	-0.77547000	4.36755600
C	0.82718500	-2.16659800	0.69526800
O	0.40011000	-3.22121700	1.25235500
C	1.91738800	-1.41695100	1.09241700
C	2.76724100	-1.98590000	2.19712700
H	2.31823200	-0.63803000	0.45575700
H	2.22802000	-1.95450500	3.15755900
H	2.91936300	-3.05863100	2.00230200
C	5.39113000	1.54834600	-2.47969300
H	6.11492700	1.21334100	-1.73147700
H	5.83169700	1.36715200	-3.46522300
H	5.25037800	2.62558500	-2.36258400
C	2.89756400	-2.77935600	-1.84148400
H	2.98555400	-3.04961500	-0.78395100
H	1.98609000	-3.24247200	-2.22774600
H	3.75074600	-3.20276700	-2.37484200
C	0.36611100	1.61122700	-2.34821600
H	0.12340500	1.71762200	-3.41075800
H	-0.47993300	1.11869300	-1.87222400
H	0.47817300	2.61039600	-1.92150000
C	4.12669200	-1.30811500	2.35726300
C	5.06343500	-2.06907500	3.29304700
H	3.99851600	-0.28979200	2.75035900
H	4.60089100	-1.20163200	1.37029500
C	6.40396600	-1.36516300	3.48400000
H	4.57032500	-2.19934600	4.26455000
H	5.22611900	-3.07739400	2.89304800

H	7.06275300	-1.92753700	4.15063700
H	6.91942800	-1.24371700	2.52591400
H	6.26311900	-0.36811900	3.91333400
C	3.87915800	4.17386900	-0.06436900
C	2.55502300	4.58172700	-0.19362700
C	1.54147300	3.75251500	0.27174700
C	1.83258600	2.51609700	0.86763800
C	3.17616900	2.13869900	0.98463900
C	4.20113200	2.95907100	0.52761500
H	2.32214600	5.53607500	-0.65281100
H	0.50672700	4.05987100	0.16809600
H	3.43217300	1.17325700	1.40591400
H	5.23726700	2.64948400	0.61190600
C	0.75437700	1.60353600	1.30172700
C	0.91106200	0.58783200	2.19262100
H	1.81044700	0.50719400	2.79218800
H	0.04896600	0.00121600	2.48716100
N	-0.47136700	1.83201700	0.66847800
N	-1.26063200	0.85389900	0.63832900
C	-2.45824200	1.17994100	-0.07055100
O	-2.85422900	0.45283500	-0.95817100
O	-3.02667100	2.29008700	0.36447800
C	-4.20058500	2.85334200	-0.31183100
C	-3.87768900	3.11161600	-1.77998300
C	-5.39292400	1.92407700	-0.12486800
C	-4.41551900	4.16615600	0.42999900
H	-2.94582500	3.67917100	-1.86102600
H	-3.78028900	2.18162800	-2.33960300
H	-4.68199600	3.70684700	-2.22030500
H	-5.58060300	1.76840400	0.94052400
H	-6.27940600	2.38422800	-0.56969400
H	-5.21969800	0.95906900	-0.60417200
H	-5.29191400	4.67848000	0.02605500
H	-4.57698300	3.97947200	1.49450700
H	-3.54402600	4.81547500	0.31500200
Cl	5.15986900	5.20183900	-0.67007600

NHC-1

C	-0.06965000	-0.37425500	-0.18862900
C	1.31248100	-1.84294400	-1.21450500
C	2.28986200	0.35421200	-0.74037400
H	1.88175000	1.36756300	-0.72442600
N	0.23624900	-2.53557800	-1.01783000
N	-0.58172500	-1.61350500	-0.38521600

N	1. 16195200	-0. 56144400	-0. 75004200
C	2. 58835000	-2. 17235500	-1. 91745300
H	2. 45865500	-3. 02802400	-2. 57991300
H	3. 38649900	-2. 39672300	-1. 19566400
C	3. 21443300	0. 13734600	-1. 99454500
O	2. 91032800	-1. 04767900	-2. 71868000
C	4. 52575500	-0. 03074700	0. 04384700
C	3. 19854000	0. 09540500	0. 44138800
C	2. 82012900	-0. 03936800	1. 77264500
C	3. 80864900	-0. 29334200	2. 72012000
C	5. 14573500	-0. 41242700	2. 33071800
C	5. 51375000	-0. 28387400	0. 99283800
C	4. 66306000	0. 13773800	-1. 44866800
H	1. 77349900	0. 04150600	2. 05571200
H	5. 90547000	-0. 61385300	3. 07926200
H	6. 55283600	-0. 38862500	0. 69492000
H	5. 23999500	-0. 66284200	-1. 92203200
H	5. 16112300	1. 08186500	-1. 69229000
C	-1. 87256600	-2. 02726600	0. 01688500
C	-2. 12834200	-2. 38390100	1. 34299100
C	-2. 91842600	-2. 10619200	-0. 90537200
C	-3. 39126500	-2. 79349500	1. 75217000
C	-4. 18952600	-2. 51932800	-0. 52749800
C	-4. 40438500	-2. 85503600	0. 80356700
H	-3. 57600200	-3. 06219000	2. 78492100
H	-4. 99017600	-2. 57429500	-1. 25455300
H	3. 05942200	0. 93800000	-2. 71819100
H	3. 54074600	-0. 40448300	3. 76574100
Cl	-5. 98966600	-3. 36924500	1. 29741900
Cl	-0. 84607000	-2. 32396000	2. 50829300
Cl	-2. 63009300	-1. 66821400	-2. 55675500

NHC-2

C	-0. 53448400	-0. 04003100	0. 70577900
C	-1. 21014500	-1. 60760800	-0. 77841600
C	-3. 03403700	-0. 79255500	0. 48514500
H	-3. 19977500	-0. 81595700	1. 56437200
N	0. 06250100	-1. 51606500	-1. 00521400
N	0. 44546300	-0. 54842900	-0. 08225900
N	-1. 59230600	-0. 75522300	0. 22144100
C	-2. 37836400	-2. 37971900	-1. 30233700
H	-2. 15335900	-3. 43536200	-1. 45604200
H	-2. 70694400	-1. 96060000	-2. 25826500
C	-3. 41990200	-2. 14100300	-0. 17743200

C	1. 82368700	-0. 16996700	-0. 03077500
C	2. 34479800	0. 60552400	-1. 07053200
C	2. 60626500	-0. 59617300	1. 04637900
C	3. 69330200	0. 95614400	-1. 01193700
C	3. 94814800	-0. 21688200	1. 06684600
C	4. 50760100	0. 55749400	0. 04903800
H	4. 11569300	1. 55883000	-1. 81261300
H	4. 57349600	-0. 54112300	1. 89542800
H	-3. 34176700	-2. 94322900	0. 56016500
C	2. 01230000	-1. 43989900	2. 14264800
H	2. 78292300	-1. 75213200	2. 84952600
H	1. 24000300	-0. 88485000	2. 68192600
H	1. 53410300	-2. 33329400	1. 72923700
C	5. 95411900	0. 97745600	0. 10969900
H	6. 36313100	1. 13249200	-0. 89123700
H	6. 06182400	1. 91780000	0. 66011700
H	6. 56237100	0. 22660600	0. 61942400
C	1. 46503600	1. 04709400	-2. 20944300
H	0. 54645000	1. 50638700	-1. 83066700
H	1. 98394800	1. 77006700	-2. 84113700
H	1. 16618900	0. 19419900	-2. 82532400
H	-4. 44410300	-2. 12245800	-0. 55374000
C	-3. 75650700	0. 40031800	-0. 14249100
H	-4. 82307000	0. 29892100	0. 10143100
H	-3. 67410300	0. 32323700	-1. 23571600
C	-3. 26821800	1. 78179800	0. 30702300
C	-3. 27676500	1. 92177200	1. 82928700
C	-4. 12440900	2. 86597200	-0. 34754800
H	-2. 23173500	1. 90144200	-0. 03368700
H	-2. 53180100	1. 26624400	2. 28842600
H	-3. 04088300	2. 94921500	2. 12182000
H	-4. 26417600	1. 67401300	2. 23765700
H	-4. 12581600	2. 77019200	-1. 43780400
H	-5. 16238000	2. 79540200	-0. 00229500
H	-3. 75437800	3. 86355800	-0. 09436100

M3_{NHC-1}

C	-0. 07689400	-0. 35803100	-0. 23612300
C	1. 28879300	-1. 77693000	-1. 20531800
C	2. 31802500	0. 41219700	-0. 68889400
H	1. 90908900	1. 42006800	-0. 62739400
N	0. 18649700	-2. 44672900	-1. 06688200
N	-0. 65329200	-1. 55339200	-0. 44998600
N	1. 17170600	-0. 50568900	-0. 70973300

C	2. 55767800	-2. 11116500	-1. 91790400
H	2. 40731300	-2. 96001300	-2. 58418100
H	3. 35912600	-2. 34708000	-1. 20500100
C	3. 21418900	0. 18463800	-1. 96389300
O	2. 86173100	-0. 97627700	-2. 70688200
C	4. 54351600	-0. 08039400	0. 04968700
C	3. 23127900	0. 10157900	0. 47615900
C	2. 87442400	-0. 00382400	1. 81697100
C	3. 87050500	-0. 31846200	2. 73775800
C	5. 19031100	-0. 51068600	2. 31907300
C	5. 53791500	-0. 38768800	0. 97547900
C	4. 66736300	0. 11832600	-1. 43946800
H	1. 84560700	0. 18667900	2. 11015900
H	5. 95449300	-0. 75529300	3. 05026300
H	6. 56523600	-0. 53378100	0. 65523300
H	5. 20887600	-0. 68800400	-1. 94384700
H	5. 19431500	1. 05087800	-1. 66532200
C	-1. 93142200	-1. 99824500	-0. 02280200
C	-2. 17496800	-2. 25250900	1. 32922500
C	-2. 94403900	-2. 22930200	-0. 95481600
C	-3. 41390300	-2. 71305600	1. 75251100
C	-4. 18818100	-2. 69834200	-0. 55428600
C	-4. 40291300	-2. 93028600	0. 79905900
H	-3. 59936500	-2. 90352200	2. 80230200
H	-4. 97033900	-2. 86929500	-1. 28332900
H	3. 07270600	1. 00388500	-2. 66850500
H	3. 62313300	-0. 40941200	3. 79050900
C	-0. 59402400	0. 89041300	0. 41873800
O	0. 30140800	1. 56127900	1. 03521300
C	-1. 92258100	1. 14105400	0. 21745200
C	-2. 57186600	2. 38574900	0. 73823600
H	-2. 51520400	0. 46924300	-0. 39669600
H	-3. 43430600	2. 13419300	1. 37401200
H	-1. 84882500	2. 90746900	1. 37505600
C	-3. 05228700	3. 33069400	-0. 37030400
C	-3. 73786500	4. 58471500	0. 16722600
H	-3. 74445100	2. 79317500	-1. 03367300
H	-2. 19355300	3. 61831800	-0. 99075000
C	-4. 20441500	5. 52240700	-0. 94304700
H	-4. 59417300	4. 28949100	0. 78704100
H	-3. 04517100	5. 11476200	0. 83321300
H	-4. 68823800	6. 41666100	-0. 54093100
H	-3. 35886300	5. 84565000	-1. 55871000
H	-4. 92017800	5. 02006500	-1. 60178600

C1	-5.95443200	-3.50930600	1.31684000
C1	-0.92328900	-1.98952000	2.49193300
C1	-2.65941600	-1.89357200	-2.62779700

M3_{NHC-2}

C	0.85479300	-0.30627700	-0.34832800
C	2.21235200	-1.96043100	-0.82354500
C	3.36833400	0.11171200	-0.97704300
H	3.12030900	1.00745900	-1.54837200
N	1.08520900	-2.54905800	-0.54676400
N	0.24676100	-1.49756700	-0.25112400
N	2.10912800	-0.60567300	-0.70805500
C	3.58623300	-2.33952700	-1.27646300
H	3.56768200	-3.11307500	-2.04389900
H	4.17338300	-2.70968800	-0.43110100
C	4.10892800	-0.97369600	-1.80095200
C	-1.14459300	-1.73321400	0.01128900
C	-1.50335400	-2.24852600	1.25622400
C	-2.06881900	-1.43092600	-0.99224200
C	-2.86084700	-2.46551100	1.49131200
C	-3.41272200	-1.65939500	-0.70622700
C	-3.82513900	-2.17198900	0.52681600
H	-3.17028200	-2.86696200	2.45301000
H	-4.15668200	-1.43500000	-1.46685900
H	3.85000900	-0.87036300	-2.85707000
C	0.29258200	1.08816300	-0.30617200
O	0.71419600	1.81575000	-1.27078200
C	-0.55070300	1.36891500	0.72676200
C	-1.21106500	2.71236900	0.81938800
H	-0.82086500	0.58261300	1.42569600
H	-1.54738800	2.90974500	1.84498600
H	-0.48103800	3.49369900	0.56624000
C	-1.62019100	-0.88395100	-2.32128100
H	-2.46234700	-0.82268700	-3.01210500
H	-1.18553300	0.11619000	-2.21611200
H	-0.85472500	-1.52732300	-2.76748900
C	-5.28996700	-2.37984900	0.81236300
H	-5.43720800	-3.07882300	1.63815500
H	-5.76609600	-1.43289600	1.08635100
H	-5.81123300	-2.76636800	-0.06679100
C	-0.45794400	-2.53770900	2.29988100
H	0.15463900	-1.65017500	2.49326600
H	-0.92428600	-2.84413300	3.23719700
H	0.21794700	-3.33218000	1.97073600

C	-2.40367900	2.85013300	-0.13828100
C	-3.09001000	4.21122300	-0.05664700
H	-3.13173100	2.05436200	0.07195200
H	-2.03815500	2.67889000	-1.15912200
C	-4.26113300	4.34065100	-1.02724800
H	-3.44034600	4.37838100	0.97031800
H	-2.35199500	4.99746400	-0.26077000
H	-4.73998500	5.32131000	-0.95781300
H	-3.92558300	4.20265800	-2.06009800
H	-5.02151900	3.58006200	-0.82235300
H	5.19063100	-0.87816600	-1.69900000
C	4.10372000	0.43717500	0.32536800
H	5.05271800	0.91232000	0.04253600
H	4.36404300	-0.51176100	0.81561400
C	3.37309700	1.33833200	1.32580400
C	3.11356700	2.73444000	0.75923300
C	4.18965700	1.42149500	2.61657700
H	2.40195900	0.88205800	1.56398500
H	2.45324900	2.70060400	-0.11231700
H	2.63442200	3.36362200	1.51633800
H	4.06121800	3.21153500	0.47959700
H	4.36055000	0.43147200	3.05089100
H	5.16723600	1.87742100	2.42092600
H	3.67715500	2.03619500	3.36179500

TS4S_{NHC-1}

C	-0.53115100	0.72794000	-0.52568200
C	0.69335300	2.18224800	-1.62313900
C	1.75253200	-0.02732600	-1.41885900
H	1.71263300	-0.78078500	-0.63291000
N	-0.37021000	2.84961900	-1.30096600
N	-1.12784000	1.92986100	-0.62354400
N	0.63676400	0.89312200	-1.17529800
C	1.94217000	2.62112200	-2.30996800
H	1.99736800	3.70896300	-2.33291000
H	1.96530800	2.23601600	-3.33894500
C	3.12518800	0.73386700	-1.40928500
O	3.03004000	2.14516800	-1.54518800
C	2.89831400	-0.54646800	-3.45136500
C	1.67211100	-0.64234800	-2.79845400
C	0.57014800	-1.24017500	-3.40094100
C	0.71479400	-1.73396500	-4.69589700
C	1.93978600	-1.63538000	-5.36096400
C	3.04120700	-1.04640600	-4.74282300

C	3. 93117000	0. 10826200	-2. 56970500
H	-0. 36344700	-1. 32904000	-2. 85361300
H	2. 03480400	-2. 02418100	-6. 36991100
H	3. 99242600	-0. 97364100	-5. 26174600
H	4. 51533100	0. 88194300	-3. 07609200
H	4. 63658500	-0. 63552300	-2. 18393400
C	-2. 44937900	2. 28812700	-0. 25663000
C	-3. 51583500	1. 97199900	-1. 10118400
C	-2. 69456200	2. 97053100	0. 93474400
C	-4. 81697000	2. 31157900	-0. 75953400
C	-3. 98897300	3. 32729900	1. 29331800
C	-5. 03051100	2. 98719300	0. 43785900
H	-5. 64248100	2. 05758300	-1. 41263400
H	-4. 17695200	3. 85237600	2. 22151200
H	3. 61395200	0. 58709300	-0. 44468600
H	-0. 12905400	-2. 20310100	-5. 19126500
C	-1. 04275400	-0. 60376700	-0. 05187900
O	-0. 32688200	-1. 58480500	-0. 41980500
C	-2. 20174900	-0. 65598300	0. 69428700
C	-2. 96471900	-1. 94647600	0. 79890100
H	-2. 70596900	0. 25352300	0. 99731200
H	-2. 25815000	-2. 78462800	0. 79687000
H	-3. 52475900	-1. 99178200	1. 74163100
C	-3. 94776000	-2. 10892700	-0. 36897900
C	-4. 77579900	-3. 38878600	-0. 28532600
H	-3. 37730200	-2. 09547900	-1. 30718800
H	-4. 61864000	-1. 23813800	-0. 40281700
C	-5. 74996000	-3. 53371100	-1. 45149600
H	-4. 09967500	-4. 25230700	-0. 25659300
H	-5. 32883600	-3. 39890700	0. 66270500
H	-6. 33389800	-4. 45519200	-1. 37912900
H	-6. 45042800	-2. 69279600	-1. 47945000
H	-5. 21371500	-3. 54970400	-2. 40570300
C	1. 28792700	-5. 99942900	1. 69840700
C	1. 76251800	-5. 02444200	0. 82162300
C	1. 43641900	-3. 68698000	1. 01406600
C	0. 63539200	-3. 29709100	2. 09428100
C	0. 17571200	-4. 28147600	2. 97677000
C	0. 49003900	-5. 62268300	2. 77550500
H	1. 53883900	-7. 04383900	1. 54249300
H	2. 37838700	-5. 31015900	-0. 02551100
H	1. 76894200	-2. 93197500	0. 31092500
H	-0. 41630700	-3. 99262600	3. 84028000
H	0. 12187700	-6. 37081700	3. 47057800

C	0.29313600	-1.87262400	2.31601500
C	-0.85630900	-1.45041300	2.88861200
H	-1.61880500	-2.15906500	3.18907200
H	-0.98993800	-0.40786300	3.14518800
N	1.28783200	-0.94612000	1.93070700
N	0.92198100	0.25427500	2.00252600
C	1.94914900	1.21662400	1.77319100
O	1.73282600	2.20020300	1.10048400
O	3.04946800	0.95456900	2.46922800
C	4.08628200	1.97936200	2.65029600
C	4.77728800	2.27550000	1.32522600
C	3.47110900	3.22970300	3.27115500
C	5.04618000	1.31243400	3.62664700
H	5.25257100	1.36945200	0.93678200
H	4.07415900	2.66492400	0.58648900
H	5.56198800	3.01847200	1.49463300
H	2.89870400	2.96248100	4.16405500
H	4.27575600	3.90688800	3.56985800
H	2.81989100	3.74767200	2.56711100
H	4.54050900	1.09259600	4.57027600
H	5.42823300	0.37853500	3.20675400
H	5.88949100	1.97816600	3.82653300
Cl	-3.21130900	1.12443300	-2.57741800
Cl	-1.37529600	3.33758200	1.98633700
Cl	-6.65305400	3.41812300	0.87680100

TS4S_{NHC-2}

C	-0.31555000	-0.99483600	0.76002800
C	0.99483900	-2.16234300	2.07024000
C	1.03667300	0.10788700	2.74372400
H	1.22297800	1.02544000	2.18717800
N	0.45898000	-3.05492800	1.29717100
N	-0.36507100	-2.31181800	0.48507500
N	0.52400800	-0.91165600	1.80507800
C	2.03841800	-2.12852800	3.13732200
H	2.91761200	-2.70163400	2.83843200
H	1.65402400	-2.54216600	4.07483600
C	2.32340500	-0.60592100	3.23082700
C	-1.18060400	-3.00280200	-0.46964500
C	-2.52241900	-3.22718600	-0.14740400
C	-0.58703600	-3.46943600	-1.64297900
C	-3.30133000	-3.90292500	-1.08290900
C	-1.40980100	-4.14273200	-2.54565200
C	-2.76248400	-4.36193600	-2.28686300

H	-4.35216400	-4.07993500	-0.86492200
H	-0.97842400	-4.50860500	-3.47464500
H	3.14676400	-0.36104300	2.55855100
C	-0.96707400	0.22671200	0.17803900
O	-0.46485100	1.31205300	0.58152800
C	-2.01334800	0.11286300	-0.72422900
C	-2.84806000	1.33933400	-0.97410800
H	-2.38950400	-0.85745700	-1.02820900
H	-2.18803100	2.20262500	-1.11632400
H	-3.44504500	1.22328600	-1.88784900
C	-3.61996100	-5.11674400	-3.27022400
H	-4.65067300	-4.75221800	-3.25910000
H	-3.23263600	-5.02104100	-4.28788700
H	-3.64423800	-6.18403400	-3.02346600
C	0.88026500	-3.26159600	-1.90029100
H	1.14295000	-2.19981500	-1.84632400
H	1.47861500	-3.77066100	-1.13749500
H	1.15564200	-3.65254800	-2.88254400
C	-3.09580600	-2.72916400	1.15296500
H	-2.47404100	-3.03862700	1.99995300
H	-3.14753300	-1.63286600	1.16049000
H	-4.10394200	-3.12079700	1.30425800
C	-3.77305000	1.64328700	0.21291000
C	-4.54796600	2.94824700	0.04698000
H	-3.15198500	1.70549900	1.11716500
H	-4.47540000	0.81043000	0.36373700
C	-5.43797900	3.25430600	1.24878600
H	-3.83173600	3.76608500	-0.10403700
H	-5.15834000	2.89946100	-0.86459500
H	-5.97042700	4.20257400	1.12857400
H	-6.18441800	2.46583100	1.39508200
H	-4.84151200	3.31850800	2.16605100
C	-0.37374400	5.80682200	-2.08799100
C	0.21307900	5.21768500	-0.96909900
C	0.47197900	3.85255900	-0.94666200
C	0.15504600	3.05245500	-2.05101100
C	-0.42173300	3.65397200	-3.17435000
C	-0.69171200	5.01897200	-3.19064200
H	-0.58058400	6.87279700	-2.10027100
H	0.45875600	5.82466300	-0.10247400
H	0.89536200	3.37624300	-0.06942900
H	-0.64561200	3.05001700	-4.04976900
H	-1.13966300	5.46892400	-4.07180900
C	0.42057000	1.59535000	-2.01964800

C	-0.37832900	0.67397900	-2.62645100
H	-1.23668800	0.98343600	-3.21247600
H	-0.07559100	-0.36468600	-2.68093400
N	1.55510200	1.22125400	-1.30137500
N	1.71388000	-0.02424000	-1.14984800
C	2.93229000	-0.36894800	-0.51678500
O	2.99612900	-1.32486700	0.23320000
O	3.95983300	0.38205400	-0.90574900
C	5.32110300	0.05431400	-0.50909800
C	5.47172300	0.08117300	1.00961000
C	5.71084000	-1.29934300	-1.09481000
C	6.13224800	1.17694200	-1.14539200
H	5.01520300	0.99015600	1.41546200
H	5.00815300	-0.79383800	1.46698600
H	6.53572500	0.08962500	1.26681900
H	5.58465000	-1.28858600	-2.18159900
H	6.76276500	-1.50362500	-0.87171400
H	5.09942000	-2.09772300	-0.67015800
H	5.97399300	1.19025700	-2.22703800
H	5.82411800	2.14457300	-0.73956800
H	7.19758100	1.03059000	-0.94516500
H	2.58842600	-0.29444200	4.24340900
C	0.04574800	0.31077600	3.89713400
H	-0.13558800	-0.67624000	4.35002900
H	0.55812000	0.91068000	4.66284300
C	-1.29376200	0.97915000	3.56702800
C	-1.12044000	2.47380200	3.30078900
C	-2.27870500	0.75067100	4.71476700
H	-1.70760600	0.51261600	2.66359100
H	-0.44702300	2.65385400	2.46085000
H	-2.08308800	2.93233600	3.04950700
H	-0.73577100	2.97482400	4.19886000
H	-2.46322200	-0.31611000	4.88267400
H	-1.89243800	1.17706500	5.64890300
H	-3.23910700	1.23119700	4.50157600