

Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

**A DFT Study of NHC-Catalyzed Reactions between 2-Bromo-2-enals and
Acylhydrazones: Mechanisms, Chemo- and Stereoselectivities**

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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).

Table S1 Different computational levels.

	Optimization			Single Point Energy		
	Functional	Basis Set	Solvation Model	Functional	Basis Set	Solvation Model
L1	M062-2X	6-31G(d,p)	IEF-PCM	M062-2X-D3	6-311++G(2df,2pd)	IEF-PCM
L2	B3LYP-D3	6-31G(d,p)	IEF-PCM	B3LYP-D3	6-311++G(2df,2pd)	IEF-PCM
L3	B3PW91-D3	6-31G(d,p)	IEF-PCM	B3PW91-D3	6-311++G(2df,2pd)	IEF-PCM
L4	wB97-XD	6-31G(d,p)	IEF-PCM	wB97-XD	6-311++G(2df,2pd)	IEF-PCM
L5	M06-2X	6-31G(d,p)	SMD	M06-2X-D3	6-311++G(2df,2pd)	SMD

Table 2. Comparison of relative energies for stereoselective transition states at different levels. Energies are in kcal/mol.

	L1	L2	L3	L4	L5
TS6(R)	0.0	0.0	0.0	0.0	0.0
TS6(S)	12.4	12.1	12.8	12.0	10.6

Fig. S1 Energy profiles and optimized structures for direct proton transfer. Bond distances are given in Å.

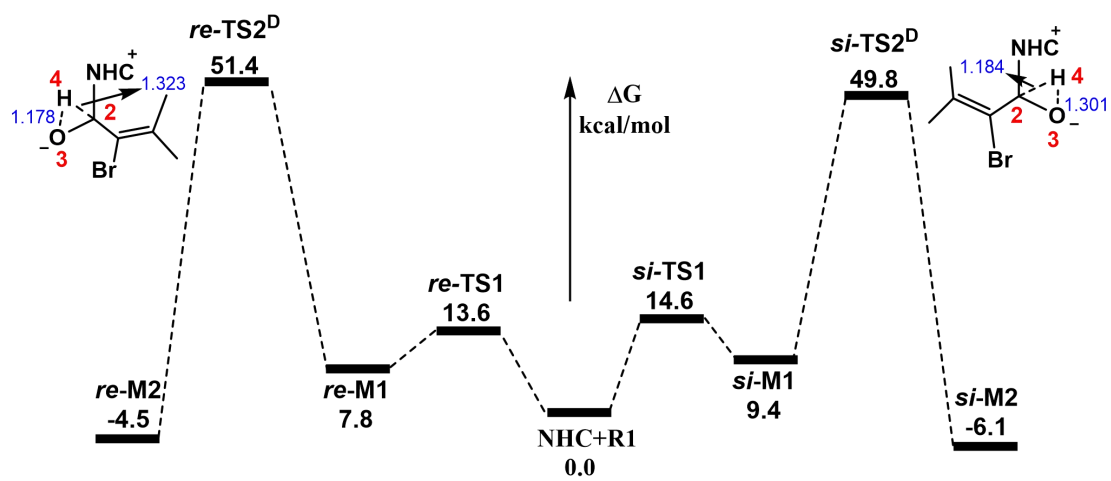


Fig. S2 Energy profiles and optimized structures for water-assisted proton transfer. Bond distances are given in Å.

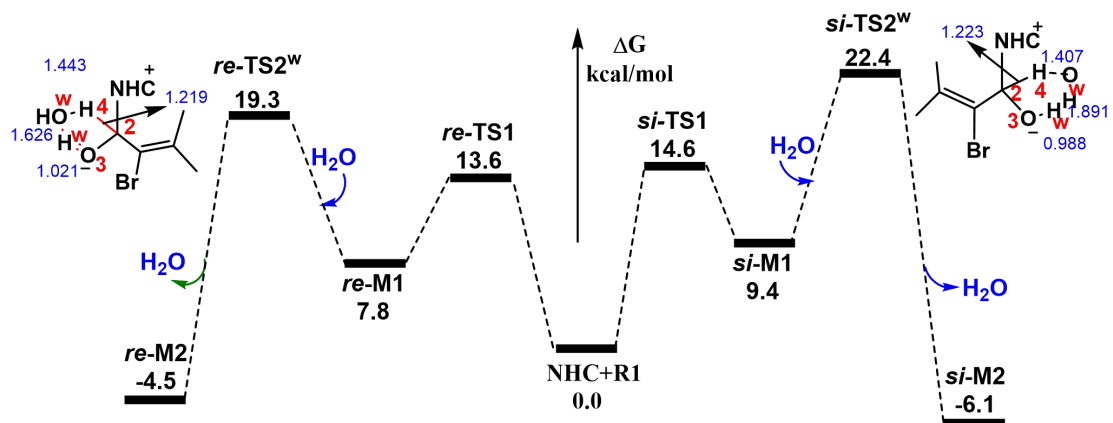


Fig. S3 Energy profiles and optimized structures for **M3** → **M4** conversion. Bond distances are given in Å.

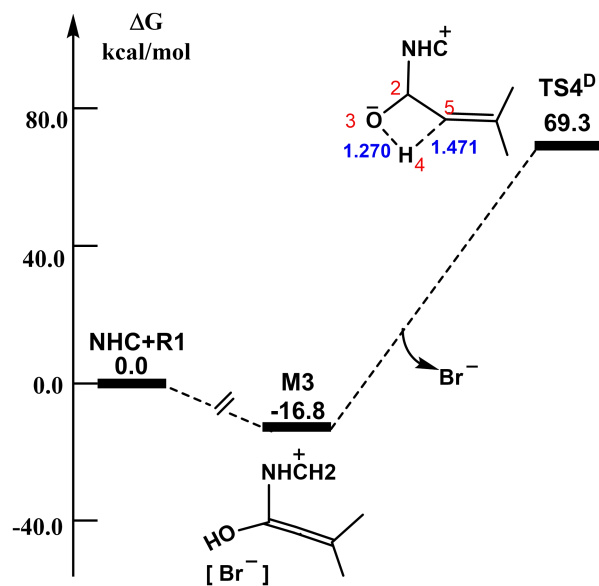
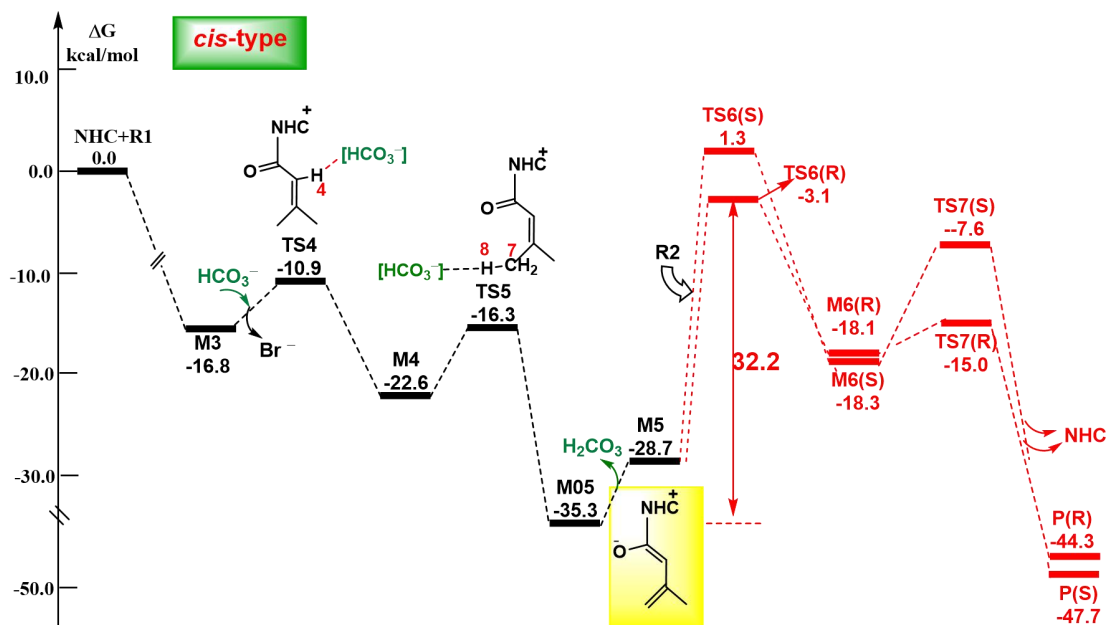
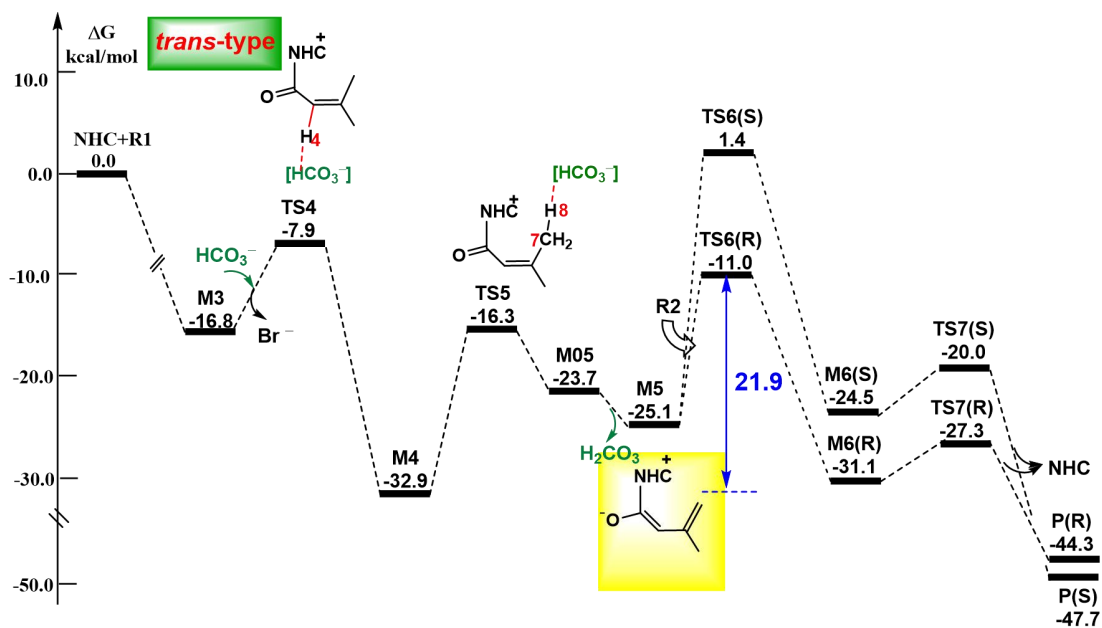


Fig. S4 Energy profiles for other possible pathways of steps 4-7.



Cartesian Coordinates

NHC

C	-4.52239000	0.92294200	-0.37102600
C	-3.61226100	0.77949300	0.67830400
C	-3.23749400	1.86391800	1.46215500
C	-3.80305000	3.10779300	1.18932000
C	-4.72354600	3.25430800	0.14985400
C	-5.08869400	2.16444200	-0.63928600
C	-4.72755300	-0.38981900	-1.08553400
C	-4.22055600	-1.40884300	-0.04158200
C	-3.14746700	-0.65207200	0.78446200
H	-2.51187300	1.74042600	2.25938800
H	-3.52891400	3.96896200	1.78988500
H	-5.16081600	4.22859500	-0.04494500
H	-5.80482200	2.28424000	-1.44683400
H	-4.12127400	-0.41881400	-1.99888000
H	-5.04326200	-1.64474700	0.63822600
H	-5.76386700	-0.58153500	-1.37304300
H	-3.09243600	-1.01253000	1.81461000
N	-1.83332000	-0.85321600	0.16892300
O	-3.78528900	-2.65772200	-0.53556200
C	-0.68028200	-0.21389000	0.54545900
C	-1.58987000	-1.76120100	-0.82889300
N	0.19342400	-0.80782100	-0.29812800
N	-0.33486700	-1.75460700	-1.15490900
C	-2.68520900	-2.59234900	-1.42108600
H	-2.98030700	-2.18703900	-2.39810800
H	-2.33589100	-3.61502500	-1.57294600
C	1.57871800	-0.47325700	-0.40298700
C	1.89627100	0.87863700	-0.52573100
C	2.57011400	-1.46256000	-0.37227200
C	3.22130700	1.27433200	-0.64459600
C	3.89401300	-1.03487100	-0.52172800
C	4.22409500	0.30848400	-0.65749600
H	3.46593800	2.32697200	-0.73887500
H	4.68828300	-1.77580700	-0.51669000
H	1.08646400	1.59982300	-0.52133500
H	5.26371300	0.60071100	-0.76512400
C	2.26244900	-2.93671100	-0.17287100
C	3.18451600	-3.57958400	0.86916300
C	2.34079000	-3.68930500	-1.50601400
H	1.23733300	-3.01714100	0.19882800
H	3.18468800	-3.01429900	1.80484200
H	2.84888300	-4.59877400	1.08173700

H	4.21639600	-3.64537900	0.51060900
H	1.63042400	-3.27317700	-2.22299200
H	3.34929200	-3.61317000	-1.92735800
H	2.11386200	-4.75022700	-1.36061900

R1

C	-0.02946600	1.35287500	0.01525800
C	1.20255600	0.80941700	0.01461600
Br	1.42116100	-1.07037900	0.14997100
C	2.47574400	1.54870600	-0.08757700
O	3.56823100	1.03164000	-0.08370600
H	2.37262200	2.64357000	-0.17173000
C	-1.26003300	0.49508000	0.12448300
H	-1.24385400	-0.07371400	1.05929500
H	-2.16657200	1.10108400	0.09157300
H	-1.28749900	-0.23756400	-0.68760900
C	-0.29597500	2.83023900	-0.08918000
H	-0.87822400	3.14668400	0.78245200
H	0.59016600	3.45668600	-0.15657300
H	-0.91969100	3.01599600	-0.96990000

R2

C	-1.62176700	1.11959900	-0.03607500
N	-0.38626600	0.80121500	0.00146900
N	0.50310900	1.77056800	0.22855100
O	2.56466500	2.60695500	0.25461500
C	2.48503200	0.23551800	0.09543300
C	1.87611300	-0.95546800	0.50605000
C	2.57830600	-2.15375500	0.41447400
C	3.87527000	-2.17695100	-0.09063600
C	4.48524000	-0.99154900	-0.49589500
C	3.79625500	0.20933100	-0.39288500
H	0.86330300	-0.95700000	0.88522100
H	2.10432500	-3.07433200	0.73843200
H	5.49739700	-1.00305400	-0.88630000
H	4.25861700	1.14586300	-0.68495100
C	-2.60677500	0.02770900	-0.26408200
O	-2.34345900	-1.14595200	-0.35838900
O	-3.83931500	0.54694200	-0.34849200
C	-4.90792600	-0.39575200	-0.55424800
C	-5.29487800	-1.06879600	0.74860600
H	-4.58941600	-1.12777700	-1.29986900
H	-5.72573900	0.20228600	-0.95835700
H	-6.15042600	-1.72847300	0.58428000

H	-4.46407600	-1.66669400	1.12781900
H	-5.57109000	-0.32224100	1.49681600
H	-1.99436800	2.13829100	0.09032900
H	0.20603000	2.74245000	0.30855600
C	1.88194600	1.60051500	0.19779200
H	4.41152100	-3.11776800	-0.16518800

H₂O

O	0.02545500	0.00000000	0.01817900
H	0.06657500	0.00000000	0.97972100
H	0.94804000	0.00000000	-0.25602400

HCO₃⁻

H	1.68282400	-0.44242300	0.00003000
C	-0.12706100	0.08170900	0.00000400
O	-1.29244200	-0.33520000	-0.00001200
O	0.34030300	1.24059200	0.00000800
O	0.85750500	-0.94114700	0.00001900

H₂CO₃

H	-1.61931800	-0.75412000	0.00002700
C	0.05420600	0.12971300	-0.00002300
O	0.73702000	1.11572700	0.00001900
O	-1.27760000	0.15075400	-0.00001600
O	0.51689100	-1.13353700	0.00004700
H	1.48358600	-1.08770800	-0.00028800

re-TS1

C	3.69180000	-1.92000300	-0.03485000
C	2.70324100	-1.01801000	0.34917900
C	2.67707200	-0.45388300	1.62193600
C	3.67722000	-0.82616500	2.51761300
C	4.67362400	-1.73108300	2.14257700
C	4.69092700	-2.28338600	0.86389700
C	3.49767000	-2.36452200	-1.46297000
C	2.08580500	-1.86976000	-1.84904300
C	1.72947700	-0.77036300	-0.78290100
H	1.90287400	0.26205800	1.89764300
H	3.68341500	-0.40619100	3.51824700
H	5.44275300	-2.00834200	2.85694600
H	5.46575200	-2.98794900	0.57586300
H	3.56103600	-3.44864200	-1.59787100
H	2.06490700	-1.44297900	-2.85286200
H	4.25028500	-1.91152400	-2.11745200

H	1.84905400	0.23255000	-1.19952400
N	0.34260100	-0.90819200	-0.34774900
O	1.14367400	-2.93315300	-1.90402700
C	-0.55891000	0.02929000	0.02947300
C	-0.20158700	-2.15409100	-0.17266300
N	-1.60364900	-0.71812200	0.41448400
N	-1.41026300	-2.07590400	0.29081800
C	0.59762900	-3.31881800	-0.65375500
H	1.38094400	-3.58544500	0.06878100
H	-0.04575500	-4.18230900	-0.82239100
C	-2.83633100	-0.22653900	0.95899600
C	-2.76631800	0.50554300	2.14319800
C	-4.04347800	-0.48996800	0.30267000
C	-3.93955400	0.98326900	2.71361500
C	-5.20617600	-0.01401000	0.91701600
C	-5.16163000	0.70831000	2.10457600
H	-3.89811100	1.56019300	3.63095100
H	-6.16689600	-0.20607900	0.44853600
H	-1.79025800	0.71174300	2.57750500
H	-6.08435500	1.06637000	2.54987400
C	-4.11198600	-1.25590000	-1.00633700
C	-5.01871000	-0.56385600	-2.02910000
C	-4.56542800	-2.69955900	-0.75793500
H	-3.10293400	-1.28943300	-1.43042400
H	-4.72991400	0.48060400	-2.17644600
H	-4.95271100	-1.07896200	-2.99158300
H	-6.06757600	-0.58607800	-1.71813800
H	-3.88059100	-3.20500800	-0.07346200
H	-5.56917100	-2.71290100	-0.31962400
H	-4.59808400	-3.25735700	-1.69876900
C	0.04880500	2.89879300	-1.56939000
C	0.55548100	2.47057700	-0.40784300
Br	2.40986200	2.62081000	-0.00121300
C	-0.25028400	1.85669200	0.72265800
O	0.23654400	1.70846200	1.86278400
H	-1.31652600	2.12850500	0.61313900
C	0.83396900	3.57579500	-2.65500700
H	0.86453900	2.93858500	-3.54667500
H	0.33216100	4.50445700	-2.94786600
H	1.85437200	3.80308200	-2.35062400
C	-1.42303800	2.70258600	-1.86680700
H	-1.80023200	1.74834700	-1.48691800
H	-2.02401800	3.50397100	-1.42320000
H	-1.58845600	2.72782100	-2.94693900

si-TS1

C	4. 95902900	-0. 20281000	0. 18973400
C	3. 65300300	-0. 67045300	0. 06706200
C	3. 32204900	-1. 70290700	-0. 80518000
C	4. 34243200	-2. 25636200	-1. 57594300
C	5. 65439200	-1. 78894900	-1. 46681800
C	5. 97417000	-0. 76265200	-0. 58063600
C	5. 05098000	0. 89275400	1. 22123100
C	3. 58751800	1. 28919000	1. 51641300
C	2. 71829400	0. 08487400	0. 98917100
H	2. 29816900	-2. 06958000	-0. 85897000
H	4. 11579800	-3. 06213200	-2. 26658500
H	6. 43428200	-2. 23191300	-2. 07842600
H	6. 99527600	-0. 40248900	-0. 49631300
H	5. 61152600	1. 76978600	0. 88393600
H	3. 41388700	1. 44255900	2. 58242300
H	5. 53654600	0. 52765300	2. 13286200
H	2. 37644400	-0. 53592700	1. 82171500
N	1. 53244900	0. 58030300	0. 29721400
O	3. 24557400	2. 53486300	0. 92438900
C	0. 27076200	0. 08661000	0. 25118300
C	1. 61320500	1. 69504900	-0. 49654700
N	-0. 33676600	0. 94288600	-0. 58154600
N	0. 47191500	1. 95370200	-1. 05433600
C	2. 88639200	2. 47172300	-0. 44687500
H	3. 66922700	1. 99545000	-1. 05225900
H	2. 72853400	3. 49122100	-0. 79820800
C	-1. 70197900	0. 86597000	-1. 00892400
C	-2. 09275300	-0. 30070700	-1. 65666200
C	-2. 58802300	1. 91601900	-0. 73963900
C	-3. 41112300	-0. 44286600	-2. 06877600
C	-3. 90041500	1. 75424200	-1. 19506000
C	-4. 31053900	0. 59662900	-1. 84991000
H	-3. 72876800	-1. 36287900	-2. 54702400
H	-4. 62128600	2. 54791800	-1. 02268500
H	-1. 36753300	-1. 10149600	-1. 78010800
H	-5. 34030900	0. 50339400	-2. 17960900
C	-2. 16789300	3. 17805000	-0. 00700900
C	-3. 17791500	3. 58682000	1. 07035000
C	-1. 93894600	4. 32221600	-1. 00220000
H	-1. 21384000	2. 97806400	0. 49300700
H	-3. 38275800	2. 76469500	1. 76312800
H	-2. 78594700	4. 43052300	1. 64547000

H	-4.12871300	3.90466900	0.63197600
H	-1.17410200	4.04840900	-1.73221400
H	-2.86657200	4.55133600	-1.53743800
H	-1.61672400	5.22663500	-0.47702400
C	-2.31094700	-0.89455700	1.82641600
C	-1.65322600	-1.74412300	1.03069800
Br	-2.57927800	-3.09754000	0.06003400
C	-0.14594500	-1.79743300	0.77997700
O	0.31010000	-2.51177600	-0.13207900
H	0.40800500	-1.68461500	1.73591600
C	-3.80463800	-0.82165700	1.96170600
H	-4.10702000	-1.01620300	2.99669400
H	-4.13280200	0.19581400	1.71355000
H	-4.31555900	-1.52131300	1.30278900
C	-1.57099000	0.16683100	2.60360200
H	-2.07177700	0.33983900	3.56108600
H	-0.52756900	-0.08234600	2.80129300
H	-1.59164700	1.11490000	2.04783900

re-M1

C	3.67322700	-1.81711400	-0.07512800
C	2.71207200	-0.92009600	0.38207000
C	2.71497100	-0.42758700	1.68466200
C	3.71820600	-0.87996300	2.53981400
C	4.68519100	-1.78622200	2.09621400
C	4.67366100	-2.25956100	0.78597800
C	3.46160500	-2.15679900	-1.52883200
C	2.07728800	-1.56904700	-1.88699400
C	1.73859100	-0.56741800	-0.71942500
H	1.94501300	0.28160800	1.99763800
H	3.75036900	-0.52196600	3.56386200
H	5.45593500	-2.12614700	2.78118100
H	5.42834000	-2.96183100	0.44408800
H	3.47125600	-3.23188100	-1.73462800
H	2.09520400	-1.03710100	-2.83903900
H	4.23877900	-1.70239800	-2.15237600
H	1.86317200	0.46465500	-1.04851900
N	0.34369400	-0.73519700	-0.29652900
O	1.09738600	-2.58088000	-2.07429000
C	-0.55922100	0.13671700	0.19687600
C	-0.22932800	-1.97977200	-0.26858700
N	-1.63031300	-0.61010600	0.47706700
N	-1.44094800	-1.93804400	0.19261900
C	0.54917400	-3.09806300	-0.87559300

H	1.32843200	-3.45282300	-0.18714100
H	-0.10997600	-3.92671900	-1.13300600
C	-2.85476700	-0.16436900	1.08016400
C	-2.76084100	0.46270200	2.32174700
C	-4.06769800	-0.37576600	0.41682800
C	-3.92825000	0.87559700	2.95031700
C	-5.22207300	0.03169600	1.09304300
C	-5.15943000	0.64269400	2.34064300
H	-3.87461900	1.37224800	3.91284800
H	-6.18970100	-0.12434900	0.62543800
H	-1.77131000	0.65031900	2.73670700
H	-6.07624700	0.95004200	2.83346700
C	-4.15480700	-1.01058800	-0.95952200
C	-5.06404200	-0.21244700	-1.89973300
C	-4.62027300	-2.46721200	-0.84915300
H	-3.15081600	-1.00970700	-1.39710200
H	-4.76138300	0.83716400	-1.95134500
H	-5.01707200	-0.63558100	-2.90711200
H	-6.10889400	-0.24967800	-1.57723100
H	-3.93403600	-3.04633800	-0.22733900
H	-5.61852000	-2.51397700	-0.40090400
H	-4.67136300	-2.92783200	-1.84034300
C	-0.01027100	2.59375600	-1.64723000
C	0.43608100	2.34835900	-0.41052200
Br	2.17238200	2.88127500	0.15259900
C	-0.33784600	1.58171000	0.69338100
O	0.21752300	1.46262300	1.88616200
H	-1.35947400	2.03149200	0.67967300
C	0.75634200	3.30866300	-2.72383000
H	0.77798100	2.70037400	-3.63547000
H	0.25247000	4.24718800	-2.98130300
H	1.77805100	3.53232200	-2.42075600
C	-1.37420400	2.09514100	-2.07607300
H	-2.05956300	1.92453500	-1.24196200
H	-1.84035200	2.81826000	-2.75208100
H	-1.27830500	1.15254700	-2.63145600

si-M1

C	5.02016500	0.03998300	-0.12566000
C	3.76681600	-0.56179700	-0.19469200
C	3.45331300	-1.51753300	-1.15761000
C	4.44800800	-1.85898700	-2.07176200
C	5.71053200	-1.26245500	-2.01416900
C	6.00806500	-0.31099300	-1.04093300

C	5.09803500	1.02231100	1.01492700
C	3.64483000	1.17729700	1.51942100
C	2.85571900	-0.03415100	0.89226900
H	2.45574000	-1.96502200	-1.17657000
H	4.24050500	-2.59876500	-2.83819700
H	6.46967500	-1.54353900	-2.73766400
H	6.99018900	0.15079600	-0.99990700
H	5.49383000	2.00028800	0.72309800
H	3.58707700	1.13712500	2.60765300
H	5.73938800	0.64197500	1.81680600
H	2.63925600	-0.78891100	1.65212200
N	1.57537300	0.42448000	0.35161600
O	3.09197900	2.44332700	1.19014200
C	0.39027700	-0.20696500	0.23021700
C	1.46455400	1.64383200	-0.26029400
N	-0.38543200	0.65961700	-0.42885500
N	0.27545700	1.82157500	-0.74469300
C	2.63443300	2.56337400	-0.14546700
H	3.41489800	2.29984900	-0.87249800
H	2.32611400	3.59620500	-0.30594200
C	-1.73072900	0.46151200	-0.89612800
C	-1.95916900	-0.64383000	-1.70891900
C	-2.73393800	1.36849200	-0.53633600
C	-3.23969800	-0.85868300	-2.20310600
C	-4.00260700	1.13214600	-1.07254800
C	-4.25680400	0.03956000	-1.89661300
H	-3.43803900	-1.73037300	-2.81723300
H	-4.81183200	1.81524500	-0.83155300
H	-1.14206000	-1.34414600	-1.87498900
H	-5.25693800	-0.11501800	-2.28871000
C	-2.49548900	2.55247200	0.38340400
C	-3.54573000	2.62465200	1.49722000
C	-2.45471900	3.85870100	-0.41831900
H	-1.51704700	2.42487400	0.85776000
H	-3.62773500	1.67263800	2.03052800
H	-3.27576700	3.40396200	2.21583600
H	-4.53444600	2.87292300	1.09964000
H	-1.66755200	3.82228100	-1.17483000
H	-3.41245500	4.02589600	-0.92232500
H	-2.26645900	4.70884900	0.24445500
C	-1.84759800	-1.22232600	2.06894500
C	-1.26870900	-1.90187000	1.07579900
Br	-2.22112800	-3.29996700	0.22079500
C	0.16086600	-1.70572700	0.50397400

O	0.45336100	-2.31417900	-0.63539200
H	0.84105400	-1.93047100	1.36785200
C	-3.28364700	-1.43790700	2.47441200
H	-3.42974000	-2.43930800	2.89233300
H	-3.59368800	-0.70344300	3.22229500
H	-3.94191800	-1.35554100	1.60355200
C	-1.08798600	-0.16560800	2.83574600
H	-1.31639600	-0.25223200	3.90261000
H	-0.00367500	-0.24497600	2.72481000
H	-1.39123600	0.84314300	2.52521500

re-TS2

C	4.17200100	1.38492900	-0.43273400
C	2.98965200	0.65980000	-0.54689400
C	2.45903400	0.29627500	-1.78409800
C	3.16546300	0.67495600	-2.92375100
C	4.35993700	1.39419100	-2.82197000
C	4.87208100	1.75619300	-1.57835000
C	4.50601100	1.66065400	1.01354600
C	3.24580300	1.24105300	1.81213200
C	2.38518400	0.39518700	0.81409100
H	1.52639600	-0.27028800	-1.86468600
H	2.78230200	0.40642300	-3.90294000
H	4.89191100	1.67953500	-3.72444400
H	5.79507900	2.32444700	-1.50521800
H	4.74180100	2.71136500	1.21316500
H	3.50648700	0.63864400	2.68303600
H	5.37074800	1.07127000	1.33605000
H	2.41132900	-0.66271900	1.07352100
N	0.98960200	0.84723400	0.82479500
O	2.54573500	2.34853800	2.36112900
C	-0.06285100	0.25516700	0.18763200
C	0.73640700	2.19581300	0.86312300
N	-0.89772500	1.27646100	-0.08834100
N	-0.40407100	2.48956800	0.33129800
C	1.79813800	3.08927600	1.41969900
H	2.43303900	3.46567200	0.60368100
H	1.35338100	3.94038800	1.93710800
C	-2.13442500	1.23436300	-0.82270300
C	-2.04410700	1.12400300	-2.20643700
C	-3.35324300	1.32218000	-0.14561700
C	-3.20605200	1.11642700	-2.96321000
C	-4.50559400	1.30625600	-0.93661900
C	-4.43727800	1.20844700	-2.32117100

H	-3.15109600	1.01239800	-4.04146900
H	-5.47607600	1.33798800	-0.45350000
H	-1.06655300	0.99758000	-2.65668800
H	-5.35461800	1.18160000	-2.90088600
C	-3.42628600	1.43002000	1.36521300
C	-4.65254100	0.71952800	1.94276200
C	-3.39881200	2.90330700	1.79798500
H	-2.53824100	0.92537800	1.76349600
H	-4.75229900	-0.28409500	1.52090200
H	-4.55213600	0.64874100	3.03081500
H	-5.56718200	1.29010300	1.74102700
H	-2.50072800	3.41209900	1.43884400
H	-4.27338300	3.42717700	1.39556500
H	-3.43411400	2.97980200	2.89007500
C	0.60600300	-2.36909600	1.90696700
C	0.58337300	-2.08980600	0.59452800
Br	1.89757300	-2.90531800	-0.57909900
C	-0.34019200	-1.15410100	-0.12440600
O	-0.55061200	-1.36482200	-1.46036400
H	-1.48709500	-1.31637500	0.40921200
C	1.61528500	-3.24703200	2.59380400
H	1.10580600	-4.07398700	3.10184900
H	2.35263600	-3.65727400	1.90598200
H	2.13727700	-2.67631000	3.37329300
C	-0.38378500	-1.71080500	2.84398600
H	-1.35887300	-1.55271400	2.37905800
H	-0.52338000	-2.33555000	3.73213300
H	0.00184000	-0.74201500	3.19232100
H	-1.94761300	-1.68645800	-1.50635000
C	-3.56360000	-1.78563300	-0.30867200
O	-4.78591100	-1.93857500	-0.20113700
O	-2.78996800	-1.52509400	0.71001600
O	-2.99049400	-1.87865600	-1.51011500

re-TS2^w

C	-4.81327300	-0.20562700	0.09092400
C	-3.57615000	0.43123500	0.14951200
C	-3.39989000	1.74075700	-0.29262800
C	-4.51674900	2.40906700	-0.79214400
C	-5.76491200	1.78462700	-0.84447800
C	-5.92302000	0.47186800	-0.40527200
C	-4.72644300	-1.61827400	0.61285000
C	-3.21361400	-1.90905100	0.74785000
C	-2.52617800	-0.49671100	0.72030900

H	-2.42784700	2.23980000	-0.27337200
H	-4.41046000	3.42849200	-1.14861500
H	-6.61979800	2.32452700	-1.23986000
H	-6.89182900	-0.01628800	-0.45860200
H	-5.18812300	-2.35725900	-0.04939500
H	-2.97949700	-2.41835100	1.68332100
H	-5.21655900	-1.70697300	1.58826500
H	-2.19782500	-0.19057800	1.71220000
N	-1.33800300	-0.52097600	-0.13600800
O	-2.74324700	-2.79987700	-0.25621000
C	-0.18530000	0.16855800	-0.08123100
C	-1.30542000	-1.27855300	-1.27751200
N	0.48488700	-0.19541300	-1.17720900
N	-0.19391400	-1.11536900	-1.92871100
C	-2.45445900	-2.20290500	-1.50600600
H	-3.31811700	-1.65626800	-1.90980000
H	-2.17250500	-2.99392400	-2.20071600
C	1.75091500	0.33087700	-1.60249200
C	1.78263400	1.65821800	-2.02406200
C	2.88031100	-0.48872100	-1.55007700
C	2.99153000	2.18577200	-2.46206300
C	4.07661200	0.07339200	-2.00605700
C	4.13310300	1.38582900	-2.46509300
H	3.04121900	3.21732100	-2.79346100
H	4.98038800	-0.52878000	-1.99685100
H	0.88302200	2.26813000	-1.94771500
H	5.07737700	1.79059500	-2.81536300
C	2.82143200	-1.91018500	-1.02319500
C	3.92096500	-2.17444300	0.00831600
C	2.88205100	-2.91285500	-2.18094300
H	1.86500800	-2.03985000	-0.50585000
H	3.86599400	-1.44875300	0.82356100
H	3.79572500	-3.17345400	0.43590100
H	4.91802500	-2.12632200	-0.44061000
H	2.06165300	-2.74574800	-2.88346700
H	3.82715000	-2.81277700	-2.72541800
H	2.81478700	-3.93685800	-1.80200900
C	2.67107900	1.42238000	1.69395900
C	1.52859100	0.74092500	1.56760300
Br	1.34471500	-1.03150000	2.34138600
C	0.27656300	1.17848100	0.89032300
O	-0.76319700	1.52499700	1.78340700
H	0.29906700	2.21503800	0.24108800
C	3.89057000	0.93052000	2.42008000

H	4.71138300	0.79753800	1.70514200
H	4.21801200	1.68275000	3.14508900
H	3.71865600	-0.00992600	2.94184300
C	2.83370000	2.78958300	1.07726200
H	1.93485900	3.15605700	0.58115700
H	3.12197600	3.50397700	1.85635600
H	3.65022000	2.76056000	0.34651200
O	-0.50473700	3.28573900	-0.19162800
H	-1.00906100	2.40377600	1.40341000
H	-0.20714900	4.18288700	-0.00671700

re-TS2^D

C	3.60832600	-1.84203200	0.10672400
C	2.61195300	-0.91176900	0.38806300
C	2.38505100	-0.43561600	1.67851000
C	3.20591200	-0.91596100	2.69610000
C	4.21711000	-1.84220900	2.42471200
C	4.42565500	-2.31371800	1.13119900
C	3.63041400	-2.20332900	-1.35783700
C	2.37847400	-1.52649300	-1.97004700
C	1.83550700	-0.55868000	-0.86038200
H	1.59205400	0.28484200	1.89972900
H	3.05781200	-0.56539900	3.71226500
H	4.84383600	-2.20304900	3.23430800
H	5.20596500	-3.04124900	0.92769800
H	3.59570000	-3.28352800	-1.53558300
H	2.63191900	-0.95464900	-2.86266400
H	4.53788200	-1.83121100	-1.84366400
H	1.97061500	0.48504800	-1.14739200
N	0.40501700	-0.78846600	-0.63451100
O	1.40970900	-2.45944100	-2.42785200
C	-0.44135100	-0.03344200	0.11658300
C	-0.11747000	-2.05370900	-0.69400700
N	-1.44291200	-0.87781200	0.43353400
N	-1.25009000	-2.14001700	-0.07027800
C	0.68595100	-3.09884900	-1.39832500
H	1.35358400	-3.59910300	-0.68127800
H	0.03457300	-3.84615300	-1.85237000
C	-2.67494500	-0.53049600	1.07632400
C	-2.64974400	-0.26000800	2.44180300
C	-3.84588000	-0.47203300	0.31109300
C	-3.83859400	0.05075000	3.08962000
C	-5.02630800	-0.17110200	0.99697100
C	-5.02761800	0.08140900	2.36501600

H	-3.83466300	0.26760400	4.15194800
H	-5.96104500	-0.12661100	0.44631400
H	-1.69575000	-0.25991800	2.95570700
H	-5.96172300	0.31506800	2.86571900
C	-3.84991200	-0.73098100	-1.18467900
C	-4.68805600	0.30024900	-1.94677300
C	-4.33469400	-2.15602500	-1.47913300
H	-2.81762600	-0.64376600	-1.54427700
H	-4.39772600	1.32262600	-1.68946800
H	-4.55314000	0.16368500	-3.02350600
H	-5.75538200	0.18567900	-1.73385000
H	-3.69766800	-2.89242300	-0.98392000
H	-5.36069900	-2.28749300	-1.11921300
H	-4.32448200	-2.34834400	-2.55619300
C	0.08889100	2.59851900	-1.62531400
C	0.42475100	2.22326600	-0.38140900
Br	2.11637700	2.82253200	0.33857600
C	-0.34046100	1.34911400	0.51299400
O	-0.24842000	1.56510500	1.95611300
H	-1.25109600	1.75717200	1.15016700
C	0.99157500	3.42347400	-2.50703200
H	0.54660800	3.56375200	-3.49434700
H	1.16977700	4.40811500	-2.06251200
H	1.97294900	2.95516800	-2.63121200
C	-1.24005700	2.18620500	-2.20680200
H	-1.92311600	1.83776000	-1.42841700
H	-1.69923500	3.02842000	-2.73495700
H	-1.11441200	1.37888400	-2.94029700

re-M2

C	3.93112400	1.25798000	-0.40710400
C	2.81301300	0.42705100	-0.43297200
C	2.66262900	-0.55229500	-1.41279000
C	3.64543100	-0.66616300	-2.39235200
C	4.75883200	0.17730900	-2.38325400
C	4.91354800	1.13851600	-1.38728100
C	3.90179000	2.18523500	0.78130400
C	2.50963300	1.98276800	1.43065900
C	1.86486100	0.74275200	0.70276300
H	1.81073300	-1.22559600	-1.40147000
H	3.54700000	-1.42087900	-3.16567400
H	5.51586300	0.07536600	-3.15439400
H	5.78749600	1.78336800	-1.37497300
H	4.04222900	3.23834500	0.51477700

H	2.59737800	1.77311000	2.49770600
H	4.69417700	1.93199200	1.49281500
H	1.78596200	-0.09730500	1.39462200
N	0.51672800	1.07722500	0.24173100
O	1.70699800	3.15006100	1.37340900
C	-0.45060600	0.22831100	-0.29424200
C	0.27696300	2.32917400	-0.29472900
N	-1.20520800	1.05572500	-1.11745400
N	-0.75327600	2.37598500	-1.05639800
C	1.22009800	3.42537900	0.07655800
H	2.03838300	3.48882300	-0.65619000
H	0.69956700	4.38341100	0.10256200
C	-2.58937000	0.85813100	-1.42693700
C	-2.92186200	0.34579100	-2.67816600
C	-3.57074400	1.20330900	-0.48958800
C	-4.25458100	0.17497000	-3.02670200
C	-4.90727200	1.02964700	-0.86662500
C	-5.24957800	0.52383900	-2.11528900
H	-4.51580500	-0.22474200	-4.00075400
H	-5.69484400	1.29975300	-0.16861400
H	-2.11831500	0.07766700	-3.35484200
H	-6.29560700	0.40052800	-2.37768000
C	-3.21753500	1.78450500	0.86740800
C	-3.98555500	1.10409200	2.00493400
C	-3.45203700	3.30005700	0.87255600
H	-2.14933700	1.61446700	1.04478900
H	-3.86719600	0.01677300	1.97144100
H	-3.61775000	1.46113800	2.97157600
H	-5.05563800	1.32854700	1.95700300
H	-2.86084900	3.78189500	0.08987500
H	-4.50947700	3.52293400	0.69383200
H	-3.17131800	3.72817300	1.83980100
C	0.16680800	-1.61606000	2.20913100
C	0.04578300	-1.89111900	0.89546700
Br	0.84667200	-3.51202500	0.17649300
C	-0.63572900	-1.11522600	-0.11154000
O	-1.40938000	-1.77180100	-1.05909600
C	1.03076500	-2.37894100	3.17373900
H	0.40365300	-2.93773100	3.87866700
H	1.69819100	-3.07908500	2.67362100
H	1.63013600	-1.68165400	3.77057200
C	-0.57332100	-0.44616600	2.80578600
H	-1.47608100	-0.21346000	2.23663600
H	-0.84619500	-0.66581500	3.84259100

H	0.04405100	0.46452400	2.81809500
H	-2.18267500	-2.15160300	-0.62349700

si-TS2

C	-4.68022800	0.06529100	-0.34601200
C	-3.40604700	0.44248400	0.06785200
C	-3.06782600	1.77625300	0.27754800
C	-4.04101000	2.74226200	0.03252300
C	-5.31983300	2.37592000	-0.39683700
C	-5.65126100	1.03573000	-0.58253200
C	-4.80225300	-1.43406800	-0.44440900
C	-3.36658600	-1.98150600	-0.24138700
C	-2.50679900	-0.75664200	0.25164700
H	-2.07212500	2.02288900	0.64115000
H	-3.80657100	3.79132900	0.18495300
H	-6.06558200	3.14381500	-0.58050900
H	-6.64944400	0.75277200	-0.90537500
H	-5.19722900	-1.77654000	-1.40728300
H	-3.33728900	-2.76165000	0.51955200
H	-5.47076500	-1.82291000	0.33048800
H	-2.20175100	-0.88893300	1.28896700
N	-1.27465800	-0.63201800	-0.54062500
O	-2.87802500	-2.62356300	-1.41299700
C	-0.06175500	-0.10658000	-0.22725100
C	-1.21916800	-1.05037600	-1.84245700
N	0.66418800	-0.26424000	-1.35642700
N	-0.05172300	-0.85991000	-2.36863800
C	-2.42252700	-1.72606000	-2.40343100
H	-3.19494400	-0.98856600	-2.66877200
H	-2.15463900	-2.29990900	-3.29073300
C	2.06939900	-0.02828100	-1.52278400
C	2.46706900	1.19117900	-2.05958000
C	2.97794600	-1.02350500	-1.13957200
C	3.82182300	1.46253600	-2.20132700
C	4.33418100	-0.72118700	-1.30106200
C	4.75376700	0.50189400	-1.81582400
H	4.14669200	2.41756900	-2.60091300
H	5.07607800	-1.45744200	-1.00758600
H	1.71015500	1.92896500	-2.30012600
H	5.81557100	0.70511500	-1.91680800
C	2.51105600	-2.37719900	-0.63483100
C	3.47254100	-3.02058100	0.36430500
C	2.27591500	-3.31275300	-1.83095200
H	1.56524100	-2.24478000	-0.09966900

H	3.71190000	-2.33655100	1.18096800
H	2.99715400	-3.89974600	0.80559200
H	4.40323400	-3.34296700	-0.11722900
H	1.55456800	-2.88927200	-2.53452400
H	3.21692000	-3.48473800	-2.36632800
H	1.89828800	-4.27861500	-1.48259000
C	2.64203900	1.47997500	1.47545600
C	1.38725200	1.41732400	1.02728000
Br	0.65797200	3.05049600	0.20926600
C	0.35295300	0.34630300	1.10162100
O	-0.70750100	0.66377200	1.91582500
H	0.78772400	-0.78637100	1.56499100
C	3.49634100	2.71666900	1.34277700
H	3.06649300	3.55058600	1.90723600
H	4.50735100	2.52836800	1.71205400
H	3.55641500	3.03522300	0.29735000
C	3.30001600	0.29901300	2.14095400
H	3.69624900	0.60792600	3.11551500
H	2.62633900	-0.54653200	2.28997700
H	4.15587100	-0.02494300	1.53459300
H	-0.84474200	-0.44840800	2.67690200
C	-0.09030100	-2.33727500	2.91671100
O	-0.19371700	-3.45718300	3.41780800
O	0.90252600	-1.98824600	2.13608500
O	-1.02966500	-1.41237600	3.15741800

si-TS2^w

C	4.71038800	0.13098300	0.10536400
C	3.41381600	-0.31801300	0.34026900
C	3.06669500	-1.65731400	0.18944800
C	4.05445600	-2.54950700	-0.21886200
C	5.35845800	-2.10818500	-0.45747500
C	5.69677600	-0.76711700	-0.29456700
C	4.83383800	1.61239200	0.35310600
C	3.38774500	2.11691400	0.57792500
C	2.51085800	0.81816500	0.75925800
H	2.04980600	-1.98957800	0.37663600
H	3.80975300	-3.59856900	-0.35011700
H	6.11562800	-2.81793200	-0.77592400
H	6.71107200	-0.42664300	-0.48146400
H	5.28983900	2.15413800	-0.48214200
H	3.31158300	2.72843900	1.47697200
H	5.44750300	1.81344900	1.23701700
H	2.16821400	0.72083000	1.78717300

N	1.30259600	0.88619000	-0.07733400
O	2.95191100	2.97826200	-0.46309800
C	0.06895200	0.36218500	0.08134300
C	1.30538900	1.55971900	-1.27198900
N	-0.62133300	0.78208900	-0.98862300
N	0.14468700	1.52338400	-1.84862600
C	2.54411100	2.30503000	-1.63660800
H	3.31936300	1.61894200	-2.00649900
H	2.32728300	3.05017500	-2.40161500
C	-2.02714300	0.60335300	-1.22917500
C	-2.39484100	-0.33071300	-2.18932900
C	-2.95256300	1.35157000	-0.48658900
C	-3.74414400	-0.56795400	-2.42161400
C	-4.30039900	1.08550400	-0.74629000
C	-4.69344500	0.13921500	-1.68990700
H	-4.04885900	-1.30116000	-3.16045800
H	-5.06222600	1.62732500	-0.19636400
H	-1.62025000	-0.88588600	-2.70644800
H	-5.75053700	-0.04161700	-1.85646400
C	-2.51552500	2.42613400	0.49921300
C	-3.61364100	2.83787900	1.48022200
C	-2.01992300	3.66325500	-0.26773700
H	-1.68735700	2.04279500	1.10818100
H	-4.04529000	1.97652600	1.99659200
H	-3.18669700	3.50327800	2.23443100
H	-4.42066700	3.38093200	0.97670800
H	-1.20047200	3.42344300	-0.94934800
H	-2.83761400	4.08882600	-0.85903300
H	-1.67183900	4.42457200	0.43585000
C	-2.63568400	-1.72181100	1.21302200
C	-1.38395500	-1.50004500	0.80448100
Br	-0.61284000	-2.72357000	-0.47857300
C	-0.44609800	-0.42112700	1.21805100
O	0.60761200	-0.87236400	2.03645600
H	-0.88391400	0.39541100	2.01090100
C	-3.46007800	-2.87302000	0.69646500
H	-2.98173600	-3.83046700	0.92393000
H	-4.45873300	-2.86426100	1.13735900
H	-3.55553600	-2.81076600	-0.39256400
C	-3.31688900	-0.82058900	2.20753800
H	-3.66570400	-1.41841100	3.05700400
H	-2.67613100	-0.02277600	2.58650300
H	-4.20474900	-0.37771900	1.74007300
O	-0.44116200	1.08032900	3.20156700

H	-0.98579300	0.90485400	3.97704600
H	0.43199400	-0.23608800	2.81541600

si-TS2^D

C	4.88125700	0.05385100	-0.08818000
C	3.62947800	-0.53680600	0.05416300
C	3.26105500	-1.65821600	-0.68236600
C	4.17624900	-2.17328000	-1.59659200
C	5.43063700	-1.57769100	-1.75841500
C	5.79515000	-0.46649800	-1.00202500
C	5.05100400	1.21849400	0.85280000
C	3.65731900	1.44130200	1.49233800
C	2.78390700	0.19696800	1.07091300
H	2.29191100	-2.11952900	-0.50182500
H	3.91782900	-3.04791500	-2.18476600
H	6.13141000	-1.98989200	-2.47767000
H	6.77464600	-0.01338400	-1.12431500
H	5.38188300	2.13565500	0.35391500
H	3.72115200	1.48677400	2.57976500
H	5.79304900	0.99319000	1.62527200
H	2.54374000	-0.44109500	1.92017500
N	1.51577300	0.63530000	0.48092000
O	3.09412500	2.69149800	1.12707900
C	0.31203300	-0.00669000	0.37896500
C	1.41899300	1.80177800	-0.22798300
N	-0.43173200	0.81057600	-0.41543700
N	0.25739700	1.95410300	-0.77170500
C	2.59176000	2.72164800	-0.19427400
H	3.35132100	2.40730200	-0.92493100
H	2.28070400	3.74155500	-0.41982400
C	-1.60521700	0.46825600	-1.16447200
C	-1.53874300	-0.66702100	-1.96781700
C	-2.75159600	1.26684700	-1.09328100
C	-2.63941500	-1.04001400	-2.72781500
C	-3.83397500	0.88233200	-1.89006800
C	-3.78870600	-0.25404600	-2.69102600
H	-2.59456800	-1.92813000	-3.34967100
H	-4.74087100	1.47829800	-1.86814500
H	-0.62185700	-1.25006600	-1.98139200
H	-4.65368200	-0.52698900	-3.28685700
C	-2.82553500	2.49222700	-0.20267300
C	-4.17930800	2.61305000	0.50426100
C	-2.52791100	3.76282400	-1.01020600
H	-2.05494100	2.37778500	0.56801500

H	-4.45252000	1.67651000	0.99670300
H	-4.13339200	3.40423800	1.25782100
H	-4.97612700	2.87830300	-0.19791300
H	-1.54341300	3.70704000	-1.47843700
H	-3.28125600	3.89486600	-1.79452400
H	-2.55914200	4.64219200	-0.35948000
C	-1.89640900	-2.81470400	0.42666700
C	-1.45131700	-1.67900000	0.97151300
Br	-2.68165400	-0.45401900	1.82842000
C	-0.05811200	-1.19404400	1.07629600
O	1.01046700	-2.13140600	1.38620900
H	0.40836600	-1.23998600	2.15649500
C	-3.32732000	-3.26234500	0.40316000
H	-3.68879800	-3.24404900	-0.63303000
H	-3.40879200	-4.29634600	0.75464000
H	-3.97650900	-2.62678900	1.00365600
C	-0.92839200	-3.70218500	-0.31256900
H	0.10733300	-3.44169800	-0.08543500
H	-1.09702700	-4.74988000	-0.04134700
H	-1.11067100	-3.62010600	-1.39219400

si-M2

C	-4.56974000	0.48198400	-0.69230800
C	-3.38057000	0.71223700	-0.00469400
C	-2.75346300	1.95647600	-0.04565400
C	-3.33950800	2.97050600	-0.79918400
C	-4.53275900	2.74418100	-1.48964800
C	-5.15646500	1.50048600	-1.43910100
C	-5.06044000	-0.92877700	-0.48842800
C	-3.93051700	-1.65436200	0.28452000
C	-2.91620600	-0.53214700	0.72101100
H	-1.82698500	2.13682500	0.49424100
H	-2.86652200	3.94595700	-0.84960500
H	-4.97661800	3.54585400	-2.07145100
H	-6.08411900	1.32645700	-1.97673900
H	-5.26600900	-1.45162100	-1.42872300
H	-4.31898800	-2.15517800	1.17186100
H	-5.98918900	-0.94207100	0.09081600
H	-2.94148500	-0.39447400	1.80057800
N	-1.55204600	-0.90527000	0.35459100
O	-3.34039600	-2.70111300	-0.46915500
C	-0.35282100	-0.31199100	0.74678200
C	-1.30044600	-1.58554000	-0.81172500
N	0.57368500	-0.77876700	-0.19564700

N	-0.06959500	-1.56138600	-1.17063300
C	-2.46182800	-2.24671500	-1.47755500
H	-2.95954700	-1.53485100	-2.15359600
H	-2.13156200	-3.10887400	-2.05716600
C	1.71807900	-0.05443400	-0.65717000
C	1.65034000	1.33628500	-0.74533800
C	2.87602100	-0.74962600	-1.03772400
C	2.75254500	2.06799900	-1.16301300
C	3.96028100	0.01111400	-1.49030900
C	3.91377900	1.39989600	-1.54431300
H	2.69637700	3.15102000	-1.20045800
H	4.86672800	-0.50114000	-1.80014600
H	0.73526200	1.84008200	-0.45073700
H	4.78068000	1.95784400	-1.88353800
C	2.95960200	-2.26549000	-1.00938900
C	4.28278300	-2.77005900	-0.42146200
C	2.75424600	-2.83541700	-2.41945700
H	2.14080600	-2.62866100	-0.37900900
H	4.50091800	-2.31164000	0.54778000
H	4.23973500	-3.85455000	-0.28631800
H	5.12380400	-2.55906800	-1.08931300
H	1.78917100	-2.52380700	-2.82267600
H	3.54618800	-2.48323100	-3.08975800
H	2.79020500	-3.92922200	-2.39742800
C	2.30000800	0.45589000	2.38845200
C	1.11522500	1.04353700	2.19415900
Br	0.97597500	3.01332300	2.15919300
C	-0.15397700	0.44994600	1.86305400
O	-1.26380100	0.80724500	2.62376900
C	3.62455900	1.15714500	2.39731500
H	3.52206500	2.24096600	2.36657300
H	4.20609700	0.87252300	3.27990900
H	4.19189800	0.83820300	1.51243500
C	2.36032000	-1.04484000	2.50188800
H	3.07901900	-1.33228300	3.27593600
H	1.38477000	-1.47383500	2.73515100
H	2.70520400	-1.47788300	1.55608900
H	-1.19187800	1.75910500	2.80002900
TS3			
C	4.66096100	-0.37540400	0.05432300
C	3.39263200	0.17007000	-0.12680700
C	3.00113900	1.33933400	0.51901800
C	3.92148000	1.96598000	1.35586500

C	5.19989500	1.43138000	1.53575000
C	5.57854000	0.25772600	0.88817200
C	4.83017000	-1.64598800	-0.74033800
C	3.42029600	-1.98272700	-1.28442100
C	2.56818100	-0.67833700	-1.06867000
H	2.00393600	1.75823700	0.39460700
H	3.63979300	2.87707300	1.87348800
H	5.90293500	1.93254300	2.19358700
H	6.56950000	-0.16087500	1.03788300
H	5.20648100	-2.48287000	-0.14289600
H	3.44987200	-2.23029600	-2.34585300
H	5.53259200	-1.50169600	-1.56764100
H	2.38749900	-0.17183400	-2.01451700
N	1.26397700	-1.00012500	-0.48346400
O	2.86544300	-3.14002200	-0.67696100
C	0.07808700	-0.31587400	-0.49020100
C	1.14790400	-2.01301700	0.43252600
N	-0.69103600	-0.98628700	0.41008700
N	-0.02172200	-2.04955600	0.97723700
C	2.32288600	-2.91633500	0.60854300
H	3.05856800	-2.46268400	1.28851500
H	2.00462900	-3.87556000	1.01696600
C	-2.01650100	-0.69306500	0.86355900
C	-2.22081200	0.48379700	1.58365700
C	-3.04673900	-1.60094500	0.59706300
C	-3.49116300	0.77689700	2.05812100
C	-4.31195600	-1.28549400	1.10733100
C	-4.53606100	-0.11755800	1.82595700
H	-3.66380800	1.70001600	2.60101400
H	-5.13660100	-1.97014900	0.93310700
H	-1.40407400	1.19212300	1.69577200
H	-5.53054800	0.09869100	2.20338200
C	-2.81828100	-2.88702700	-0.17644300
C	-3.89989100	-3.13204100	-1.23273400
C	-2.72405100	-4.07358200	0.79194900
H	-1.85894000	-2.80074700	-0.69761300
H	-3.99633200	-2.28088400	-1.91224200
H	-3.64537900	-4.01591100	-1.82421300
H	-4.87628900	-3.31603200	-0.77459800
H	-1.92255200	-3.91840600	1.51737900
H	-3.66701400	-4.19422000	1.33615900
H	-2.52784400	-4.99956500	0.24298200
C	-2.64451800	1.73293700	-1.33610800
C	-1.35600700	1.56171400	-1.11361300

Br	-0.38400200	3.39418000	0.14318500
C	-0.24457400	0.78653300	-1.31133000
O	0.81257000	1.33862600	-2.02651500
C	-3.53707800	2.78247600	-0.74427700
H	-3.01553500	3.38322500	-0.00261500
H	-3.90880100	3.43510800	-1.54219700
H	-4.40573800	2.29969600	-0.28389300
C	-3.33463800	0.73681200	-2.24307000
H	-3.87088500	1.26007900	-3.04170100
H	-2.62815400	0.03116100	-2.68235600
H	-4.07370200	0.18013000	-1.65383000
H	0.89441700	2.25072900	-1.68230300

M3

C	4.65702100	-0.62639700	-0.20753900
C	3.41625900	0.00636300	-0.22769700
C	3.18164600	1.18628500	0.47009800
C	4.23725900	1.73419100	1.19571700
C	5.48761800	1.11311400	1.21693100
C	5.70748600	-0.07235100	0.51735700
C	4.63901200	-1.88425000	-1.03985600
C	3.14493300	-2.15154200	-1.32597600
C	2.43882200	-0.76938300	-1.08437300
H	2.20985200	1.67741600	0.47078200
H	4.07792500	2.65478900	1.74742800
H	6.29656700	1.55537100	1.78992700
H	6.67845800	-0.55807400	0.54401800
H	5.08194800	-2.75028200	-0.53915200
H	2.97856900	-2.48886100	-2.34980600
H	5.18161100	-1.73780400	-1.98007200
H	2.21852800	-0.25606200	-2.02046500
N	1.16581500	-0.96897900	-0.38138600
O	2.62263300	-3.20353500	-0.52354700
C	-0.01869200	-0.32917000	-0.44606300
C	1.06664500	-1.90262000	0.61293500
N	-0.76894500	-0.88553800	0.51080900
N	-0.10719600	-1.88371500	1.16877400
C	2.22330700	-2.83184200	0.78321400
H	3.03468100	-2.34815800	1.34264100
H	1.90849300	-3.73308200	1.30895900
C	-2.07142000	-0.47797400	0.96927700
C	-2.15902600	0.75896100	1.60098200
C	-3.15782600	-1.33657400	0.79599300
C	-3.38753000	1.15609600	2.11274200

C	-4.37630300	-0.90680100	1.33176000
C	-4.49132500	0.31477700	1.98835700
H	-3.47852400	2.12159300	2.59845500
H	-5.25041700	-1.54408200	1.23444500
H	-1.29089200	1.41511600	1.63184400
H	-5.45159400	0.61627200	2.39467900
C	-3.03891000	-2.66890300	0.08085800
C	-4.12105400	-2.83511700	-0.99015500
C	-3.07259700	-3.82242300	1.09036200
H	-2.06832400	-2.69638600	-0.42670500
H	-4.10623600	-2.00074500	-1.69693400
H	-3.95711000	-3.76262600	-1.54578500
H	-5.11940000	-2.88941100	-0.54568400
H	-2.26772500	-3.72094300	1.82249100
H	-4.02648900	-3.83226700	1.62813900
H	-2.96157200	-4.78244200	0.57784200
C	-2.85525200	1.34650700	-1.96135700
C	-1.63518200	0.95524000	-1.70680400
Br	0.11653500	3.36537100	0.42836800
C	-0.37693400	0.72076900	-1.39910700
O	0.68732000	1.43497000	-1.87676600
C	-3.46060200	2.43711600	-1.10867200
H	-2.70462800	2.87781200	-0.45408700
H	-3.87053000	3.21397400	-1.76255300
H	-4.28198500	2.03014100	-0.50962400
C	-3.69667600	0.76837900	-3.06783600
H	-3.96671700	1.55781400	-3.77621200
H	-3.17905300	-0.02780500	-3.60410200
H	-4.62880700	0.37285400	-2.65030800
H	0.67322300	2.26933500	-1.31480900

TS3'

C	4.48400700	0.20079400	-0.54018400
C	3.34475700	-0.35398800	0.03890900
C	2.86500600	-1.60134600	-0.36120300
C	3.53143400	-2.26537600	-1.38910200
C	4.66232700	-1.70431000	-1.98693100
C	5.15261500	-0.47328900	-1.55897900
C	4.85238400	1.51504300	0.09741500
C	3.76587500	1.76443300	1.17518500
C	2.75857500	0.55917400	1.09433700
H	2.01097300	-2.05052400	0.13779400
H	3.17407100	-3.23516500	-1.72086700
H	5.17077000	-2.23810700	-2.78389400

H	6.04445600	-0.04752500	-2.01009200
H	4.88206400	2.34135500	-0.62110900
H	4.21163300	1.77285000	2.17042600
H	5.84425100	1.47072600	0.55707600
H	2.64042800	0.03873800	2.04632800
N	1.42821600	1.04785500	0.72433800
O	3.15274700	3.03953300	1.06316900
C	0.25612400	0.29853300	0.65694400
C	1.20617000	2.20303200	0.03345200
N	-0.62899100	1.12841300	-0.04090600
N	0.00922000	2.31233000	-0.43325600
C	2.33436800	3.17502000	-0.07855900
H	2.89420300	2.98894700	-1.00615300
H	1.95400100	4.19662800	-0.10257100
C	-1.74590200	0.69304100	-0.79654900
C	-1.65086000	-0.51210800	-1.49375600
C	-2.92117400	1.46591800	-0.83182300
C	-2.73448000	-0.99127700	-2.21889800
C	-3.98152300	0.97697000	-1.59757400
C	-3.90295000	-0.23806200	-2.27756700
H	-2.65519200	-1.94043100	-2.73899900
H	-4.89908400	1.55572300	-1.65430000
H	-0.72140600	-1.06993500	-1.44752200
H	-4.75473200	-0.59079800	-2.85019900
C	-3.04472600	2.78383900	-0.09036300
C	-4.36466300	2.88984800	0.68084900
C	-2.88380100	3.95846900	-1.06373600
H	-2.22234100	2.83844100	0.63057500
H	-4.36586500	3.79417300	1.29567000
H	-5.22234600	2.95384900	0.00424700
H	-4.51764500	2.02773300	1.33803900
H	-1.91450100	3.90792800	-1.56406500
H	-3.67344700	3.93584300	-1.82275500
H	-2.95372500	4.91025500	-0.52823500
C	-2.38520300	-1.22783400	1.53290400
C	-1.11137300	-1.76862500	1.24080000
Br	-0.98281200	-3.33442800	0.07351300
C	0.08775600	-0.91968400	1.27377100
O	0.94237600	-1.45488700	2.15250100
C	-3.67159900	-1.73116500	0.99295500
H	-4.14980900	-0.93560400	0.40132200
H	-3.54458200	-2.60895200	0.36199200
H	-4.35393600	-1.95547200	1.82196600
C	-2.43030100	-0.05052500	2.44355500

H	-3.36457100	-0.02382500	3.01115200
H	-1.56248200	-0.03325600	3.10924400
H	-2.37448500	0.87522700	1.84508000
H	-0.43547100	-2.15034600	2.21521700

M3'

C	4.38623700	0.88820300	0.43482200
C	3.29452200	0.13556900	-0.00316800
C	3.44047600	-0.84629600	-0.97450900
C	4.71447600	-1.08579500	-1.48961500
C	5.81249700	-0.35408900	-1.03808800
C	5.65533700	0.64120300	-0.07339200
C	3.94381400	1.92850300	1.43692400
C	2.43517900	2.04293300	1.17320700
C	2.04013400	0.61042600	0.70683700
H	2.58291000	-1.41155100	-1.32117700
H	4.85040600	-1.84540600	-2.25233600
H	6.79625300	-0.55029200	-1.45252400
H	6.50749800	1.22624300	0.25946600
H	4.43163400	2.89799100	1.31380900
H	1.85338200	2.33125100	2.05043200
H	4.12111600	1.58564400	2.46331600
H	1.76010100	0.00221700	1.57195000
N	0.86521400	0.70163200	-0.14353100
O	2.17680900	3.04581000	0.18516600
C	-0.34911700	0.13297000	-0.00893900
C	0.77215100	1.68360300	-1.08424600
N	-1.11041300	0.76175000	-0.91179200
N	-0.42343900	1.73724100	-1.59259100
C	1.91831300	2.63878700	-1.15155100
H	2.79446000	2.17812400	-1.62209600
H	1.63027000	3.52986400	-1.70897100
C	-2.50360300	0.55838100	-1.21048700
C	-2.79461700	-0.00752300	-2.44587800
C	-3.48794500	0.92730300	-0.28376200
C	-4.11564600	-0.26851400	-2.78421200
C	-4.80679800	0.63729700	-0.65245100
C	-5.11966900	0.04424300	-1.87257000
H	-4.35411400	-0.72028100	-3.74056500
H	-5.61106800	0.88666100	0.03045800
H	-1.97860400	-0.25655000	-3.11684300
H	-6.15675000	-0.16516100	-2.11444000
C	-3.14958800	1.66503600	1.00041500
C	-4.28685100	1.65462700	2.02137600

C	-2.76213100	3.11539700	0.66703200
H	-2.28499400	1.18429600	1.47678000
H	-3.93013100	2.08687000	2.95936300
H	-5.14204000	2.25221200	1.68596300
H	-4.63672700	0.63979600	2.23186400
H	-1.91482500	3.16448700	-0.02232900
H	-3.60514900	3.63949900	0.20349000
H	-2.48701600	3.64709000	1.58229800
C	-1.69271700	-1.83755600	1.15883600
C	-0.21696300	-2.09168100	1.35251900
Br	0.78060100	-3.01532000	-0.02010400
C	-0.70520000	-0.65494000	1.22488200
O	-0.60039000	0.16707500	2.24793900
C	-2.32407600	-2.34496300	-0.11957900
H	-3.31471600	-1.90420000	-0.26585200
H	-1.71573000	-2.13182500	-1.00116100
H	-2.43309000	-3.43426000	-0.05620900
C	-2.56424000	-1.98331500	2.38554400
H	-2.70088700	-3.03632200	2.65286200
H	-2.11735700	-1.44067300	3.22102900
H	-3.55186600	-1.55121900	2.18786000
H	0.15125700	-2.35460500	2.33807700

TS4'

C	-4.57949400	-0.06770400	-0.68456400
C	-3.60286900	0.62294700	0.03384200
C	-3.36016700	1.97509900	-0.18746700
C	-4.12437900	2.63328700	-1.14904200
C	-5.10982700	1.95062800	-1.86467000
C	-5.34538800	0.59625700	-1.63704300
C	-4.62581200	-1.52176500	-0.29458500
C	-3.81315600	-1.56127800	1.01869600
C	-2.90281400	-0.29609700	1.01128900
H	-2.59563900	2.49020500	0.38634200
H	-3.95593100	3.68836600	-1.33851600
H	-5.70000300	2.48103500	-2.60536200
H	-6.11390600	0.06839700	-2.19396100
H	-4.16567400	-2.14030800	-1.07336000
H	-4.49811500	-1.45468900	1.86244800
H	-5.63951000	-1.90082800	-0.14491300
H	-2.78513500	0.14800600	2.00295900
N	-1.56382100	-0.67400000	0.54692900
O	-3.11635400	-2.76596100	1.26877800
C	-0.44111100	0.13071500	0.49560700

C	-1.16518100	-1.91772800	0.20923900
N	0.56214200	-0.67406100	-0.01927000
N	0.08542500	-1.97183800	-0.16573900
C	-2.11529300	-3.06825600	0.32125600
H	-2.53583600	-3.31237400	-0.66227600
H	-1.57403800	-3.94273500	0.68537800
C	1.47678400	-0.23444300	-1.05671400
C	1.10975900	0.89143800	-1.79038900
C	2.65879500	-0.94087100	-1.33166600
C	1.94194500	1.37464800	-2.78962600
C	3.46904700	-0.42950000	-2.34916200
C	3.13241900	0.71444500	-3.06556100
H	1.65834800	2.26384600	-3.34176900
H	4.39323000	-0.94627400	-2.58809100
H	0.17917600	1.39769100	-1.55582600
H	3.79737600	1.08099500	-3.84059000
C	3.05092600	-2.23696400	-0.64188200
C	4.55951600	-2.35049400	-0.38676400
C	2.59184400	-3.43812800	-1.48336700
H	2.53181900	-2.27837900	0.32045800
H	4.75505000	-3.18548100	0.29261200
H	5.10279700	-2.55792500	-1.31376700
H	4.97810300	-1.44263900	0.05263400
H	1.51329200	-3.41729100	-1.64057300
H	3.09163100	-3.42040900	-2.45795600
H	2.85867300	-4.37451600	-0.98288000
C	1.90638700	-0.10750400	1.94727500
C	1.26461500	1.18968100	1.87420100
Br	2.45764800	2.60550100	0.64166000
C	-0.17002600	1.19848300	1.42906100
O	-0.99756000	2.00714900	1.85301600
C	3.39552900	-0.16775800	1.97177700
H	3.78937800	0.20953900	1.02017500
H	3.80785800	0.49190900	2.74859400
H	3.75251100	-1.18470300	2.15073300
C	1.18027900	-1.24926700	2.59151100
H	1.40356100	-1.24626100	3.66790100
H	0.09308400	-1.17619200	2.51006200
H	1.51014600	-2.21801700	2.19529600
H	1.36121000	1.85707900	2.73084200
M4'			
C	4.57996100	-0.24052500	-0.06110600
C	3.41356300	0.51210700	0.04940300

C	3.25879300	1.48119700	1.03617500
C	4.30631100	1.68312500	1.92972900
C	5.48002400	0.93219400	1.82712100
C	5.62757000	-0.03079500	0.83185900
C	4.50303200	-1.20814400	-1.21403200
C	3.02281000	-1.19685400	-1.65324400
C	2.41476500	0.11003900	-1.01323500
H	2.34856800	2.06922500	1.09789900
H	4.21175000	2.43103000	2.70953300
H	6.28609000	1.10103600	2.53341800
H	6.54151300	-0.61185700	0.75813100
H	4.80411500	-2.22697600	-0.95317100
H	2.91549500	-1.16861900	-2.73747700
H	5.14388300	-0.88302400	-2.03965900
H	2.25102300	0.89021400	-1.75931700
N	1.10976600	-0.20264200	-0.40513600
O	2.33222100	-2.37569500	-1.26559300
C	-0.01128600	0.51772200	-0.27186400
C	0.90597100	-1.38129400	0.25627800
N	-0.83375700	-0.21674300	0.47960100
N	-0.27238400	-1.40943100	0.81271100
C	1.95596600	-2.43358300	0.09699400
H	2.79999500	-2.25531400	0.77582200
H	1.53426900	-3.41908700	0.29234800
C	-2.10192900	0.19397500	1.02678400
C	-2.12307500	1.43596700	1.66120300
C	-3.23044300	-0.62687100	0.91491500
C	-3.31317600	1.90984000	2.19114200
C	-4.40871600	-0.11892800	1.47477800
C	-4.45889700	1.12388400	2.09499600
H	-3.34071300	2.87355300	2.68629100
H	-5.31182900	-0.71788700	1.42247900
H	-1.20701400	2.01341200	1.75064100
H	-5.39548800	1.47716900	2.51269600
C	-3.21661700	-2.00818900	0.28245400
C	-4.45759400	-2.27117800	-0.57915800
C	-3.08850300	-3.08078200	1.37337800
H	-2.33568300	-2.08356900	-0.36362500
H	-4.32395800	-3.20096800	-1.13757100
H	-5.35377600	-2.38984200	0.03616300
H	-4.64819000	-1.46445400	-1.29383900
H	-2.17688000	-2.94041800	1.95730500
H	-3.94712500	-3.03455900	2.05062400
H	-3.06565900	-4.07575400	0.92008100

C	-2.28100300	1.50789900	-2.16849800
C	-1.45553100	2.30230500	-1.45858400
C	-0.20038100	1.92186500	-0.81791100
O	0.72950500	2.67942300	-0.62238100
C	-3.56000200	2.06647400	-2.71622900
H	-4.40036300	1.45814200	-2.36199800
H	-3.72136000	3.10136300	-2.41424200
H	-3.56430800	2.00689800	-3.80918200
C	-2.03961200	0.06572500	-2.51279500
H	-2.26042700	-0.08742600	-3.57318000
H	-1.02255600	-0.28588100	-2.33604400
H	-2.73653400	-0.56880400	-1.95508400
H	-1.67602900	3.36121700	-1.35880000

TS4

C	4.21856500	0.56682800	0.27987900
C	3.16095400	0.95972200	-0.54896100
C	2.70779300	2.27710300	-0.55787200
C	3.29979100	3.18678900	0.31710300
C	4.32865000	2.78835800	1.17093500
C	4.80450600	1.47806500	1.15007500
C	4.58407600	-0.87712200	0.04788000
C	3.93602700	-1.15124400	-1.32705600
C	2.69798700	-0.22033200	-1.37615000
H	1.91288200	2.58783100	-1.22534800
H	2.95855700	4.21629100	0.32741900
H	4.77696400	3.51109500	1.84489600
H	5.62655600	1.17845500	1.79274400
H	4.15656600	-1.51210900	0.83325400
H	4.61491500	-0.81707200	-2.11428100
H	5.66068200	-1.05796200	0.03361000
H	2.35708700	0.02141100	-2.38227400
N	1.59324400	-0.96583200	-0.70461900
O	3.63910000	-2.49572100	-1.63268900
C	0.41526200	-0.49320200	-0.26050000
C	1.65159400	-2.28186000	-0.33578000
N	-0.17999200	-1.50721800	0.35900700
N	0.58030500	-2.63477500	0.31926800
C	2.82399000	-3.14658400	-0.68761300
H	3.37523200	-3.41309000	0.22249100
H	2.46380800	-4.06763200	-1.14901400
C	-1.44307600	-1.52814100	1.06342300
C	-1.34717800	-1.74270000	2.43330200
C	-2.65727100	-1.34163400	0.38877000

C	-2.50443900	-1.75772500	3.20104800
C	-3.79637700	-1.34442200	1.20007700
C	-3.72860500	-1.54552800	2.57613000
H	-2.44600900	-1.92267800	4.27102100
H	-4.76464300	-1.18293000	0.74339400
H	-0.36894600	-1.89061800	2.87945200
H	-4.64265600	-1.53771200	3.16026000
C	-2.74889100	-1.17622600	-1.12313900
C	-4.16741100	-0.87650700	-1.60941900
C	-2.22458600	-2.42929000	-1.84394200
H	-2.13306000	-0.31602200	-1.41503800
H	-4.59846200	-0.00966100	-1.10583600
H	-4.13932900	-0.65380200	-2.67870900
H	-4.82134800	-1.74312000	-1.46121700
H	-1.18973900	-2.67500500	-1.59328500
H	-2.84254100	-3.29385500	-1.58217200
H	-2.28402200	-2.28349700	-2.92549000
C	-0.70267400	1.63165600	1.73583700
C	-0.95402000	1.50249700	0.42216600
C	-0.11612800	0.89989600	-0.55040100
O	0.09433100	1.26652200	-1.71168700
C	0.64029900	1.41675800	2.38805700
H	1.04053700	2.36791200	2.75865400
H	0.53468700	0.75917100	3.25946000
H	1.38742000	0.99921300	1.70580000
C	-1.80113400	2.05058200	2.67545000
H	-1.53097700	2.96567500	3.21510700
H	-2.73695100	2.21233500	2.13856700
H	-1.95456200	1.26883900	3.42989800
H	-1.70293000	2.14589000	-2.00485600
H	-2.19730400	1.81648000	-0.04552600
C	-3.61865200	2.24242800	-1.61153300
O	-4.72222600	2.42232100	-2.08838900
O	-2.55174300	2.21356700	-2.46895300
O	-3.36216700	2.03730600	-0.35518100

Z-TS4

C	-4.39517800	-0.48507400	0.25360500
C	-3.11126300	-0.09756500	0.62106500
C	-2.71681700	1.23550700	0.60770500
C	-3.63292900	2.19862100	0.19795800
C	-4.92562400	1.81670100	-0.17373200
C	-5.31808700	0.48051400	-0.14228800
C	-4.57304300	-1.97751700	0.36209600

C	-3.16478100	-2.54132900	0.67707800
C	-2.25616700	-1.28857100	0.97991000
H	-1.71290200	1.52722100	0.90054700
H	-3.32608100	3.23839300	0.15140200
H	-5.63250900	2.57397100	-0.49713300
H	-6.32467900	0.19547200	-0.43345400
H	-4.96037700	-2.43356200	-0.55519500
H	-3.18105800	-3.19176000	1.55128600
H	-5.27188100	-2.23645200	1.16331800
H	-1.90266100	-1.27250800	2.01170600
N	-1.05169100	-1.31941900	0.13218600
O	-2.66235100	-3.37113800	-0.35907500
C	0.12166000	-0.68996800	0.28816600
C	-1.04122500	-1.88159900	-1.11283700
N	0.80376700	-0.92073600	-0.83015100
N	0.09240700	-1.66869800	-1.71910600
C	-2.24229500	-2.67253100	-1.51348200
H	-3.02497300	-2.00484000	-1.90046600
H	-1.98196900	-3.40203000	-2.28010700
C	2.14058300	-0.47271300	-1.13177500
C	2.25860800	0.53236400	-2.08186000
C	3.22792300	-1.02243700	-0.43935300
C	3.52177700	1.03662100	-2.36782100
C	4.47933500	-0.48467400	-0.74822500
C	4.62715800	0.52891700	-1.69349200
H	3.63451800	1.82943200	-3.09841600
H	5.35997500	-0.86204000	-0.24033900
H	1.36296600	0.94182100	-2.53583200
H	5.61689000	0.92326800	-1.90043700
C	3.05467200	-2.17001000	0.54548500
C	4.27815900	-2.40583500	1.43062900
C	2.70761600	-3.46357600	-0.20954300
H	2.21737000	-1.92763800	1.21375300
H	4.58323100	-1.49953300	1.95994100
H	4.04565000	-3.17193900	2.17429800
H	5.12777900	-2.76670500	0.84209700
H	1.81525700	-3.35716400	-0.83112200
H	3.53915000	-3.74226000	-0.86430600
H	2.54014300	-4.28020800	0.49819400
C	2.36004400	1.83613400	1.54012600
C	1.17738900	1.37088000	1.10693900
C	0.55051700	0.14648400	1.49836400
O	0.14940900	-0.26239700	2.58251500
C	2.89610500	3.15546500	1.04975000

H	3. 15371800	3. 81036500	1. 88984200
H	3. 81745600	2. 99234300	0. 47724200
H	2. 17821200	3. 66783600	0. 40546900
C	3. 28552500	1. 07514100	2. 45326800
H	3. 52867600	1. 67702900	3. 33632700
H	2. 84677100	0. 13270400	2. 78978800
H	4. 23314100	0. 86936200	1. 93967500
H	-0. 13794100	3. 23830200	1. 03341200
H	0. 57092800	1. 93150800	-0. 08655200
C	-0. 73129700	3. 35437100	-0. 79926700
O	-1. 44551900	3. 91215000	-1. 60015600
O	-0. 74402300	3. 78184700	0. 50194500
O	0. 06544100	2. 34899600	-1. 04851200

M4

C	-4. 39517800	-0. 48507400	0. 25360500
C	-3. 11126300	-0. 09756500	0. 62106500
C	-2. 71681700	1. 23550700	0. 60770500
C	-3. 63292900	2. 19862100	0. 19795800
C	-4. 92562400	1. 81670100	-0. 17373200
C	-5. 31808700	0. 48051400	-0. 14228800
C	-4. 57304300	-1. 97751700	0. 36209600
C	-3. 16478100	-2. 54132900	0. 67707800
C	-2. 25616700	-1. 28857100	0. 97991000
H	-1. 71290200	1. 52722100	0. 90054700
H	-3. 32608100	3. 23839300	0. 15140200
H	-5. 63250900	2. 57397100	-0. 49713300
H	-6. 32467900	0. 19547200	-0. 43345400
H	-4. 96037700	-2. 43356200	-0. 55519500
H	-3. 18105800	-3. 19176000	1. 55128600
H	-5. 27188100	-2. 23645200	1. 16331800
H	-1. 90266100	-1. 27250800	2. 01170600
N	-1. 05169100	-1. 31941900	0. 13218600
O	-2. 66235100	-3. 37113800	-0. 35907500
C	0. 12166000	-0. 68996800	0. 28816600
C	-1. 04122500	-1. 88159900	-1. 11283700
N	0. 80376700	-0. 92073600	-0. 83015100
N	0. 09240700	-1. 66869800	-1. 71910600
C	-2. 24229500	-2. 67253100	-1. 51348200
H	-3. 02497300	-2. 00484000	-1. 90046600
H	-1. 98196900	-3. 40203000	-2. 28010700
C	2. 14058300	-0. 47271300	-1. 13177500
C	2. 25860800	0. 53236400	-2. 08186000
C	3. 22792300	-1. 02243700	-0. 43935300

C	3. 52177700	1. 03662100	-2. 36782100
C	4. 47933500	-0. 48467400	-0. 74822500
C	4. 62715800	0. 52891700	-1. 69349200
H	3. 63451800	1. 82943200	-3. 09841600
H	5. 35997500	-0. 86204000	-0. 24033900
H	1. 36296600	0. 94182100	-2. 53583200
H	5. 61689000	0. 92326800	-1. 90043700
C	3. 05467200	-2. 17001000	0. 54548500
C	4. 27815900	-2. 40583500	1. 43062900
C	2. 70761600	-3. 46357600	-0. 20954300
H	2. 21737000	-1. 92763800	1. 21375300
H	4. 58323100	-1. 49953300	1. 95994100
H	4. 04565000	-3. 17193900	2. 17429800
H	5. 12777900	-2. 76670500	0. 84209700
H	1. 81525700	-3. 35716400	-0. 83112200
H	3. 53915000	-3. 74226000	-0. 86430600
H	2. 54014300	-4. 28020800	0. 49819400
C	2. 36004400	1. 83613400	1. 54012600
C	1. 17738900	1. 37088000	1. 10693900
C	0. 55051700	0. 14648400	1. 49836400
O	0. 14940900	-0. 26239700	2. 58251500
C	2. 89610500	3. 15546500	1. 04975000
H	3. 15371800	3. 81036500	1. 88984200
H	3. 81745600	2. 99234300	0. 47724200
H	2. 17821200	3. 66783600	0. 40546900
C	3. 28552500	1. 07514100	2. 45326800
H	3. 52867600	1. 67702900	3. 33632700
H	2. 84677100	0. 13270400	2. 78978800
H	4. 23314100	0. 86936200	1. 93967500
H	-0. 13794100	3. 23830200	1. 03341200
H	0. 57092800	1. 93150800	-0. 08655200
C	-0. 73129700	3. 35437100	-0. 79926700
O	-1. 44551900	3. 91215000	-1. 60015600
O	-0. 74402300	3. 78184700	0. 50194500
O	0. 06544100	2. 34899600	-1. 04851200

Z-M4

C	-4. 39517800	-0. 48507400	0. 25360500
C	-3. 11126300	-0. 09756500	0. 62106500
C	-2. 71681700	1. 23550700	0. 60770500
C	-3. 63292900	2. 19862100	0. 19795800
C	-4. 92562400	1. 81670100	-0. 17373200
C	-5. 31808700	0. 48051400	-0. 14228800
C	-4. 57304300	-1. 97751700	0. 36209600

C	-3.16478100	-2.54132900	0.67707800
C	-2.25616700	-1.28857100	0.97991000
H	-1.71290200	1.52722100	0.90054700
H	-3.32608100	3.23839300	0.15140200
H	-5.63250900	2.57397100	-0.49713300
H	-6.32467900	0.19547200	-0.43345400
H	-4.96037700	-2.43356200	-0.55519500
H	-3.18105800	-3.19176000	1.55128600
H	-5.27188100	-2.23645200	1.16331800
H	-1.90266100	-1.27250800	2.01170600
N	-1.05169100	-1.31941900	0.13218600
O	-2.66235100	-3.37113800	-0.35907500
C	0.12166000	-0.68996800	0.28816600
C	-1.04122500	-1.88159900	-1.11283700
N	0.80376700	-0.92073600	-0.83015100
N	0.09240700	-1.66869800	-1.71910600
C	-2.24229500	-2.67253100	-1.51348200
H	-3.02497300	-2.00484000	-1.90046600
H	-1.98196900	-3.40203000	-2.28010700
C	2.14058300	-0.47271300	-1.13177500
C	2.25860800	0.53236400	-2.08186000
C	3.22792300	-1.02243700	-0.43935300
C	3.52177700	1.03662100	-2.36782100
C	4.47933500	-0.48467400	-0.74822500
C	4.62715800	0.52891700	-1.69349200
H	3.63451800	1.82943200	-3.09841600
H	5.35997500	-0.86204000	-0.24033900
H	1.36296600	0.94182100	-2.53583200
H	5.61689000	0.92326800	-1.90043700
C	3.05467200	-2.17001000	0.54548500
C	4.27815900	-2.40583500	1.43062900
C	2.70761600	-3.46357600	-0.20954300
H	2.21737000	-1.92763800	1.21375300
H	4.58323100	-1.49953300	1.95994100
H	4.04565000	-3.17193900	2.17429800
H	5.12777900	-2.76670500	0.84209700
H	1.81525700	-3.35716400	-0.83112200
H	3.53915000	-3.74226000	-0.86430600
H	2.54014300	-4.28020800	0.49819400
C	2.36004400	1.83613400	1.54012600
C	1.17738900	1.37088000	1.10693900
C	0.55051700	0.14648400	1.49836400
O	0.14940900	-0.26239700	2.58251500
C	2.89610500	3.15546500	1.04975000

H	3. 15371800	3. 81036500	1. 88984200
H	3. 81745600	2. 99234300	0. 47724200
H	2. 17821200	3. 66783600	0. 40546900
C	3. 28552500	1. 07514100	2. 45326800
H	3. 52867600	1. 67702900	3. 33632700
H	2. 84677100	0. 13270400	2. 78978800
H	4. 23314100	0. 86936200	1. 93967500
H	-0. 13794100	3. 23830200	1. 03341200
H	0. 57092800	1. 93150800	-0. 08655200
C	-0. 73129700	3. 35437100	-0. 79926700
O	-1. 44551900	3. 91215000	-1. 60015600
O	-0. 74402300	3. 78184700	0. 50194500
O	0. 06544100	2. 34899600	-1. 04851200

TS5

C	-4. 39517800	-0. 48507400	0. 25360500
C	-3. 11126300	-0. 09756500	0. 62106500
C	-2. 71681700	1. 23550700	0. 60770500
C	-3. 63292900	2. 19862100	0. 19795800
C	-4. 92562400	1. 81670100	-0. 17373200
C	-5. 31808700	0. 48051400	-0. 14228800
C	-4. 57304300	-1. 97751700	0. 36209600
C	-3. 16478100	-2. 54132900	0. 67707800
C	-2. 25616700	-1. 28857100	0. 97991000
H	-1. 71290200	1. 52722100	0. 90054700
H	-3. 32608100	3. 23839300	0. 15140200
H	-5. 63250900	2. 57397100	-0. 49713300
H	-6. 32467900	0. 19547200	-0. 43345400
H	-4. 96037700	-2. 43356200	-0. 55519500
H	-3. 18105800	-3. 19176000	1. 55128600
H	-5. 27188100	-2. 23645200	1. 16331800
H	-1. 90266100	-1. 27250800	2. 01170600
N	-1. 05169100	-1. 31941900	0. 13218600
O	-2. 66235100	-3. 37113800	-0. 35907500
C	0. 12166000	-0. 68996800	0. 28816600
C	-1. 04122500	-1. 88159900	-1. 11283700
N	0. 80376700	-0. 92073600	-0. 83015100
N	0. 09240700	-1. 66869800	-1. 71910600
C	-2. 24229500	-2. 67253100	-1. 51348200
H	-3. 02497300	-2. 00484000	-1. 90046600
H	-1. 98196900	-3. 40203000	-2. 28010700
C	2. 14058300	-0. 47271300	-1. 13177500
C	2. 25860800	0. 53236400	-2. 08186000
C	3. 22792300	-1. 02243700	-0. 43935300

C	3. 52177700	1. 03662100	-2. 36782100
C	4. 47933500	-0. 48467400	-0. 74822500
C	4. 62715800	0. 52891700	-1. 69349200
H	3. 63451800	1. 82943200	-3. 09841600
H	5. 35997500	-0. 86204000	-0. 24033900
H	1. 36296600	0. 94182100	-2. 53583200
H	5. 61689000	0. 92326800	-1. 90043700
C	3. 05467200	-2. 17001000	0. 54548500
C	4. 27815900	-2. 40583500	1. 43062900
C	2. 70761600	-3. 46357600	-0. 20954300
H	2. 21737000	-1. 92763800	1. 21375300
H	4. 58323100	-1. 49953300	1. 95994100
H	4. 04565000	-3. 17193900	2. 17429800
H	5. 12777900	-2. 76670500	0. 84209700
H	1. 81525700	-3. 35716400	-0. 83112200
H	3. 53915000	-3. 74226000	-0. 86430600
H	2. 54014300	-4. 28020800	0. 49819400
C	2. 36004400	1. 83613400	1. 54012600
C	1. 17738900	1. 37088000	1. 10693900
C	0. 55051700	0. 14648400	1. 49836400
O	0. 14940900	-0. 26239700	2. 58251500
C	2. 89610500	3. 15546500	1. 04975000
H	3. 15371800	3. 81036500	1. 88984200
H	3. 81745600	2. 99234300	0. 47724200
H	2. 17821200	3. 66783600	0. 40546900
C	3. 28552500	1. 07514100	2. 45326800
H	3. 52867600	1. 67702900	3. 33632700
H	2. 84677100	0. 13270400	2. 78978800
H	4. 23314100	0. 86936200	1. 93967500
H	-0. 13794100	3. 23830200	1. 03341200
H	0. 57092800	1. 93150800	-0. 08655200
C	-0. 73129700	3. 35437100	-0. 79926700
O	-1. 44551900	3. 91215000	-1. 60015600
O	-0. 74402300	3. 78184700	0. 50194500
O	0. 06544100	2. 34899600	-1. 04851200

Z-TS5

C	-3. 62115700	2. 04015400	0. 18096700
C	-2. 61882100	1. 10479200	-0. 06071700
C	-2. 67315400	-0. 18045600	0. 47347000
C	-3. 76071100	-0. 51769800	1. 27532900
C	-4. 76860500	0. 41810400	1. 52532500
C	-4. 70943500	1. 69826200	0. 98022600
C	-3. 35526300	3. 34353800	-0. 52586600

C	-1.98361700	3.16466300	-1.22201700
C	-1.54118400	1.67606800	-0.95008200
H	-1.90445700	-0.92736900	0.28536500
H	-3.81445300	-1.52215600	1.68142600
H	-5.61333000	0.14053100	2.14794700
H	-5.49925600	2.41864300	1.17256400
H	-3.32288400	4.20046200	0.15614000
H	-2.06732500	3.30950600	-2.29895800
H	-4.13039900	3.56318000	-1.26575600
H	-1.40508800	1.11095600	-1.87223300
N	-0.22980000	1.65220500	-0.27158800
O	-1.02785700	4.13422900	-0.81959900
C	0.64820200	0.64402000	-0.15650100
C	0.23908300	2.68391700	0.48876100
N	1.61833000	1.10586400	0.63174100
N	1.37847700	2.38468200	1.04456800
C	-0.54597100	3.95323800	0.49440600
H	-1.36118700	3.89334900	1.22921000
H	0.09723700	4.79680400	0.74420000
C	2.82305000	0.43192400	1.04341300
C	2.94531400	0.15520100	2.39936900
C	3.79702100	0.09594800	0.09508400
C	4.08237000	-0.49975100	2.85562900
C	4.92227100	-0.56895300	0.58913100
C	5.06580700	-0.86528400	1.94230300
H	4.19220500	-0.72701900	3.90984900
H	5.70718400	-0.86260800	-0.09839200
H	2.14815500	0.44774000	3.07488200
H	5.95543600	-1.38502000	2.28247000
C	3.67371000	0.50336400	-1.36532800
C	4.57024300	-0.31111700	-2.29702400
C	3.97207700	2.00443300	-1.50301400
H	2.64380500	0.33102300	-1.69551500
H	4.34463400	-0.05341300	-3.33443400
H	5.62921300	-0.09261600	-2.12715300
H	4.40918900	-1.38496200	-2.16946400
H	3.31261800	2.61032200	-0.87463900
H	5.00425800	2.21053200	-1.20252900
H	3.84596100	2.32205600	-2.54166000
C	0.61999800	-3.14201800	-0.47844500
C	0.81372600	-1.82090300	-0.07144900
C	0.49972900	-0.69995100	-0.86193000
O	0.07641600	-0.60802700	-2.02076600
C	0.07595100	-3.53912800	-1.72808600

H	0.27173800	-4.57601800	-2.00093100
H	-1.19938100	-3.54949200	-1.46184400
H	0.14717000	-2.82759600	-2.54471500
C	0.85668300	-4.20793000	0.55312200
H	1.20707500	-5.13654900	0.09812300
H	1.56580200	-3.88341300	1.31771400
H	-0.11162700	-4.39271700	1.03300100
H	1.14447700	-1.63693600	0.94490000
H	-4.62748000	-3.70396600	-0.73009300
C	-2.87089000	-3.47169600	-0.09317100
O	-2.14833900	-3.25687400	0.87810800
O	-2.53932600	-3.62771100	-1.31842800
O	-4.22050700	-3.54773600	0.13194400

M05

C	-3.70893900	-0.63720000	0.12238600
C	-2.67427000	-1.47503400	-0.30252900
C	-2.36147100	-2.64877000	0.37692200
C	-3.08776100	-2.95278900	1.52757500
C	-4.10591800	-2.10754100	1.97167800
C	-4.43192300	-0.94845400	1.26808000
C	-3.87896400	0.53010700	-0.81695400
C	-3.12571900	0.04818400	-2.07610200
C	-2.03155100	-0.90965900	-1.54519300
H	-1.56944600	-3.29464600	0.01140900
H	-2.85965500	-3.85713600	2.08154500
H	-4.66037700	-2.36269700	2.86919300
H	-5.24171000	-0.30808900	1.60471700
H	-3.39920400	1.42016300	-0.39428900
H	-3.80331900	-0.55087600	-2.68850300
H	-4.92087700	0.77682300	-1.03180300
H	-1.69431900	-1.65954000	-2.26151900
N	-0.85223000	-0.07978900	-1.21466800
O	-2.63699100	1.05197900	-2.94181300
C	0.23890800	-0.45324100	-0.52129000
C	-0.66437600	1.21529100	-1.60802000
N	1.04377300	0.61080600	-0.54173200
N	0.48829000	1.66783100	-1.20693500
C	-1.72673500	1.95660000	-2.35794500
H	-2.22189300	2.66301800	-1.67753200
H	-1.27337300	2.53011100	-3.16779300
C	2.36326200	0.73058400	0.02021900
C	2.51665300	1.64964000	1.05469300
C	3.41897000	-0.03054500	-0.49032100

C	3. 77117200	1. 82256600	1. 62426300
C	4. 66600900	0. 16301700	0. 11623100
C	4. 84535200	1. 06920800	1. 15572200
H	3. 90577900	2. 53869200	2. 42723400
H	5. 51745500	-0. 40451000	-0. 24828300
H	1. 65756000	2. 22335300	1. 38901900
H	5. 82939800	1. 19249000	1. 59658300
C	3. 28821300	-0. 97671600	-1. 67046000
C	3. 78432200	-2. 38375800	-1. 32522600
C	4. 03368000	-0. 40524500	-2. 88326500
H	2. 23426500	-1. 07643400	-1. 94151200
H	3. 57654800	-3. 06335400	-2. 15569000
H	4. 86421900	-2. 39137100	-1. 14383000
H	3. 27550200	-2. 76239800	-0. 43581700
H	3. 64882200	0. 58154400	-3. 15570800
H	5. 10342800	-0. 30477400	-2. 67207700
H	3. 91981400	-1. 07156000	-3. 74318700
C	1. 01744400	-1. 23008100	2. 21761700
C	1. 04905900	-2. 15506500	1. 09665100
C	0. 56310100	-1. 89439700	-0. 16205200
O	0. 40477800	-2. 64520400	-1. 16667800
C	-0. 07366200	-0. 49023300	2. 52009500
H	-0. 06454800	0. 20454800	3. 35753300
H	-0. 80211600	1. 23229200	1. 54992200
H	-1. 02882100	-0. 69570100	2. 03922200
C	2. 26540800	-1. 16283500	3. 06155900
H	2. 47526500	-2. 15088000	3. 48695200
H	3. 12704400	-0. 88685000	2. 44417100
H	2. 16796100	-0. 44731000	3. 88135200
H	1. 50452400	-3. 13197800	1. 24231000
H	-3. 04954200	3. 29060300	0. 76439200
C	-1. 21700600	3. 06233900	1. 20441900
O	-0. 14923200	3. 51521000	1. 51074500
O	-1. 54938800	1. 76405900	1. 20402100
O	-2. 24126400	3. 82129200	0. 79907700

Z-M05

C	-4. 07564600	1. 44017100	0. 18850400
C	-2. 93489200	0. 64562200	0. 12133500
C	-2. 78873200	-0. 49792700	0. 89965200
C	-3. 82306300	-0. 83525900	1. 76858600
C	-4. 96975900	-0. 04017800	1. 85042800
C	-5. 10600200	1. 09938200	1. 06108800
C	-4. 00848300	2. 59362900	-0. 77828400

C	-2.61504700	2.49214400	-1.44911500
C	-1.95581700	1.17002200	-0.89857600
H	-1.90866400	-1.13302400	0.83072800
H	-3.73655700	-1.73235800	2.37293600
H	-5.76810200	-0.31854800	2.53129900
H	-6.00292900	1.70893600	1.12140500
H	-4.12036200	3.56806100	-0.28997000
H	-2.70620000	2.40985600	-2.53212400
H	-4.79915200	2.52880300	-1.53155600
H	-1.75370200	0.44594400	-1.68710900
N	-0.64578400	1.45923500	-0.28649800
O	-1.82933200	3.65835100	-1.25812600
C	0.39722800	0.63952200	-0.03644900
C	-0.33643600	2.68242800	0.23629500
N	1.30228500	1.41508600	0.57844900
N	0.85164400	2.69249700	0.76152000
C	-1.32067700	3.78786700	0.05230100
H	-2.11581100	3.72303000	0.80876600
H	-0.82573400	4.75513800	0.13681700
C	2.65535900	1.10218600	0.95139500
C	2.96277200	1.17458900	2.30703100
C	3.60234800	0.78725800	-0.02793700
C	4.25910300	0.90995000	2.72621200
C	4.89633100	0.51932600	0.43111500
C	5.22555400	0.57559400	1.78041300
H	4.50974300	0.95989800	3.77985200
H	5.66554100	0.26819600	-0.29350300
H	2.18066200	1.43380300	3.01290600
H	6.24163800	0.36060500	2.09441000
C	3.30634800	0.75777100	-1.51659000
C	3.66939700	-0.59667100	-2.13418700
C	4.03857500	1.90695600	-2.22158100
H	2.23389100	0.90757900	-1.67290000
H	3.35894800	-0.62097700	-3.18253500
H	4.75081300	-0.76505800	-2.10324000
H	3.17536200	-1.41626600	-1.60599800
H	3.74940300	2.87549400	-1.80432200
H	5.12297100	1.80126300	-2.11457300
H	3.80282600	1.90448100	-3.28948400
C	1.44674500	-3.03824300	0.11108100
C	1.20985900	-1.61508500	0.36171900
C	0.48288700	-0.78867700	-0.43993700
O	-0.19760800	-1.05851500	-1.51506700
C	1.43880300	-3.57694100	-1.11821200

H	1. 63242300	-4. 63641400	-1. 25778900
H	-0. 96871200	-2. 22570600	-1. 45210600
H	1. 22334900	-2. 97866500	-1. 99602400
C	1. 70818800	-3. 87003700	1. 33951300
H	1. 97487900	-4. 89626700	1. 07764500
H	2. 51823400	-3. 44148400	1. 94037300
H	0. 80558900	-3. 89052200	1. 95841500
H	1. 62428200	-1. 20579500	1. 27855000
H	-2. 63668500	-4. 96484200	-1. 49231700
C	-1. 82108600	-3. 67464000	-0. 39055800
O	-1. 50176600	-3. 30143700	0. 71922500
O	-1. 60907600	-3. 07430800	-1. 53358700
O	-2. 49323000	-4. 83627100	-0. 54548300

M5

C	4. 27776600	-0. 22557600	0. 52643500
C	3. 15132500	0. 44113900	0. 05437500
C	3. 02839400	1. 82600800	0. 12226100
C	4. 08083500	2. 54394100	0. 68522500
C	5. 21862100	1. 88614800	1. 16058400
C	5. 32718500	0. 49928500	1. 08481900
C	4. 15751700	-1. 71504400	0. 32487100
C	2. 69235100	-1. 95266500	-0. 11259800
C	2. 14087800	-0. 53246200	-0. 50801800
H	2. 12970700	2. 32045900	-0. 24758400
H	4. 01644300	3. 62478800	0. 75589600
H	6. 02744300	2. 46302800	1. 59807000
H	6. 21208000	-0. 00633800	1. 46004300
H	4. 37338000	-2. 29570900	1. 22728400
H	2. 62743200	-2. 62638200	-0. 96744900
H	4. 84632200	-2. 06177400	-0. 45239700
H	2. 01579300	-0. 42829500	-1. 58949900
N	0. 82304400	-0. 32065800	0. 08328800
O	1. 92622600	-2. 59965900	0. 89477500
C	-0. 21198100	0. 40642500	-0. 36614500
C	0. 48456200	-0. 82238000	1. 30743400
N	-1. 12641100	0. 32762300	0. 60165600
N	-0. 71040300	-0. 44782300	1. 65356900
C	1. 46261900	-1. 75932300	1. 93590500
H	2. 28281400	-1. 20408000	2. 41188000
H	0. 97180600	-2. 38499700	2. 68095500
C	-2. 44032200	0. 90864500	0. 59138500
C	-2. 52543600	2. 29311400	0. 46696500
C	-3. 56286200	0. 07845100	0. 69505300

C	-3.77863000	2.89126600	0.47114100
C	-4.80505400	0.72008700	0.71675800
C	-4.91713300	2.10204900	0.61097300
H	-3.86223900	3.96757900	0.36906300
H	-5.70556200	0.12000500	0.80638800
H	-1.61165500	2.86282700	0.33083100
H	-5.89964800	2.56280700	0.62625800
C	-3.47367600	-1.43560900	0.78386100
C	-4.44542700	-2.12239200	-0.18166000
C	-3.70682200	-1.90137200	2.22576200
H	-2.46177400	-1.73564800	0.49355400
H	-4.27280800	-3.20227100	-0.17179400
H	-5.48738100	-1.95437500	0.10707900
H	-4.31249700	-1.76160500	-1.20541000
H	-4.70831900	-1.61314900	2.56271300
H	-3.62694200	-2.99063000	2.29201700
H	-2.97273400	-1.45450300	2.90000800
C	-0.45003400	-0.64789000	-3.07120300
C	-0.16711400	0.76065400	-2.80804400
C	-0.14487300	1.34522900	-1.56672000
O	0.06706600	2.53759400	-1.19868900
C	0.34974900	-1.27855700	-4.18804800
H	0.19500900	-0.72249100	-5.11933400
H	1.42475700	-1.24043400	-3.97818500
H	0.05987400	-2.31777800	-4.35898200
C	-1.35758300	-1.37461700	-2.39127700
H	-2.03315900	-0.90938100	-1.67917500
H	-1.47872600	-2.43971100	-2.56517900
H	0.09151600	1.40327600	-3.64587800

Z-M5

C	4.40434300	0.06794100	0.01803200
C	3.10574100	0.56162900	-0.06408700
C	2.71554500	1.70938000	0.62008800
C	3.66161800	2.36058200	1.40699300
C	4.96714000	1.87020400	1.49736600
C	5.34840700	0.72432800	0.80364500
C	4.57541600	-1.16799000	-0.82769100
C	3.15071400	-1.54190300	-1.30552800
C	2.24671700	-0.30139100	-0.95854900
H	1.69661400	2.08355000	0.54207300
H	3.38477900	3.25684400	1.95207700
H	5.69259000	2.38949500	2.11546300
H	6.36408500	0.34716400	0.87785600

H	5.01764800	-2.00863800	-0.28289800
H	3.12191300	-1.72620800	-2.37923400
H	5.22385200	-0.96757000	-1.68652100
H	1.88898700	0.22582200	-1.84662400
N	1.04126700	-0.73992400	-0.24970700
O	2.69446000	-2.76259000	-0.73652400
C	-0.15611300	-0.13437700	-0.15378700
C	1.03357800	-1.81570600	0.58898300
N	-0.85079800	-0.89307100	0.70170900
N	-0.11615400	-1.94782900	1.18146700
C	2.26116800	-2.66497800	0.60550800
H	3.02929500	-2.21914300	1.25400600
H	2.02959900	-3.66820400	0.96283200
C	-2.22175700	-0.73871400	1.10757500
C	-2.44977500	-0.47642000	2.45218800
C	-3.25105700	-0.87139700	0.16511700
C	-3.75531600	-0.31906900	2.90278800
C	-4.54878000	-0.69519400	0.65083900
C	-4.80200200	-0.42164700	1.99341000
H	-3.94832600	-0.11102300	3.94923600
H	-5.38436300	-0.77415200	-0.03522100
H	-1.60325700	-0.39309100	3.12593200
H	-5.82603000	-0.29155300	2.32791900
C	-2.97092100	-1.25297900	-1.28033600
C	-4.13253800	-0.94106500	-2.22252500
C	-2.60340500	-2.74347800	-1.35301600
H	-2.11567000	-0.67166700	-1.63958000
H	-3.82473800	-1.13563700	-3.25270200
H	-5.00279800	-1.57222100	-2.01426300
H	-4.43367000	0.10753100	-2.15056400
H	-1.74767800	-2.98392700	-0.71479200
H	-3.44918000	-3.35702800	-1.02585700
H	-2.35436000	-3.02134400	-2.38096000
C	-1.74438900	3.28625900	-0.78205500
C	-1.25898600	2.02477200	-0.24205900
C	-0.54324400	1.08722900	-0.95152500
O	-0.12438900	1.05485400	-2.14657600
C	-1.54732200	3.69575300	-2.04886400
H	-1.94394900	4.65087400	-2.38165300
H	-0.99700500	3.08474800	-2.75203400
C	-2.52250800	4.13721800	0.19473700
H	-2.86595300	5.06570900	-0.26672200
H	-3.39689600	3.59256700	0.56943300
H	-1.90958800	4.39174800	1.06689500

H	-1.50030000	1.79907700	0.79291700
TS6(R)			
C	3.78316800	-2.16915200	-0.11533200
C	2.83372700	-1.49879300	0.65143200
C	2.94040900	-1.42147900	2.03594300
C	4.02816100	-2.03975100	2.64925200
C	4.98872200	-2.70875500	1.88698400
C	4.87431700	-2.77605600	0.49967600
C	3.46944500	-2.06646200	-1.58578100
C	2.03622500	-1.49380200	-1.64988600
C	1.79474800	-0.85277000	-0.23855500
H	2.20350200	-0.86102600	2.60214900
H	4.13585500	-1.99336400	3.72830600
H	5.83181100	-3.18234300	2.38042900
H	5.62335300	-3.29626200	-0.09065200
H	3.50887300	-3.02506600	-2.11182400
H	1.91955800	-0.72810100	-2.41840600
H	4.17347200	-1.38688000	-2.07731700
H	1.90083000	0.23121100	-0.28325100
N	0.43022700	-1.11468900	0.21024500
O	1.10149000	-2.50764900	-2.00700900
C	-0.46123300	-0.33579500	0.84032700
C	-0.18148700	-2.29497400	-0.07388500
N	-1.55646200	-1.09810100	0.96475400
N	-1.39928800	-2.32429500	0.38220000
C	0.56538400	-3.25610400	-0.93705400
H	1.34614900	-3.76926900	-0.35829800
H	-0.11927800	-3.99499600	-1.35317000
C	-2.73580000	-0.83078600	1.74044600
C	-2.54847200	-0.49258900	3.07912600
C	-4.00282100	-0.94614700	1.15910600
C	-3.65152500	-0.24853400	3.88295300
C	-5.09340600	-0.70936400	2.00399300
C	-4.92887300	-0.36236300	3.33924100
H	-3.51342300	0.01781800	4.92470100
H	-6.09716100	-0.79847900	1.60145300
H	-1.54070400	-0.42706400	3.47700500
H	-5.80132200	-0.18238000	3.95890900
C	-4.22412100	-1.34300800	-0.29074800
C	-5.29697400	-0.48053700	-0.96237300
C	-4.58995400	-2.82985900	-0.38697500
H	-3.28268400	-1.19586300	-0.83360400
H	-5.37247200	-0.74096100	-2.02147800

H	-6.28301000	-0.64746900	-0.51892100
H	-5.06012100	0.58385400	-0.88071200
H	-3.81119000	-3.45250600	0.05752700
H	-5.53419000	-3.02457800	0.13288100
H	-4.71363500	-3.11896700	-1.43542700
C	-2.11642000	2.44220400	0.79498700
C	-1.07904900	2.04658200	1.62625000
C	-0.12890300	0.99493600	1.47484000
O	1.00254800	1.00853500	1.99859800
C	-2.80923300	3.75099300	1.10314100
H	-2.92480500	4.34958800	0.19321400
H	-3.81462700	3.56600900	1.49588100
H	-2.26040500	4.34001300	1.84125000
C	-2.46061900	1.79729900	-0.41202000
H	-2.40492800	0.71721100	-0.46316200
H	-3.28793900	2.21805800	-0.98196500
H	-0.75473400	2.74971400	2.39066500
C	-0.78990100	2.01933400	-1.58023000
N	0.33402900	1.90690400	-0.87505800
N	0.73648500	3.14949700	-0.39027500
O	1.99425100	4.18494000	1.17166700
C	3.03730700	2.40208000	-0.01711600
C	3.34295700	2.10242700	-1.34638500
C	4.45867500	1.32272200	-1.63955300
C	5.25614600	0.82771800	-0.60762100
C	4.94698800	1.12459200	0.71845800
C	3.84587900	1.92235900	1.01264000
H	2.70121900	2.47349500	-2.13928300
H	4.70593700	1.10027700	-2.67376200
H	5.55194500	0.71532000	1.52153700
H	3.57287300	2.15596900	2.03620600
C	-1.10115200	0.84824200	-2.44931900
O	-0.87683700	-0.31212100	-2.17346100
O	-1.69450700	1.24058700	-3.58365300
C	-2.06387200	0.19468900	-4.49973900
C	-3.36159200	-0.46267800	-4.07350300
H	-1.24976500	-0.53171600	-4.55106400
H	-2.16538800	0.69730700	-5.46255800
H	-3.67932300	-1.18939300	-4.82559200
H	-3.22440700	-0.98419600	-3.12316000
H	-4.14788800	0.28801800	-3.95984300
H	-1.06922000	2.98397600	-2.00720800
H	-0.00260900	3.76938100	-0.06118900
C	1.88916000	3.29409000	0.33973600

H	6.11329000	0.20107200	-0.83719500
TS6(S)			
C	-5.83248900	0.47663900	0.23095500
C	-4.68515400	-0.03210100	-0.37005900
C	-4.70205600	-1.21572200	-1.10200900
C	-5.91204500	-1.89280000	-1.22718300
C	-7.07095000	-1.38737000	-0.63200700
C	-7.04116500	-0.20255800	0.09961200
C	-5.54403200	1.76401900	0.96167600
C	-4.00200300	1.90609600	0.95450200
C	-3.49482700	0.85886900	-0.10451800
H	-3.79412600	-1.61214300	-1.55230700
H	-5.95466500	-2.81932100	-1.78960700
H	-8.00597500	-1.92807300	-0.73744000
H	-7.94454600	0.18059900	0.56459900
H	-5.91191400	1.76874900	1.99261700
H	-3.68767700	2.90690300	0.65755000
H	-6.00614700	2.61580000	0.45263900
H	-3.13488300	1.35540500	-1.00624700
N	-2.38191100	0.07776300	0.44277000
O	-3.43178100	1.73327800	2.24166900
C	-1.38177600	-0.58017800	-0.17510800
C	-2.35119500	-0.27406700	1.76169000
N	-0.80083400	-1.31136900	0.78262700
N	-1.39236000	-1.11623100	1.99660300
C	-3.33274200	0.38938800	2.67035100
H	-4.30324300	-0.12582600	2.63460600
H	-2.96274500	0.38649900	3.69533700
C	0.33062400	-2.20942800	0.71020300
C	0.19135700	-3.37077300	-0.04335000
C	1.47950200	-1.91963200	1.45836900
C	1.23979100	-4.28083900	-0.08860900
C	2.50253700	-2.86929000	1.40294700
C	2.39561300	-4.02795300	0.64055100
H	1.14854100	-5.17885700	-0.68895700
H	3.41541700	-2.68317900	1.96015400
H	-0.72002000	-3.53408600	-0.60123600
H	3.22091900	-4.73305500	0.61447700
C	1.61980800	-0.68747000	2.33092600
C	2.99748600	-0.03330400	2.20829100
C	1.33397100	-1.04914200	3.79577300
H	0.89488500	0.05599100	1.99057000
H	3.00440500	0.88781200	2.79852400

H	3.79627100	-0.67883200	2.58917900
H	3.21727000	0.21892100	1.16856700
H	2.07833900	-1.76526600	4.16199300
H	1.39094600	-0.15344500	4.42232000
H	0.34376600	-1.49457500	3.91203900
C	-1.04795900	1.78041600	-2.36057300
C	-1.30524400	0.42966400	-2.55556700
C	-1.19576400	-0.67977700	-1.67363000
O	-1.08510300	-1.84807800	-2.08874600
C	-1.09138300	2.68780200	-3.56823600
H	-1.33409900	2.14005700	-4.47997600
H	-1.83358000	3.48014800	-3.43055000
H	-0.12109500	3.17659800	-3.70659600
C	-0.56481600	2.33217600	-1.16460300
H	-0.78862200	1.88775000	-0.20160200
H	-0.44504900	3.41426000	-1.12971000
H	-1.44932200	0.08940200	-3.57745100
C	1.30678500	1.53211200	-1.13949400
N	1.28240800	0.22591100	-0.88921800
N	1.68765300	-0.56250900	-2.00831600
O	2.96017600	-2.36232300	-2.52171300
C	4.03045600	-0.70355100	-1.21352800
C	4.86183900	-1.59521800	-0.53387500
C	5.96852800	-1.13042900	0.16815800
C	6.27539900	0.22887400	0.16224700
C	5.48086300	1.11539000	-0.56131800
C	4.35837200	0.65359100	-1.24220200
H	4.61492200	-2.65110900	-0.56231400
H	6.59771000	-1.82769800	0.71275300
H	5.73880700	2.16854200	-0.60423200
H	3.75405600	1.34899100	-1.81281700
C	1.64840900	2.42064700	0.02300900
O	1.28470600	2.26898900	1.16607700
O	2.39903300	3.45743900	-0.39023800
C	2.74334500	4.41850100	0.62356600
C	3.94549500	3.95922700	1.42502300
H	1.87529900	4.57020200	1.26926700
H	2.95286200	5.33832500	0.07483200
H	4.16783300	4.68583400	2.21082200
H	3.74147800	2.99189000	1.88944000
H	4.82412700	3.86471200	0.78391300
H	1.67691900	1.89498600	-2.10072500
H	0.95016000	-1.17144500	-2.37019600
C	2.85703900	-1.28753000	-1.94479100

H	7.14208000	0.59346600	0.70496600
M6(R)			
C	3.55013700	2.27515300	0.61730200
C	2.51585800	1.83623700	-0.20497400
C	2.31025900	2.37710900	-1.47167900
C	3.16703400	3.38993200	-1.89712300
C	4.20758000	3.83750300	-1.07888800
C	4.40867000	3.28146800	0.18235700
C	3.59159600	1.50742500	1.91198500
C	2.30783200	0.64861200	1.91485100
C	1.75465100	0.70078500	0.44582800
H	1.51666700	1.97553700	-2.09670400
H	3.03209800	3.82962700	-2.88033200
H	4.86743700	4.62472500	-1.43042700
H	5.22037600	3.62766900	0.81581900
H	3.61195200	2.14820800	2.79979200
H	2.51025500	-0.38828500	2.18734300
H	4.47579100	0.86419000	1.95256700
H	1.90087700	-0.24277200	-0.07819100
N	0.30859700	0.95002300	0.47108700
O	1.37505500	1.10027900	2.89254600
C	-0.67346600	0.55213800	-0.35884400
C	-0.23651800	1.80979400	1.37796200
N	-1.75414200	1.22843500	0.05018700
N	-1.49787100	2.01014400	1.14638300
C	0.63552000	2.24491300	2.50821200
H	1.29238200	3.07196300	2.20510200
H	0.02799900	2.55819800	3.35678200
C	-3.03172100	1.36096900	-0.59651400
C	-3.02500200	1.85166500	-1.89999700
C	-4.20750600	1.04839000	0.09083500
C	-4.22647100	2.01776000	-2.57239900
C	-5.40346800	1.24217500	-0.61201000
C	-5.41976500	1.71180800	-1.91994900
H	-4.23121200	2.38765400	-3.59156300
H	-6.34377700	1.01779900	-0.11750900
H	-2.07325800	2.07450000	-2.37451200
H	-6.36791100	1.84380600	-2.43094200
C	-4.21968500	0.56824100	1.53113800
C	-5.17780500	-0.60923600	1.74145800
C	-4.57971700	1.73060800	2.46642700
H	-3.21219800	0.22728600	1.78823000
H	-5.04768600	-1.01264800	2.74936800

H	-6.22384800	-0.30214400	1.64373600
H	-4.99343000	-1.41501400	1.02445100
H	-3.86262700	2.54741400	2.35994600
H	-5.58083900	2.11197800	2.23752000
H	-4.57410500	1.39337200	3.50726400
C	-2.57881800	-1.66789700	-1.72341400
C	-1.69703600	-0.82606800	-2.26603500
C	-0.40992300	-0.41727300	-1.55963300
O	0.51476200	0.09603500	-2.31515800
C	-3.85849000	-2.07199200	-2.39425600
H	-3.93300200	-3.16138800	-2.48569200
H	-4.71460800	-1.73954300	-1.79381400
H	-3.94493100	-1.62700200	-3.38784500
C	-2.36003600	-2.15548600	-0.31492200
H	-2.79311600	-1.42041700	0.37572000
H	-2.90572400	-3.08927100	-0.14276300
H	-1.82901200	-0.41992900	-3.26552100
C	-0.87011700	-2.35179100	0.05684000
N	0.10433200	-1.69984200	-0.82986400
N	0.53256900	-2.59268100	-1.82502800
O	1.98308400	-2.64577300	-3.56629200
C	2.86455500	-1.90363000	-1.48979900
C	3.04192900	-2.47113700	-0.22598200
C	4.11490500	-2.06936100	0.56538900
C	4.99113600	-1.08440400	0.10655100
C	4.79742000	-0.50434000	-1.14661000
C	3.74595700	-0.92880700	-1.95324500
H	2.33064600	-3.20560400	0.13845900
H	4.26892200	-2.52358600	1.54020000
H	5.46231000	0.28116200	-1.49223200
H	3.57459700	-0.49092000	-2.93091100
C	-0.59370500	-1.88599700	1.48932600
O	-1.28252800	-1.11715100	2.12529600
O	0.52595600	-2.43747200	1.96340400
C	0.85313300	-2.13879200	3.33736900
C	0.03845100	-3.00185600	4.28135900
H	0.68521600	-1.07422700	3.51464400
H	1.91973500	-2.36147900	3.41509100
H	0.33969000	-2.80550700	5.31335600
H	-1.02451100	-2.77211700	4.18397000
H	0.19762100	-4.06146800	4.06894400
H	-0.61774400	-3.41399400	0.03584900
H	-0.16324000	-2.77655900	-2.55108300
C	1.77075400	-2.36273000	-2.40158800

H	5. 82842300	-0. 77245100	0. 72420200
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M6(S)

C	5. 32548300	0. 02391700	-0. 85108700
C	4. 01059400	-0. 41463600	-0. 98317200
C	3. 55159700	-1. 03121600	-2. 14560400
C	4. 46572400	-1. 23036200	-3. 17863400
C	5. 79275400	-0. 81461800	-3. 04771700
C	6. 23181400	-0. 18030200	-1. 88736000
C	5. 54730400	0. 70498300	0. 47566700
C	4. 13646900	0. 87355900	1. 08992400
C	3. 20568100	-0. 08028700	0. 25337400
H	2. 50613900	-1. 32823400	-2. 25100400
H	4. 13916200	-1. 70642600	-4. 09726700
H	6. 48818600	-0. 97517400	-3. 86543700
H	7. 25931900	0. 15980400	-1. 79903100
H	6. 03085100	1. 68279900	0. 38396500
H	4. 12125300	0. 57866700	2. 14024400
H	6. 17548700	0. 09580600	1. 13359900
H	2. 94419800	-0. 95816100	0. 84551700
N	1. 95637300	0. 59259300	-0. 11649500
O	3. 69884700	2. 22305100	1. 10662300
C	0. 72185700	0. 12094300	-0. 39824000
C	1. 97413800	1. 92532600	-0. 43047700
N	0. 04370500	1. 19238700	-0. 83732100
N	0. 82097300	2. 31722800	-0. 86673600
C	3. 21928000	2. 69433700	-0. 14043000
H	3. 96161600	2. 55838900	-0. 93880300
H	2. 99286000	3. 75531400	-0. 03741900
C	-1. 32629300	1. 32696200	-1. 27636400
C	-1. 77790200	0. 46367300	-2. 27255200
C	-2. 11671300	2. 35417700	-0. 74488100
C	-3. 06362200	0. 62164700	-2. 77258600
C	-3. 39368400	2. 49893100	-1. 30139700
C	-3. 86763300	1. 65340200	-2. 29655900
H	-3. 43230800	-0. 06612600	-3. 52627000
H	-4. 03878500	3. 28865900	-0. 92707100
H	-1. 11922700	-0. 33726400	-2. 59908500
H	-4. 87195300	1. 78797200	-2. 68542000
C	-1. 67197300	3. 29449000	0. 36513600
C	-2. 68669200	3. 34597000	1. 51084700
C	-1. 40541700	4. 69391800	-0. 20074000
H	-0. 74486500	2. 90925600	0. 79261200
H	-2. 32718800	4. 02603000	2. 28947300

H	-3.66395100	3.71120100	1.17926000
H	-2.80779900	2.35518900	1.95406200
H	-0.64986800	4.65463900	-0.98886300
H	-2.32190400	5.12007100	-0.62301100
H	-1.05437200	5.36577900	0.58888900
C	0.93095800	-3.10308700	1.24695500
C	1.22460100	-2.35669400	0.18073700
C	0.28450200	-1.37891000	-0.53209800
O	0.27132300	-1.65029600	-1.81754100
C	1.83025100	-4.19713200	1.74496400
H	2.71758400	-4.30728800	1.11760200
H	2.14887800	-3.98970400	2.77325200
H	1.29811300	-5.15491400	1.76433400
C	-0.36112000	-2.91088000	1.98748400
H	-0.18952000	-2.92742600	3.06893800
H	-1.03256100	-3.74743900	1.75716400
H	2.13086000	-2.56590300	-0.38476800
C	-1.04836500	-1.61663400	1.57797600
N	-1.10860600	-1.40299800	0.11860300
N	-1.82425700	-2.44704200	-0.50476800
O	-3.44609800	-3.06217100	-1.90663400
C	-4.13101500	-1.43441800	-0.32968000
C	-3.87227500	-0.31882700	0.47403400
C	-4.93455200	0.41321500	1.00354600
C	-6.25121500	0.04780300	0.74657800
C	-6.51343000	-1.05576000	-0.06330200
C	-5.46076900	-1.78403700	-0.59966300
H	-2.85625400	0.01550300	0.65021000
H	-4.72467800	1.28766700	1.61109800
H	-7.53716800	-1.34612600	-0.27774200
H	-5.64382800	-2.63712100	-1.24287200
C	-0.43350700	-0.34993200	2.17620800
O	-0.90932800	0.75300600	2.02209600
O	0.68550100	-0.56998100	2.87232200
C	1.32558700	0.59128500	3.43138400
C	2.40080500	0.09369100	4.37184600
H	0.57603100	1.19944400	3.94333700
H	1.73770900	1.19179400	2.61003000
H	2.97409500	0.93787300	4.76200200
H	1.95792800	-0.44543500	5.21205500
H	3.08460900	-0.58591500	3.85532700
H	-2.08550600	-1.61489700	1.93283700
H	-1.23477800	-2.92356600	-1.18968700
C	-3.10621100	-2.31818500	-0.99550400

H	-7.06972400	0.62333400	1.16834300
TS7(R)			
C	-3.41476600	-2.47779300	-0.47645300
C	-2.40422200	-1.67234300	-0.99490300
C	-2.18444200	-1.58045300	-2.36665500
C	-3.00305100	-2.31911100	-3.21752400
C	-4.02081600	-3.12734800	-2.70443900
C	-4.23466600	-3.21068800	-1.33100400
C	-3.47379100	-2.39342100	1.02479700
C	-2.25103700	-1.54084800	1.43537700
C	-1.66870300	-0.93493100	0.10471800
H	-1.41282500	-0.91931100	-2.74996700
H	-2.85436700	-2.26041100	-4.29102900
H	-4.65046900	-3.69548300	-3.38220100
H	-5.02560700	-3.83986700	-0.93261500
H	-3.42454800	-3.37239600	1.51419800
H	-2.53619600	-0.72703700	2.10233900
H	-4.40039200	-1.91412300	1.35515400
H	-1.82826200	0.14514300	0.05044600
N	-0.22091700	-1.15369500	0.03754100
O	-1.30789700	-2.30280600	2.18067800
C	0.73480100	-0.41895400	-0.57905500
C	0.34334500	-2.29213900	0.54392200
N	1.82768900	-1.18572100	-0.42888600
N	1.61035400	-2.34877800	0.27465500
C	-0.51627000	-3.17076200	1.38801000
H	-1.13938400	-3.82994800	0.76715700
H	0.09473500	-3.77851100	2.05502000
C	3.12246600	-0.96472800	-1.00461300
C	3.18444100	-0.79872900	-2.38703500
C	4.26755100	-0.94434900	-0.19932500
C	4.41149600	-0.60231000	-3.00499000
C	5.49248100	-0.76982500	-0.85525400
C	5.57156800	-0.59885800	-2.23248500
H	4.46200200	-0.46889100	-4.08012800
H	6.40472200	-0.76313500	-0.26601500
H	2.26224200	-0.82590000	-2.95922100
H	6.53945400	-0.46202200	-2.70393700
C	4.21842400	-1.12101900	1.30748300
C	5.06689200	-0.07313300	2.03553600
C	4.65846500	-2.54016700	1.68759800
H	3.18437500	-0.98434100	1.63220600
H	4.90326800	-0.15373300	3.11379900

H	6.13675700	-0.21620500	1.85266300
H	4.80214700	0.94274300	1.72674500
H	4.00965600	-3.28146500	1.21591100
H	5.68991400	-2.72309900	1.36650000
H	4.61153900	-2.67367300	2.77267500
C	2.46574600	2.28314500	-1.14936600
C	1.50962300	1.85426100	-1.97658900
C	0.19789300	1.34510800	-1.47181100
O	-0.73047600	1.09764100	-2.25045900
C	3.80945600	2.75036800	-1.62079600
H	4.03399100	3.75481600	-1.24585200
H	4.58468000	2.07636100	-1.23347900
H	3.87276800	2.75425300	-2.71083300
C	2.28998900	2.14310700	0.33663800
H	2.72415500	1.17692300	0.62795400
H	2.87693800	2.90521400	0.86062300
H	1.63367000	1.85815600	-3.05621200
C	0.82958200	2.18647300	0.83056500
N	-0.21117300	2.01129200	-0.19067200
N	-0.78033700	3.24901100	-0.55500300
O	-2.42844200	3.99584600	-1.91981000
C	-3.03723500	2.29398300	-0.37583500
C	-3.14414300	2.26324700	1.01539600
C	-4.12026100	1.47131500	1.61352300
C	-4.96471700	0.68890500	0.82474200
C	-4.83251600	0.69640100	-0.56346300
C	-3.88195000	1.51550000	-1.16536900
H	-2.46263000	2.85237500	1.61980000
H	-4.23005200	1.46926400	2.69425400
H	-5.47032000	0.06690700	-1.17628800
H	-3.76170800	1.53768100	-2.24308700
C	0.61315500	1.17843800	1.96766400
O	1.42322300	0.36277000	2.34709200
O	-0.58476200	1.34632100	2.53302700
C	-0.84804400	0.56398800	3.71627200
C	-0.13044500	1.14244100	4.92059600
H	-0.56241300	-0.47276200	3.52348600
H	-1.93204400	0.62480000	3.83851700
H	-0.40575600	0.58118500	5.81692600
H	0.95115700	1.07534800	4.79089700
H	-0.41048300	2.18830000	5.06789600
H	0.62255500	3.16067500	1.28203400
H	-0.18622000	3.82291100	-1.15761200
C	-2.07763700	3.22316600	-1.04913300

H	-5.73151300	0.07871000	1.29317000
TS7(S)			
C	5.23677400	-0.08455600	-1.05895200
C	3.90146500	-0.47987300	-1.07625700
C	3.36296500	-1.18778600	-2.14819300
C	4.21107400	-1.53063300	-3.19957800
C	5.55784200	-1.16119600	-3.17718600
C	6.07923700	-0.43046100	-2.11156100
C	5.54922000	0.72359200	0.17545400
C	4.17512400	1.03281900	0.81521300
C	3.17471700	0.01393700	0.15724900
H	2.30655000	-1.45524100	-2.17497600
H	3.81796000	-2.08232100	-4.04709600
H	6.20139000	-1.43346200	-4.00763900
H	7.12127700	-0.12435900	-2.10979700
H	6.07717800	1.65765400	-0.04052200
H	4.19920300	0.89214600	1.89695600
H	6.17190200	0.15391900	0.87346100
H	2.93432600	-0.78807400	0.85924300
N	1.92221000	0.66403000	-0.20712200
O	3.78711700	2.38928000	0.65471900
C	0.65960600	0.16956500	-0.28857500
C	1.94339700	1.94139500	-0.70136200
N	-0.01578000	1.20124200	-0.82242200
N	0.76237600	2.30693200	-1.08211500
C	3.22546900	2.69993100	-0.61092400
H	3.90491500	2.43085200	-1.43135500
H	3.03740000	3.77307000	-0.63907900
C	-1.40203700	1.28700900	-1.19924600
C	-1.87992100	0.36156400	-2.12245000
C	-2.18280300	2.34480800	-0.71713100
C	-3.17206500	0.49924400	-2.61545800
C	-3.46695500	2.46531000	-1.25604500
C	-3.95943700	1.56581000	-2.19540600
H	-3.55778000	-0.22665900	-3.32355500
H	-4.10257200	3.27967600	-0.91900400
H	-1.24066700	-0.46371300	-2.41968200
H	-4.96763200	1.68450900	-2.57954400
C	-1.69677400	3.34086600	0.32289200
C	-2.68710600	3.47242700	1.48422800
C	-1.42558900	4.70360000	-0.32454900
H	-0.76270400	2.96151700	0.74597300
H	-2.29212800	4.16951400	2.23004000

H	-3.65463300	3.86174100	1.15051200
H	-2.84082500	2.50490700	1.96650300
H	-0.68538600	4.61091300	-1.12220700
H	-2.34629300	5.11465600	-0.75293900
H	-1.05401200	5.41474100	0.42015200
C	1.21420300	-2.93297900	1.58743000
C	1.26558500	-2.44906200	0.34301400
C	0.12861400	-1.75585500	-0.36509700
O	-0.00602700	-2.00745600	-1.57618800
C	2.33179300	-3.73002300	2.19215300
H	3.13728200	-3.90477200	1.47559700
H	2.74044700	-3.20174900	3.06206100
H	1.96724900	-4.69844000	2.55206400
C	0.00107000	-2.71244600	2.44734100
H	0.30083500	-2.49624300	3.47798500
H	-0.59109200	-3.63629900	2.48025100
H	2.12522200	-2.65657200	-0.29010800
C	-0.87259600	-1.58645900	1.90553700
N	-1.11229500	-1.66759000	0.45211200
N	-1.90705100	-2.78946500	0.16529000
O	-3.43448100	-3.70337500	-1.17761600
C	-4.08765900	-1.61037700	-0.27417000
C	-3.88778300	-0.51840600	0.57628800
C	-4.92748500	0.38023500	0.80355500
C	-6.15664700	0.22148700	0.17197800
C	-6.34921900	-0.84651100	-0.70196300
C	-5.32343900	-1.75795100	-0.91586500
H	-2.92679300	-0.33005300	1.03607000
H	-4.76176800	1.22456000	1.46566400
H	-7.30223000	-0.97667300	-1.20510400
H	-5.46130000	-2.61078400	-1.57098300
C	-0.37604600	-0.17958000	2.24119400
O	-1.05810800	0.80783000	2.09396200
O	0.85981300	-0.15845200	2.75518400
C	1.38294900	1.12534700	3.14139600
C	2.46726000	0.87555300	4.16746800
H	0.56988800	1.73608900	3.53959400
H	1.77429500	1.62250200	2.24472700
H	2.97126300	1.81311700	4.41311300
H	2.04334300	0.45616700	5.08250400
H	3.20986600	0.17058600	3.78347400
H	-1.86360600	-1.63658700	2.36736700
H	-1.38681600	-3.60865600	-0.14369200
C	-3.11277200	-2.73067000	-0.51232900

H	-6.95848300	0.93111300	0.35272300
P(R)			
C	3.14686400	-0.80175700	0.71244300
C	2.05370100	-1.21619400	1.36834900
C	0.82012600	-1.60569600	0.64542600
O	0.01311500	-2.40755600	1.08374000
C	4.46458500	-0.55542600	1.37638800
H	5.25246900	-1.13384800	0.88160500
H	4.73477200	0.50162800	1.27654000
H	4.44312800	-0.81981300	2.43468500
C	3.06324200	-0.56829200	-0.77975400
H	3.78009400	0.19403500	-1.09086200
H	3.29805600	-1.49362300	-1.31923900
H	2.05883700	-1.43031000	2.43158900
C	1.65158100	-0.09277600	-1.11853700
N	0.66261700	-1.02834100	-0.60349000
N	-0.23966300	-1.60143100	-1.49080100
O	-2.15853800	-2.78841100	-1.46342300
C	-2.22485800	-0.73422900	-0.27416000
C	-2.25249300	0.58739700	-0.71340100
C	-3.00454300	1.52947700	-0.01543100
C	-3.70018900	1.15600900	1.13190100
C	-3.66137500	-0.16546300	1.57534900
C	-2.93876200	-1.11486900	0.86274400
H	-1.69601700	0.87095100	-1.60166700
H	-3.05379600	2.55531200	-0.36828900
H	-4.20503600	-0.45592200	2.46826100
H	-2.90675700	-2.15183300	1.18005400
C	1.50691700	1.33274800	-0.55933700
O	2.38862700	2.15336400	-0.67481300
O	0.34477100	1.54808700	0.03872100
C	0.12465100	2.87004400	0.56741700
C	-0.18455900	3.86158000	-0.53736000
H	1.00946800	3.16890800	1.13471600
H	-0.72166300	2.74341000	1.24408800
H	-0.44699800	4.82829000	-0.10024900
H	0.68116000	3.99749500	-1.18712400
H	-1.02938600	3.51451800	-1.13772100
H	1.50251100	-0.02988300	-2.19987500
H	0.10790700	-2.46684500	-1.90263200
C	-1.56378500	-1.80291800	-1.08118900
H	-4.27984300	1.89424200	1.67727200

P(S)

C	3.30942400	0.70219900	-0.26502600
C	3.03448800	-0.45211300	-0.87946600
C	2.04468600	-1.42703400	-0.36699800
O	1.98304500	-2.57226700	-0.77598800
C	4.38646200	1.63699300	-0.72090200
H	4.94691200	1.22550800	-1.56159300
H	3.95019300	2.59520300	-1.02330000
H	5.08247500	1.84679300	0.09901800
C	2.54559700	1.09548700	0.97528700
H	2.43295500	2.18428200	1.02655000
H	3.12167900	0.79821100	1.86060100
H	3.57967400	-0.78405000	-1.75627800
C	1.15839200	0.44654900	1.01745300
N	1.23536700	-0.96668100	0.66091600
N	0.46055500	-1.86890000	1.35764700
O	-1.52502200	-2.27755800	2.33358900
C	-1.61409200	-1.31099500	0.15837000
C	-1.17702800	-1.61263200	-1.13221600
C	-1.89297000	-1.13382400	-2.22463100
C	-3.02966900	-0.35278900	-2.03019100
C	-3.46981400	-0.06054100	-0.73898200
C	-2.76749200	-0.54908400	0.35705600
H	-0.29068200	-2.22524600	-1.27292600
H	-1.56038900	-1.36794500	-3.23029500
H	-4.36146700	0.54061200	-0.58822300
H	-3.10040300	-0.35282200	1.37184200
C	0.22864700	1.20498700	0.06271200
O	0.26168900	1.11301400	-1.13820100
O	-0.58345000	2.01937100	0.74263300
C	-1.49914700	2.79448500	-0.05688100
C	-2.57112400	3.31856800	0.87086200
H	-1.90810700	2.14404400	-0.83377500
H	-0.93819000	3.60004800	-0.54078300
H	-3.28244200	3.92769800	0.30834100
H	-3.11185400	2.48740900	1.33063800
H	-2.13736000	3.93312100	1.66293200
H	0.74370100	0.50984600	2.02526200
H	0.86702200	-2.21733000	2.21985400
C	-0.92228000	-1.84706400	1.36736100
H	-3.57973800	0.02404800	-2.88691800

Z-TS6(R)

C	-2.18876100	3.66699800	-1.12531000
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C	-1.81085500	2.32798200	-1.07497100
C	-2.65614100	1.34996700	-0.56530800
C	-3.88908800	1.74657300	-0.05448000
C	-4.26390300	3.09354900	-0.06778400
C	-3.42193900	4.06195900	-0.61140900
C	-1.15298600	4.51199000	-1.81576900
C	0.03775400	3.56298700	-2.09615600
C	-0.45034900	2.11061800	-1.68776700
H	-2.36227000	0.30584100	-0.55169400
H	-4.55429700	0.99032100	0.34787300
H	-5.22724000	3.38857500	0.33727200
H	-3.72480200	5.10471400	-0.64094000
H	-0.81497000	5.36322100	-1.21490300
H	0.30241700	3.55654500	-3.15381600
H	-1.54199000	4.92271200	-2.75248200
H	-0.50271400	1.44823100	-2.54940200
N	0.52420700	1.48066600	-0.76383600
O	1.21816900	3.99626800	-1.44202300
C	0.95548100	0.20398800	-0.64987500
C	1.32204000	2.24559500	0.04145900
N	2.01936200	0.26897700	0.17254300
N	2.25757600	1.53877700	0.60165000
C	1.19635400	3.72540700	-0.05183200
H	0.27171900	4.07691400	0.42388000
H	2.05559100	4.20695800	0.41420200
C	3.09936700	-0.68181500	0.31622500
C	3.21919900	-1.39089000	1.50443000
C	3.99636300	-0.82042200	-0.75012200
C	4.23724600	-2.32867300	1.62605500
C	5.00041200	-1.78200300	-0.59662000
C	5.11749800	-2.53469500	0.56655000
H	4.33294000	-2.89600000	2.54523700
H	5.70753300	-1.93818600	-1.40620000
H	2.52495800	-1.22657300	2.32096600
H	5.90656600	-3.27494600	0.65060600
C	3.91407200	0.00019600	-2.02594700
C	3.50598400	-0.87817500	-3.21497400
C	5.23741000	0.72335700	-2.30124800
H	3.15141500	0.77676600	-1.89797800
H	3.41877100	-0.27341800	-4.12211200
H	4.26008100	-1.65124900	-3.39517400
H	2.54912800	-1.37651600	-3.03409700
H	5.52999900	1.34422000	-1.45076400
H	6.04455200	0.01169100	-2.49935500

H	5.13660800	1.36481400	-3.18111200
C	0.03658900	-3.43520500	-0.98271300
C	0.78643000	-2.27635400	-0.97006300
C	0.24842100	-0.98761100	-1.27313900
O	-0.71589500	-0.70523000	-1.99863900
C	0.67857500	-4.72645200	-0.54402100
H	1.70407700	-4.57487100	-0.19807400
H	0.10137100	-5.18646400	0.26715500
H	0.69595700	-5.44967500	-1.36595900
C	-1.37240200	-3.39824500	-1.12666100
H	-1.77725200	-2.66058400	-1.80911100
H	-1.89306500	-4.35376600	-1.12234700
H	1.79922000	-2.34045300	-0.59856700
C	-1.92804500	-2.61971200	0.56510100
N	-1.27244100	-1.52011900	0.97878700
N	-0.33497400	-1.83287900	1.94744100
O	0.99074400	-1.49126300	3.70845300
C	-0.04059300	0.46956700	2.84579400
C	-1.13377500	1.09256500	2.23549400
C	-1.27576400	2.47841300	2.30715400
C	-0.33324900	3.24877800	2.98465900
C	0.75787600	2.63150700	3.59682300
C	0.89614900	1.25064100	3.53555300
H	-1.86564700	0.49221400	1.71256200
H	-2.13259400	2.94788500	1.82931300
H	1.49449000	3.22509000	4.12901200
H	1.72544200	0.74861600	4.02173600
C	-3.35446800	-2.40280500	0.15425900
O	-3.87270100	-1.34331700	-0.10772300
O	-4.00861300	-3.57751500	0.10471000
C	-5.36010800	-3.52536700	-0.38002000
C	-5.38305800	-3.42319300	-1.89348100
H	-5.87076300	-2.67816900	0.08335600
H	-5.81330300	-4.45483700	-0.03177800
H	-6.41399500	-3.44982800	-2.25551900
H	-4.92606000	-2.48542200	-2.21596200
H	-4.83666500	-4.25775200	-2.33989700
H	-1.82754200	-3.53278200	1.16382200
H	-0.06114100	-2.80495500	2.08116000
C	0.21149200	-1.01032800	2.87041300
H	-0.45163500	4.32744100	3.04297100

Z-TS-6(S)

C	-5.46429200	0.36700500	-0.71468700
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C	-4.30996800	0.78574900	-0.04482400
C	-3.78555900	2.05992700	-0.24260100
C	-4.41830800	2.90156800	-1.15489500
C	-5.55782200	2.47981800	-1.84049300
C	-6.09512100	1.21226500	-1.61925200
C	-5.86729000	-1.01966100	-0.28328200
C	-5.11305600	-1.16736400	1.05562100
C	-3.83942800	-0.29424900	0.90394400
H	-2.90767300	2.38787200	0.30438700
H	-4.02196600	3.89725300	-1.32505400
H	-6.04002600	3.15157000	-2.54356000
H	-6.99627000	0.89639100	-2.13599900
H	-5.53659800	-1.76016200	-1.02154500
H	-5.71108800	-0.71361200	1.84895700
H	-6.94483200	-1.14437600	-0.15714400
H	-3.44350900	0.08049400	1.84866300
N	-2.78450200	-1.16599800	0.32105000
O	-4.85307700	-2.48373700	1.49263800
C	-1.56562300	-0.81467000	-0.12666200
C	-2.88773000	-2.52149000	0.15366400
N	-0.98833300	-1.93377400	-0.53748700
N	-1.80496400	-3.01462100	-0.37697100
C	-4.11222800	-3.26794700	0.58660800
H	-4.70452200	-3.56077700	-0.28871400
H	-3.81122900	-4.17532200	1.11266100
C	0.36717000	-2.09968100	-1.00379200
C	0.53211900	-2.34941000	-2.36066900
C	1.42370800	-2.03532200	-0.08620100
C	1.81300100	-2.54608000	-2.85871600
C	2.69631100	-2.24335200	-0.62573900
C	2.89090800	-2.49322100	-1.98147800
H	1.96722100	-2.72524200	-3.91644900
H	3.56265300	-2.18487900	0.02343400
H	-0.34020700	-2.38189400	-3.00587200
H	3.90053000	-2.62588900	-2.35640000
C	1.19791900	-1.77844800	1.39737800
C	2.49074100	-1.46979300	2.14537300
C	0.49775100	-2.97004100	2.07055200
H	0.57561400	-0.87687900	1.47973300
H	2.25036900	-1.22372800	3.18421600
H	3.16251300	-2.33585500	2.15851300
H	2.99415100	-0.61301400	1.69668000
H	1.13911400	-3.85646300	2.02330300
H	0.31447300	-2.74456600	3.12579600

H	-0.45630800	-3.23153700	1.60882900
C	-0.32602100	2.44910700	-1.56777000
C	-0.77190400	1.15424100	-1.37506600
C	-1.03594000	0.60432400	-0.09342500
O	-1.09312700	1.12323700	1.03229100
C	-0.12852300	2.98638900	-2.96127500
H	-0.22670600	2.20908000	-3.72298900
H	-0.86945500	3.76532800	-3.17263500
H	0.85882800	3.45039800	-3.05708000
C	0.09507300	3.22551200	-0.44723700
H	-0.55741400	3.19822200	0.41795400
H	0.43220600	4.23325100	-0.68850000
H	-0.94080600	0.50438700	-2.23021100
C	1.54189600	2.34839200	0.33609500
N	1.80903600	1.07478200	-0.06134800
N	2.33499800	1.13610400	-1.36298800
O	3.66805600	0.48630100	-3.04455100
C	4.63214800	0.33127700	-0.88130000
C	4.73437300	0.78618100	0.43631800
C	5.84515500	0.44717300	1.20771600
C	6.85787900	-0.34769700	0.67899200
C	6.76849500	-0.79109700	-0.63979000
C	5.66913700	-0.44194300	-1.41440100
H	3.93783600	1.37782200	0.86849600
H	5.91308600	0.80508000	2.23045600
H	7.55916500	-1.40173800	-1.06476000
H	5.58709400	-0.75207100	-2.45065100
C	1.24380000	2.48753100	1.81638400
O	0.77263600	3.48142000	2.32367000
O	1.63133900	1.41574200	2.52035800
C	1.32595800	1.43674200	3.91999700
C	-0.09033900	0.94544500	4.15093300
H	1.46491000	2.44885700	4.30594500
H	2.06241600	0.77220400	4.37712000
H	-0.30970300	0.91351000	5.22162400
H	-0.80099300	1.61123200	3.65744800
H	-0.21416200	-0.05827700	3.73287500
H	2.26046500	3.12043800	0.02707400
H	1.65875100	1.29459400	-2.10953800
C	3.50327500	0.64364000	-1.83036300
H	7.71580100	-0.61576900	1.28795400
Z-M6(R)			
C	5.09076700	0.35199200	-0.61814800

C	4.00793600	-0.14763800	0.11165000
C	3.86564000	-1.51413800	0.34200700
C	4.79916200	-2.37807800	-0.22691900
C	5.85303400	-1.88539000	-0.99946100
C	6.01478200	-0.51458300	-1.19182200
C	5.10835700	1.85744800	-0.57754600
C	4.27007900	2.11280500	0.69244300
C	3.19408600	0.99158300	0.68528300
H	3.01165500	-1.87089700	0.91001700
H	4.70422600	-3.44751700	-0.06710000
H	6.56826100	-2.57641400	-1.43503300
H	6.85815200	-0.13009500	-1.75759600
H	4.63236200	2.28000900	-1.47084600
H	4.89915700	1.91100400	1.56303100
H	6.11048600	2.28448300	-0.49982200
H	2.77541200	0.75887200	1.66421400
N	2.01268100	1.49876900	-0.11123500
O	3.78856700	3.42229800	0.87917800
C	0.79629000	0.91487600	-0.31010800
C	1.82927900	2.84535400	-0.31751300
N	-0.04198100	1.91309300	-0.58200200
N	0.59836900	3.12513500	-0.60838800
C	2.92339000	3.84791800	-0.14532500
H	3.45463600	4.00070200	-1.09346300
H	2.48293200	4.79759600	0.16014600
C	-1.48610300	1.99500200	-0.57114600
C	-2.09882300	2.41217600	-1.74664500
C	-2.16629000	1.85100600	0.64501600
C	-3.45595200	2.70317500	-1.73842600
C	-3.53000900	2.16654500	0.61497800
C	-4.16608700	2.59003500	-0.54657200
H	-3.95012800	3.01161600	-2.65303600
H	-4.11544000	2.05975600	1.52090300
H	-1.50650000	2.49759200	-2.65155800
H	-5.22835400	2.81070500	-0.52376100
C	-1.46870500	1.40106700	1.92334500
C	-2.45115100	0.94259300	3.00150900
C	-0.58559400	2.51685900	2.50442700
H	-0.83314000	0.53754400	1.68122000
H	-1.89072100	0.55937800	3.85854300
H	-3.06882700	1.77177500	3.36350300
H	-3.10884200	0.14775800	2.63942900
H	-1.19662600	3.38489700	2.77388300
H	-0.08526900	2.15845400	3.40950800

H	0.18418900	2.86033900	1.81021400
C	1.25930400	-2.53824400	-1.61924400
C	1.47985300	-1.26645200	-1.28060400
C	0.64955100	-0.61076500	-0.15531000
O	1.03712900	-0.89233800	1.07519000
C	2.13830400	-3.27985500	-2.58475600
H	2.91287100	-2.62932500	-2.99771200
H	2.63295000	-4.11574700	-2.07588200
H	1.55437200	-3.70576500	-3.40830000
C	0.11194500	-3.32074600	-1.03165500
H	0.50258100	-4.17433100	-0.46804900
H	-0.47375700	-3.73647000	-1.86113900
H	2.30210300	-0.72117200	-1.73547100
C	-0.80545100	-2.50647900	-0.10408400
N	-0.78994200	-1.04776600	-0.37332700
N	-1.18947800	-0.80300000	-1.69636100
O	-2.58441900	-0.52279000	-3.39572800
C	-3.67740500	-0.66201600	-1.29583100
C	-3.71107900	-0.91625900	0.07954600
C	-4.93238900	-0.93446100	0.75254800
C	-6.12094300	-0.67844100	0.07805600
C	-6.09192700	-0.41192500	-1.29026000
C	-4.88122200	-0.41408500	-1.96835900
H	-2.79741000	-1.06663100	0.64100100
H	-4.94650400	-1.14564700	1.81798500
H	-7.01321900	-0.21049200	-1.82760500
H	-4.83675100	-0.21858500	-3.03358500
C	-0.52321600	-2.78503700	1.37096500
O	0.17854400	-3.68334800	1.77270300
O	-1.31035700	-2.04271300	2.16773000
C	-1.07799900	-2.20266700	3.57458900
C	0.19065200	-1.48799500	4.00196500
H	-1.02508100	-3.26961700	3.80626700
H	-1.96490800	-1.77801900	4.04967800
H	0.31735000	-1.57745900	5.08478200
H	1.05304900	-1.92305200	3.49493500
H	0.14643700	-0.43076800	3.72789300
H	-1.84411100	-2.82300900	-0.26052500
H	-0.51323700	-1.00888100	-2.42850300
C	-2.45903400	-0.65094500	-2.18100700
H	-7.06578100	-0.69048300	0.61292800

Z-M6(S)

C	3.27437000	-2.45692900	-1.17279300
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C	2. 47279100	-1. 32494200	-1. 05639800
C	2. 99585900	-0. 11348500	-0. 62527100
C	4. 33392400	-0. 06114400	-0. 24537300
C	5. 13903100	-1. 20130000	-0. 33144600
C	4. 61729200	-2. 40314800	-0. 80507700
C	2. 52284900	-3. 61412900	-1. 76594500
C	1. 11902100	-3. 05313900	-2. 10008600
C	1. 06807400	-1. 56605100	-1. 54633500
H	2. 34134500	0. 74761100	-0. 59491900
H	4. 73879700	0. 87401300	0. 12840400
H	6. 18262900	-1. 14813500	-0. 03611900
H	5. 24925600	-3. 28215100	-0. 89491800
H	2. 44129900	-4. 46133900	-1. 07552100
H	0. 97648300	-2. 99818500	-3. 18027900
H	3. 00879200	-3. 99557500	-2. 66836800
H	0. 80204800	-0. 84082200	-2. 31543300
N	-0. 02604100	-1. 41494500	-0. 53609800
O	0. 08847800	-3. 91341200	-1. 64918500
C	-0. 83813700	-0. 35992100	-0. 28047300
C	-0. 61952500	-2. 51269500	0. 03038500
N	-1. 89292200	-0. 88348700	0. 36298500
N	-1. 76693200	-2. 22566100	0. 56547900
C	-0. 06541500	-3. 86182000	-0. 24318600
H	0. 88354400	-4. 01408500	0. 28728300
H	-0. 78014900	-4. 62724900	0. 05787900
C	-3. 22907500	-0. 33298400	0. 43517300
C	-3. 65686600	0. 31033900	1. 58645800
C	-4. 03376200	-0. 49245400	-0. 70349900
C	-4. 92468600	0. 88363200	1. 59979400
C	-5. 29693200	0. 10203000	-0. 65483500
C	-5. 73474300	0. 79247600	0. 47285100
H	-5. 27147200	1. 39852800	2. 48900000
H	-5. 95379400	0. 02294100	-1. 51483100
H	-3. 01171800	0. 36385900	2. 45760900
H	-6. 72052000	1. 24647100	0. 47319300
C	-3. 55812200	-1. 23777000	-1. 94546400
C	-2. 89322400	-0. 30102800	-2. 96853300
C	-4. 69799900	-2. 01284100	-2. 61567700
H	-2. 81498300	-1. 97874100	-1. 63033500
H	-2. 66422600	-0. 86251200	-3. 87953600
H	-3. 57442600	0. 51395800	-3. 23686800
H	-1. 95913700	0. 14610500	-2. 61295400
H	-5. 25207900	-2. 61779700	-1. 89331100
H	-5. 40210100	-1. 33890300	-3. 11365100

H	-4.28878300	-2.67703100	-3.38115400
C	-1.54688800	3.33979000	-0.67459200
C	-1.73479500	2.02062000	-0.74258000
C	-0.48499100	1.13561000	-0.61781800
O	0.34377500	1.19273400	-1.62174800
C	-2.64420400	4.34774000	-0.85336500
H	-3.61201300	3.86119500	-0.99760000
H	-2.71247100	5.00894400	0.01804700
H	-2.44352400	4.98755900	-1.72044400
C	-0.13811000	3.84427100	-0.50672300
H	0.35619000	3.76557500	-1.47696700
H	-0.12144500	4.89596400	-0.20585800
H	-2.72366600	1.62271000	-0.93541700
C	0.66896300	3.01085400	0.51864800
N	0.22707600	1.60767400	0.69321600
N	-0.60091300	1.53700400	1.81775300
O	-1.36841800	0.69086900	3.73509500
C	0.41676900	-0.52874600	2.76234700
C	1.72065400	-0.46305900	2.26726900
C	2.50847700	-1.61398100	2.26243300
C	2.00293700	-2.82242900	2.73435800
C	0.70421000	-2.88533600	3.23931400
C	-0.07942000	-1.73787700	3.26635000
H	2.11304900	0.47149100	1.88004400
H	3.51849000	-1.56351500	1.86756300
H	0.30586100	-3.82205500	3.61672300
H	-1.08906300	-1.76062500	3.66276700
C	2.17690700	3.10031100	0.30846300
O	2.98380400	2.42507300	0.90606400
O	2.51310800	4.08572900	-0.52923300
C	3.91660200	4.26640300	-0.78656600
C	4.35382700	3.36873400	-1.92754200
H	4.47471600	4.05820000	0.12844100
H	4.01905800	5.32223800	-1.04287200
H	5.41503300	3.52264100	-2.13964900
H	4.19854700	2.31850800	-1.66898200
H	3.77995500	3.59227300	-2.82934100
H	0.53946800	3.46992300	1.50527100
H	-1.39149100	2.17752300	1.87614200
C	-0.54384600	0.62144200	2.82408300
H	2.62374600	-3.71380900	2.71558000

Z-TS7(R)

C	-5.01390600	-0.10500000	-0.62671300
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C	-4.03416200	0.25119000	0.30847400
C	-3.81266500	1.58026700	0.64717600
C	-4.53459200	2.56439200	-0.02820700
C	-5.46479200	2.21721100	-1.00784500
C	-5.72333400	0.87772500	-1.30556100
C	-5.19516900	-1.60242500	-0.64866300
C	-4.63647400	-1.96441200	0.74682300
C	-3.43870900	-0.99356400	0.91996900
H	-3.04993500	1.84226600	1.37252900
H	-4.36335100	3.60988100	0.20630600
H	-6.01346300	2.99705900	-1.52686100
H	-6.48408600	0.61054100	-2.03303100
H	-4.59983800	-2.06223300	-1.44720200
H	-5.37816000	-1.67918800	1.49755300
H	-6.23304100	-1.91702300	-0.77673700
H	-3.14498000	-0.86438500	1.96440600
N	-2.26802400	-1.59153400	0.21428800
O	-4.35287200	-3.31703500	0.99931300
C	-1.01539300	-1.05533200	0.01780500
C	-2.19585600	-2.95863800	0.04196000
N	-0.28190900	-2.15115400	-0.23384800
N	-0.99003000	-3.33373700	-0.23491100
C	-3.38335800	-3.86199900	0.13383800
H	-3.79737700	-4.03359800	-0.86914300
H	-3.07512600	-4.82423600	0.54476300
C	1.14877000	-2.31306400	-0.21696300
C	1.71796300	-2.97202500	-1.30131400
C	1.88439400	-1.97473400	0.93018900
C	3.05939800	-3.32936800	-1.26665100
C	3.22786300	-2.36656700	0.93719300
C	3.81037600	-3.03760200	-0.13284800
H	3.50986200	-3.82837300	-2.11781800
H	3.84328500	-2.12193700	1.79550300
H	1.09787200	-3.19596400	-2.16252800
H	4.86073000	-3.30759000	-0.08876500
C	1.25576400	-1.25468100	2.11738400
C	2.28830000	-0.67382200	3.08526700
C	0.30753100	-2.18930200	2.88557700
H	0.67798900	-0.40808400	1.72901300
H	1.77602100	-0.08798700	3.85401900
H	2.85255100	-1.46093000	3.59745100
H	2.99592300	-0.01431400	2.57364500
H	0.87057200	-3.01663100	3.33075400
H	-0.18869100	-1.64116000	3.69263600

H	-0.46474900	-2.62427300	2.24526000
C	-0.99516600	2.60463000	-1.87736900
C	-1.40905000	1.56041800	-1.14892300
C	-0.54125700	1.15966200	0.01469700
O	-0.77293000	1.50281300	1.16534500
C	-1.83294900	3.19475900	-2.97477400
H	-2.78911200	2.67431600	-3.06418200
H	-2.03239700	4.25268300	-2.77216800
H	-1.30918600	3.14568700	-3.93591700
C	0.35004500	3.25626500	-1.64495500
H	0.20364200	4.30017800	-1.34812500
H	0.88279700	3.27648600	-2.60327600
H	-2.36462500	1.08847200	-1.32989800
C	1.22671300	2.56164400	-0.58339600
N	0.88517900	1.12131700	-0.39446700
N	1.06073900	0.43797500	-1.60760100
O	2.18424400	-0.45453200	-3.29608400
C	3.54302400	0.05817900	-1.41866900
C	3.73763200	0.52493900	-0.11482900
C	5.01521700	0.52587500	0.44171300
C	6.10361600	0.05265500	-0.28306500
C	5.91442600	-0.42034300	-1.58122300
C	4.64513800	-0.41225200	-2.14303300
H	2.89787200	0.85701300	0.48146100
H	5.15146600	0.89447800	1.45451500
H	6.75775900	-0.79191800	-2.15472000
H	4.47456600	-0.78039400	-3.14838000
C	1.19889500	3.27011300	0.77158000
O	0.68248600	4.34326600	0.96953300
O	1.90115700	2.58996200	1.68178800
C	1.88193500	3.11367000	3.02059700
C	0.55922000	2.82360100	3.70355900
H	2.08499300	4.18697900	2.98280800
H	2.71104000	2.60692800	3.51860900
H	0.60631100	3.15165600	4.74552700
H	-0.25245300	3.34987400	3.19934000
H	0.33989700	1.75431600	3.66988300
H	2.27613700	2.58224200	-0.89994400
H	0.30658400	0.49654000	-2.28631700
C	2.23201400	-0.00650400	-2.15416800
H	7.09592000	0.05339800	0.15788000

Z-TS7(S)

C	3.87238300	-1.10489100	-1.11579100
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C	2. 65227000	-0. 42723600	-1. 16708000
C	2. 61724900	0. 96300300	-1. 09059500
C	3. 81550100	1. 66114400	-0. 95748900
C	5. 03546600	0. 98415800	-0. 92523500
C	5. 07003200	-0. 40576300	-0. 99975200
C	3. 68406000	-2. 58574300	-1. 26500100
C	2. 29542800	-2. 68066600	-1. 92445000
C	1. 51588600	-1. 36532000	-1. 53847800
H	1. 67356400	1. 49230000	-1. 14928000
H	3. 78282000	2. 74354900	-0. 88827900
H	5. 96338200	1. 54297200	-0. 84379500
H	6. 01624600	-0. 93964900	-0. 98213800
H	3. 70338800	-3. 07425000	-0. 28343200
H	2. 42777400	-2. 64524700	-3. 00850500
H	4. 44713900	-3. 06514000	-1. 88313700
H	0. 98479300	-0. 96829600	-2. 40764500
N	0. 43548500	-1. 66267600	-0. 56212900
O	1. 61833300	-3. 89495000	-1. 68324600
C	-0. 67504300	-0. 90170600	-0. 31741600
C	0. 20346300	-2. 93486500	-0. 09111100
N	-1. 48584300	-1. 77575700	0. 29652600
N	-0. 97418200	-3. 04050100	0. 44319600
C	1. 17903200	-4. 02827000	-0. 34541800
H	2. 01263100	-3. 98032900	0. 36813800
H	0. 68521300	-4. 99516500	-0. 24901200
C	-2. 88757300	-1. 54892100	0. 51340000
C	-3. 33808600	-1. 21688100	1. 78564900
C	-3. 74172800	-1. 63898400	-0. 59368300
C	-4. 67939900	-0. 89401000	1. 96505100
C	-5. 08210200	-1. 30180100	-0. 38171100
C	-5. 54566900	-0. 92208600	0. 87516800
H	-5. 04400000	-0. 62230400	2. 95003600
H	-5. 77861500	-1. 34241900	-1. 21358400
H	-2. 62466800	-1. 20727600	2. 60490800
H	-6. 59169600	-0. 66271900	1. 00524900
C	-3. 23915900	-2. 06308500	-1. 96574400
C	-2. 92343200	-0. 84977100	-2. 85286700
C	-4. 22791300	-2. 99586600	-2. 67248700
H	-2. 31081300	-2. 62652200	-1. 81772400
H	-2. 61624800	-1. 18459600	-3. 84847000
H	-3. 81539200	-0. 22327400	-2. 96975900
H	-2. 11979000	-0. 23198100	-2. 43927800
H	-4. 51410200	-3. 83496100	-2. 03310100
H	-5. 13760400	-2. 46515100	-2. 97031500

H	-3.77276200	-3.39491300	-3.58306300
C	-2.71320900	2.49392900	0.65963300
C	-2.33246100	1.50672300	-0.16043700
C	-0.86646700	1.31990600	-0.40919200
O	-0.36303500	1.66443500	-1.46970200
C	-4.15861900	2.83751700	0.87888100
H	-4.81231400	2.17560400	0.30681700
H	-4.41747200	2.74499800	1.94015900
H	-4.35996900	3.87409400	0.58770900
C	-1.71334500	3.32584400	1.43448700
H	-1.88091600	4.38398500	1.20990400
H	-1.92627900	3.20743700	2.50488800
H	-3.05458100	0.94339900	-0.74092200
C	-0.23537500	2.96593300	1.17691900
N	-0.06537900	1.52701800	0.83980300
N	-0.53896500	0.79628800	1.93521400
O	-0.53864600	-1.02587000	3.22807500
C	1.57116000	-0.47794100	2.31859000
C	2.49446200	0.54653900	2.10615700
C	3.85440600	0.24893500	2.08872400
C	4.29275100	-1.06333700	2.23552400
C	3.36969500	-2.09180700	2.42478600
C	2.01443100	-1.79430700	2.48699800
H	2.16288700	1.56488000	1.93419900
H	4.57315600	1.04529800	1.93127500
H	3.70896900	-3.11629900	2.54853500
H	1.27438900	-2.56465500	2.68221500
C	0.48499400	3.78707100	0.10960100
O	1.69071800	3.79873800	0.01847600
O	-0.33849300	4.49823700	-0.65720600
C	0.27833100	5.22692500	-1.73661800
C	0.64741100	4.30045900	-2.87892200
H	1.15466000	5.75059100	-1.34627600
H	-0.47599700	5.95644100	-2.03534600
H	1.03335100	4.88985700	-3.71504600
H	1.41317400	3.58980400	-2.56150200
H	-0.22639000	3.73569300	-3.20783500
H	0.34621700	3.12793400	2.08910200
H	-1.54795000	0.77843100	2.07675900
C	0.10448700	-0.26682800	2.51003500
H	5.35506200	-1.28543300	2.19735000

When the reaction in 1,4-dioxane:

M4-NHC

C	3.54047800	0.56417100	-0.10040200
C	2.60972100	1.05336900	-1.02383700
C	2.27949100	2.40399100	-1.08101100
C	2.86888000	3.26939000	-0.16060900
C	3.77354600	2.78298000	0.78462100
C	4.12369900	1.43359200	0.81410900
C	3.78919300	-0.90787900	-0.29623600
C	3.19315600	-1.15575800	-1.70073000
C	2.08171100	-0.08675400	-1.85851700
H	1.58951900	2.78007000	-1.82997300
H	2.62862100	4.32738500	-0.18531400
H	4.22231700	3.46854900	1.49672200
H	4.84336400	1.06587200	1.53860800
H	3.28460500	-1.51347000	0.46787400
H	3.94536900	-0.93721800	-2.46308600
H	4.85264700	-1.15972800	-0.27118300
H	1.84509700	0.15609600	-2.89563500
N	0.85533100	-0.65430700	-1.24374300
O	2.74312700	-2.46140700	-1.98388400
C	-0.23016000	0.00187500	-0.81330400
C	0.69795500	-1.95660500	-0.86680600
N	-1.00317900	-0.90570000	-0.23515000
N	-0.45034300	-2.13884200	-0.27129100
C	1.78918900	-2.95915100	-1.06427000
H	2.21525500	-3.17079900	-0.07329100
H	1.37768700	-3.87612400	-1.48938500
C	-2.23048800	-0.66698300	0.47602400
C	-2.13718000	-0.70316500	1.86514500
C	-3.40996600	-0.40880200	-0.22345500
C	-3.28281900	-0.43969600	2.60509500
C	-4.54016200	-0.14698900	0.55869600
C	-4.47953800	-0.15466900	1.94781100
H	-3.24035100	-0.45810700	3.68854200
H	-5.48661200	0.05586000	0.06599200
H	-1.17358300	-0.92401500	2.32421000
H	-5.37638500	0.05441900	2.52207900
C	-3.50636400	-0.46926900	-1.73782700
C	-4.11710100	0.80432900	-2.32891100
C	-4.30380800	-1.71095500	-2.15794800
H	-2.49719900	-0.57222700	-2.15123100
H	-4.12686600	0.74228100	-3.42025800
H	-5.14925500	0.94244100	-1.99250500
H	-3.54474700	1.69029500	-2.04269200
H	-3.84870600	-2.62221000	-1.76147800

H	-5.33096300	-1.65310600	-1.78372300
H	-4.34266100	-1.78631400	-3.24825500
C	-0.92288400	2.63424200	0.88642100
C	-1.21813300	2.39432500	-0.40790600
C	-0.65344500	1.37869500	-1.28921400
O	-0.58506900	1.51303800	-2.49940100
C	0.10460400	1.91453800	1.69700800
H	0.80396700	2.65561100	2.10224300
H	-0.36789000	1.42350500	2.55454100
H	0.68406600	1.15825600	1.17097700
C	-1.63243000	3.74612400	1.60339900
H	-0.90904800	4.46767800	1.99615000
H	-2.34767900	4.26618900	0.96481000
H	-2.16504800	3.33078200	2.46639800
H	-1.88697000	3.06788900	-0.93776100
H	0.87180000	-2.86027500	3.80441900
C	1.40327000	-1.87096200	2.28797100
O	1.17275300	-0.83550400	1.63175600
O	2.22349300	-2.78678300	2.07436000
O	0.60500900	-2.01578600	3.41986900

TS6(R)-NHC

C	-3.78445900	-2.16819200	0.09863400
C	-2.83423600	-1.49311700	-0.66301500
C	-2.94107900	-1.40474500	-2.04683000
C	-4.02978600	-2.01669100	-2.66473300
C	-4.99109000	-2.69040800	-1.90759000
C	-4.87652400	-2.76874700	-0.52089900
C	-3.47074000	-2.07663200	1.56983800
C	-2.03677800	-1.50633700	1.63818200
C	-1.79505700	-0.85451400	0.23202900
H	-2.20365900	-0.84076800	-2.60881400
H	-4.13762600	-1.96160700	-3.74337500
H	-5.83490800	-3.15903500	-2.40452400
H	-5.62623800	-3.29243300	0.06547600
H	-3.51155400	-3.03888900	2.08907700
H	-1.91896400	-0.74692700	2.41273000
H	-4.17384800	-1.39947900	2.06603600
H	-1.90102900	0.22911500	0.28538200
N	-0.43062400	-1.11312300	-0.21881300
O	-1.10332300	-2.52426600	1.98697000
C	0.46117200	-0.32943900	-0.84243900
C	0.18086000	-2.29572300	0.05615600
N	1.55626800	-1.09096200	-0.97258800

N	1. 39878900	-2. 32173000	-0. 39976800
C	-0. 56661200	-3. 26367100	0. 91116000
H	-1. 34699400	-3. 77208000	0. 32762800
H	0. 11786100	-4. 00589400	1. 32166400
C	2. 73553100	-0. 81743900	-1. 74618800
C	2. 54799800	-0. 46905000	-3. 08221800
C	4. 00263100	-0. 93631100	-1. 16574600
C	3. 65085100	-0. 21767500	-3. 88403800
C	5. 09303700	-0. 69178900	-2. 00865200
C	4. 92824800	-0. 33442500	-3. 34111300
H	3. 51258500	0. 05682400	-4. 92365200
H	6. 09683600	-0. 78304300	-1. 60670000
H	1. 54016400	-0. 40110300	-3. 47956800
H	5. 80054900	-0. 14856600	-3. 95924300
C	4. 22399000	-1. 34502300	0. 28079700
C	5. 29664100	-0. 48802400	0. 95967100
C	4. 58975800	-2. 83265400	0. 36451700
H	3. 28252000	-1. 20247900	0. 82481700
H	5. 37200700	-0. 75719800	2. 01659500
H	6. 28278700	-0. 65116200	0. 51504600
H	5. 05960800	0. 57697200	0. 88683600
H	3. 81117800	-3. 45130600	-0. 08584000
H	5. 53426200	-3. 02297500	-0. 15645700
H	4. 71277000	-3. 13091600	1. 41048300
C	2. 11710700	2. 44801600	-0. 77588600
C	1. 07987100	2. 05865000	-1. 61009200
C	0. 12927200	1. 00631600	-1. 46614400
O	-1. 00238800	1. 02471200	-1. 98918800
C	2. 81079500	3. 75841100	-1. 07516400
H	2. 93274200	4. 34809300	-0. 16029600
H	3. 81358700	3. 57510100	-1. 47532600
H	2. 25918800	4. 35554700	-1. 80467000
C	2. 46111200	1. 79430200	0. 42664200
H	2. 40633500	0. 71379600	0. 46967800
H	3. 28833000	2. 21107700	0. 99967200
H	0. 75514400	2. 76753400	-2. 36898400
C	0. 79086200	2. 00595300	1. 59613500
N	-0. 33288700	1. 89931900	0. 88962900
N	-0. 73480900	3. 14591600	0. 41454100
O	-1. 98902600	4. 18891900	-1. 14565300
C	-3. 03548500	2. 40179300	0. 03409500
C	-3. 34234700	2. 09664000	1. 36182800
C	-4. 45873800	1. 31639300	1. 65084900
C	-5. 25587400	0. 82653000	0. 61621300

C	-4.94533700	1.12864500	-0.70833800
C	-3.84327700	1.92660400	-0.99837100
H	-2.70101600	2.46413000	2.15673900
H	-4.70703300	1.08979500	2.68391800
H	-5.54982700	0.72299400	-1.51362500
H	-3.56868400	2.16376700	-2.02067800
C	1.10154800	0.82764000	2.45559500
O	0.87708700	-0.33034100	2.17004600
O	1.69461400	1.21011300	3.59347100
C	2.06213400	0.15628300	4.50107300
C	3.35931300	-0.49927500	4.07029100
H	1.24713400	-0.56961100	4.54572900
H	2.16367100	0.65084600	5.46806500
H	3.67585900	-1.23240000	4.81665900
H	3.22193800	-1.01298900	3.11574000
H	4.14654500	0.25137700	3.96299300
H	1.06956900	2.96696200	2.03162700
H	0.00499800	3.76672700	0.08867000
C	-1.88629100	3.29462400	-0.31760600
H	-6.11377400	0.19968200	0.84247100

M4-NHC1

C	-3.68888700	0.63252300	-0.22249000
C	-2.71880800	1.27721300	0.55016000
C	-2.31561600	2.57893600	0.26159200
C	-2.86437200	3.21627900	-0.85033900
C	-3.81108200	2.56482200	-1.64117400
C	-4.23868400	1.27709900	-1.32415200
C	-4.00651300	-0.73768100	0.30868800
C	-3.39718600	-0.69852000	1.72593700
C	-2.27135900	0.37537300	1.67727400
H	-1.61112700	3.10364200	0.89754700
H	-2.56425300	4.23104800	-1.09051500
H	-4.23191400	3.07358900	-2.50275400
H	-4.99048000	0.78118300	-1.93019300
H	-3.53661600	-1.50027100	-0.32276600
H	-4.14428300	-0.32362400	2.43023800
H	-5.08029300	-0.93776000	0.34943300
H	-2.12647900	0.88582900	2.63060800
N	-0.98980700	-0.31651500	1.38044100
O	-2.97238900	-1.92981200	2.26714500
C	0.18496400	0.22853600	1.04601000
C	-0.82952300	-1.66867000	1.28924100
N	1.01437800	-0.78229800	0.80623400

N	0.39997100	-1.97933800	0.97409100
C	-1.98481200	-2.58934600	1.49612300
H	-2.34534800	-2.89985800	0.50379100
H	-1.66273100	-3.46455400	2.06228500
C	2.40966900	-0.70460200	0.46157700
C	2.79335600	-1.15795100	-0.80734000
C	3.30708100	-0.18091200	1.39581300
C	4.13505600	-1.00218800	-1.14903400
C	4.63854200	-0.05575100	0.99805300
C	5.06684900	-0.44798300	-0.26838700
H	4.46084200	-1.33117100	-2.13288300
H	5.35720700	0.35297300	1.70400000
C	1.43866300	2.27571300	-1.03244100
C	1.39197800	2.40784500	0.30880100
C	0.54214700	1.68332000	1.24737800
O	0.15508300	2.15336600	2.30341700
C	0.54746100	1.40907200	-1.86576100
H	-0.12040600	0.72725900	-1.33697200
H	-0.08714300	2.06910500	-2.47066100
H	1.14744300	0.82607800	-2.57264500
C	2.41249100	3.10844800	-1.81514300
H	1.89233000	3.67784500	-2.59178400
H	2.97740200	3.79470900	-1.18299500
H	3.11558000	2.44201800	-2.32754400
H	1.98659700	3.17665700	0.79578700
H	-1.40790100	-2.95337300	-3.55682600
C	-1.67660000	-2.04675800	-1.93277000
O	-1.34509600	-1.04690600	-1.25850300
O	-2.47089200	-2.96467900	-1.63916900
O	-1.06190900	-2.13826700	-3.17182300
C	2.89522700	0.23680100	2.78529800
H	2.67903100	1.30861400	2.83807900
H	2.00974300	-0.30019900	3.13384900
H	3.70840000	0.03458400	3.48496600
C	6.51375000	-0.32193900	-0.66847500
H	7.03271800	0.41640000	-0.05397700
H	7.02990200	-1.27966300	-0.54843900
H	6.60770400	-0.02808100	-1.71661700
C	1.82127600	-1.81352700	-1.74985400
H	1.73072000	-2.87780900	-1.50787300
H	0.81559700	-1.39205700	-1.68746400
H	2.17717900	-1.73258300	-2.77908000

TS6(R)-NHC1

C	3.90547500	-0.82864800	-1.78449000
C	2.80257100	-1.23246000	-1.03598500
C	2.70462300	-2.52107400	-0.52145700
C	3.74383200	-3.41316800	-0.77656800
C	4.85793800	-3.01407500	-1.51919800
C	4.94745200	-1.71908900	-2.02643500
C	3.79182400	0.62016500	-2.18540500
C	2.33822400	1.01712800	-1.84479200
C	1.84900500	-0.07603200	-0.83189700
H	1.84957500	-2.79380400	0.08904200
H	3.69288000	-4.42463300	-0.38617200
H	5.66082200	-3.72106900	-1.70421100
H	5.81489800	-1.41188300	-2.60380400
H	3.98516100	0.79910600	-3.24739600
H	2.26393600	2.00102300	-1.37928300
H	4.49705300	1.23034100	-1.61128600
H	1.87048700	0.30369700	0.18970800
N	0.46216100	-0.43694600	-1.11136700
O	1.54794400	1.11873100	-3.02561500
C	-0.57421200	-0.67734100	-0.29502000
C	0.00389500	-0.50103400	-2.39032700
N	-1.60356800	-0.93536300	-1.11376600
N	-1.25936300	-0.81129500	-2.43082700
C	0.94812900	-0.08103000	-3.46677500
H	1.69034400	-0.86811700	-3.65960000
H	0.40145000	0.13302500	-4.38505800
C	-2.92981500	-1.36207400	-0.76499000
C	-3.09265400	-2.58712900	-0.10690300
C	-4.00358500	-0.54362900	-1.12911400
C	-4.38966400	-2.95162000	0.24619100
C	-5.27932000	-0.95882100	-0.74887300
C	-5.48975200	-2.14540700	-0.04917300
H	-4.54394300	-3.89913800	0.75642500
H	-6.13047600	-0.33586200	-1.01329700
C	-2.43686100	0.40346100	2.12929900
C	-1.50612400	-0.62558000	2.11459200
C	-0.44859100	-0.88851000	1.19631900
O	0.58725100	-1.51226700	1.50455900
C	-3.30761700	0.55979400	3.35510200
H	-3.34492600	1.60724000	3.67214100
H	-4.33527500	0.25507400	3.12984400
H	-2.95062300	-0.04565700	4.19113300
C	-2.51248100	1.40494300	1.14249300
H	-2.30977100	1.13245500	0.11702300

H	-3.28697300	2.16362200	1.24760700
H	-1.36679000	-1.18813700	3.03579600
C	-0.69259700	2.36605500	1.27012800
N	0.30127400	1.50837000	1.48346000
N	0.53439300	1.34131500	2.84582500
O	1.47962500	-0.00900400	4.38878300
C	2.80923700	0.51846700	2.48050500
C	3.30148900	1.67161600	1.86539700
C	4.50148800	1.62253000	1.16208700
C	5.20266100	0.42063500	1.06082200
C	4.71053500	-0.72906200	1.67497700
C	3.52062600	-0.67778300	2.39401600
H	2.73710500	2.59613400	1.93320200
H	4.89095900	2.52183300	0.69345300
H	5.24078500	-1.67053600	1.56933500
H	3.10703000	-1.56121800	2.86900700
C	-0.76866300	2.90062600	-0.11937300
O	-0.47776100	2.28784000	-1.12658500
O	-1.23353300	4.15602900	-0.11726400
C	-1.37096500	4.79474500	-1.39875100
C	-2.66984800	4.39349200	-2.06997300
H	-0.50875200	4.53396400	-2.01600300
H	-1.34910000	5.86218000	-1.17456800
H	-2.80949700	4.97145500	-2.98706100
H	-2.65055100	3.33375400	-2.33014800
H	-3.51727800	4.58435200	-1.40669900
H	-0.97989100	3.07610400	2.04686100
H	-0.28874700	1.28739300	3.44390800
C	1.55864100	0.54898500	3.30347100
H	6.12760700	0.37747900	0.49269600
C	-1.93692500	-3.50494700	0.19720500
H	-1.16031000	-3.44799600	-0.57095100
H	-1.47041700	-3.25932000	1.15587500
H	-2.28873800	-4.53709100	0.24741000
C	-6.87462800	-2.54793300	0.38619700
H	-7.63428300	-2.14420100	-0.28675000
H	-6.97980000	-3.63484300	0.41508800
H	-7.08565300	-2.16867800	1.39138400
C	-3.83299000	0.71629200	-1.93907000
H	-4.02277900	0.50941900	-2.99696200
H	-4.54559300	1.47583000	-1.60736400
H	-2.82452100	1.12856600	-1.86999900

