
Supplementary information

Unraveling the origins of selectivities in an N-heterocyclic carbene-catalyzed Friedel-Crafts alkylation/annulation cascade reaction

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Content

Part 1: Full names for Gaussian 09	S3
Part 2: Test of different functionals	S3
Part 3: Conformational searching for stereoselective transition states	S3
Part 4: IRC calculations	S4
Part 5: HCO_3^- and NaHCO_3 -assisted proton transfer pathways for <i>Si</i> -face addition mode	S4
Part 6: Energy profile for <i>R</i> -configured pathway	S5
Part 7: 3D structures for transition states TS5R and TS5S	S5
Part 8: Structures and energy barriers of transition states involving α -protonation process	S6
Part 9: POCV results of intermediate M4 and 4-aminoindole	S6
Part 10: POCV results of intermediate M4 and 4-hydroxyindole	S7
Part 11: Energy information for all stationary points	S7
Part 12: Cartesian coordinates for all stationary points	S9

Part 1: Full names for Gaussian 09

Frisch M, Trucks G, Schlegel H, Scuseria G, Robb M, Cheeseman J, Scalmani G, Barone V, Petersson G, Nakatsuji H, Li X, Caricato M, Marenich A, Bloino J, Janesko B, Gomperts R, Mennucci B, Hratchian H, Ortiz J, Izmaylov A, Sonnenberg J, Williams-Young D, Ding F, Lipparini F, Egidi F, Goings J, Peng B, Petrone A, Henderson T, Ranasinghe D, Zakrzewski V, Gao J, Rega N, Zheng G, Liang W, Hada M, Ehara M, Toyota K, Fukuda R, Hasegawa J, Ishida M, Nakajima T, Honda Y, Kitao O, Nakai H, Vreven T, Throssell K, Montgomery J, Peralta J, Ogliaro F, Bearpark M, Heyd J, Brothers E, Kudin K, Staroverov V, Keith T, Kobayashi R, Normand J, Raghavachari K, Rendell A, Burant J, Iyengar S, Tomasi J, Cossi M, Millam J, Klene M, Adamo C, Cammi R, Ochterski J, Martin R, Morokuma K, Farkas O, Foresman J, Fox D, Gaussian 09, Revision D.01, Gaussian, Inc., Wallingford CT, 2013.

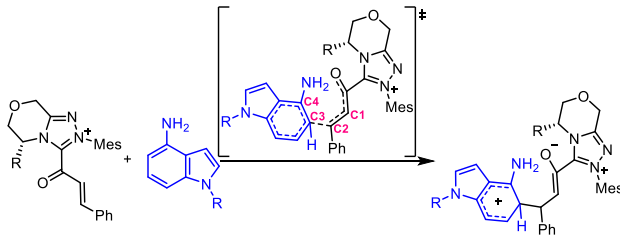
Part 2: Test of different functionals

Table S1. Test of different functionals involved in the stereoselectivity-determining step

	M06-2X	B3LYP	B3PW91	CAM-B3LYP	mPW1PW91	ωB97X-D
TS5S	0.0	0.0	0.0	0.0	0.0	0.0
TS5R	2.1	1.0	2.1	3.1	2.6	2.1

Part 3: Conformational searching for stereoselective transition states

Table S2. Conformational searching for stereoselective transition states **TS5R** and **TS5S**

					
$\Phi(\text{C1-C2-C3-C4}) / ^\circ$	0	90	180	270	
TS5R	0	0.1	2.8	2.3	
TS5S	0	3.7	3.2	4.0	

Part 4: IRC calculations

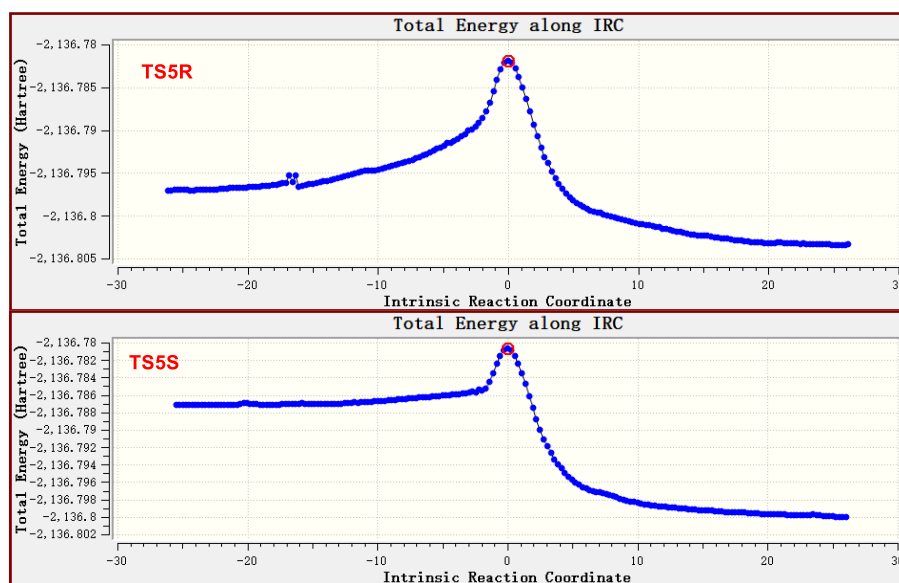
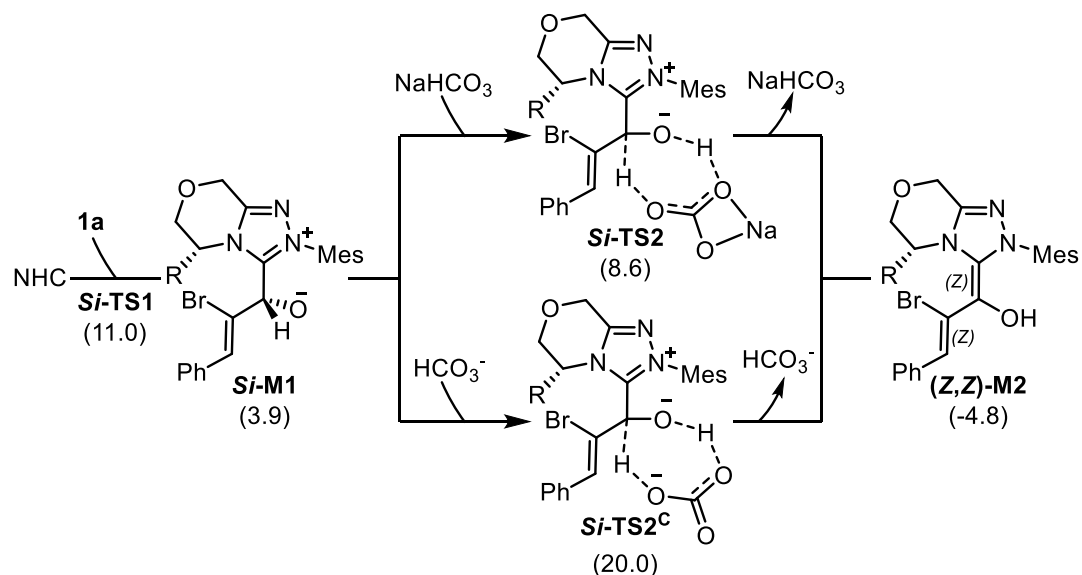


Figure S1. IRC calculations for the key stereoselective transition states TS5R and TS5S

Part 5: HCO_3^- and NaHCO_3 -assisted proton transfer pathways for *Si*-face addition mode



Scheme S1. HCO_3^- and NaHCO_3 -assisted proton transfer pathways

Part 6: Energy profile for *R*-configured pathway

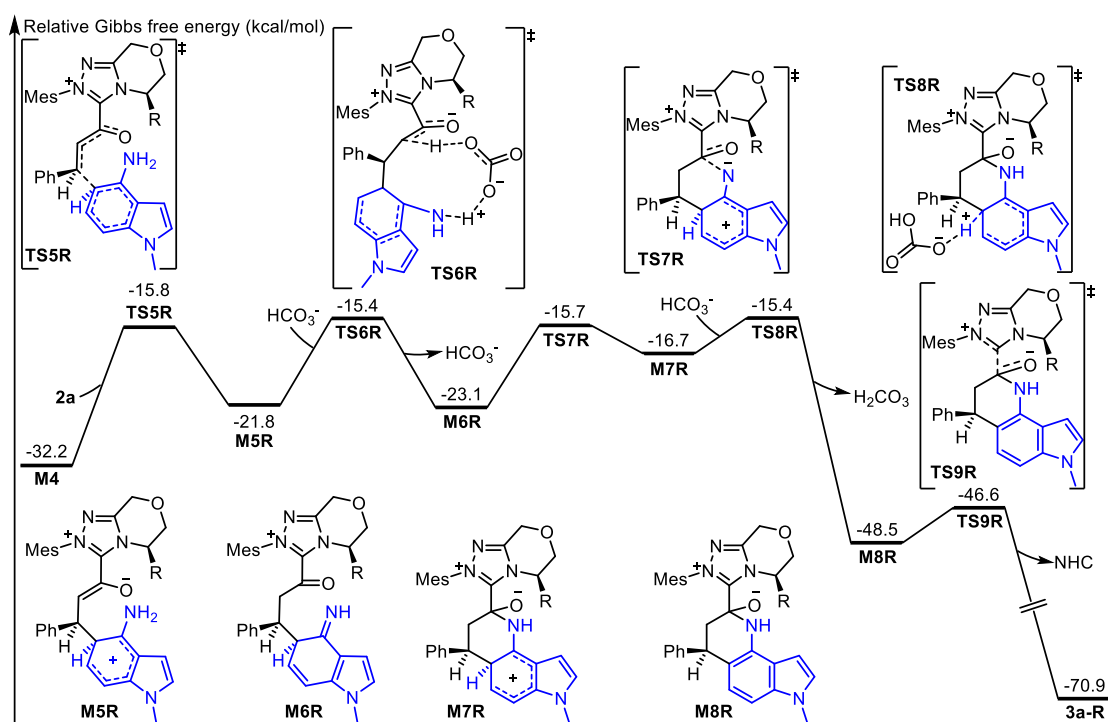


Figure S2. Relative Gibbs free energy profile for the transformation of α,β -unsaturated acylazolium intermediate involved in *R*-configured pathway

Part 7: 3D structures for transition states TS5R and TS5S

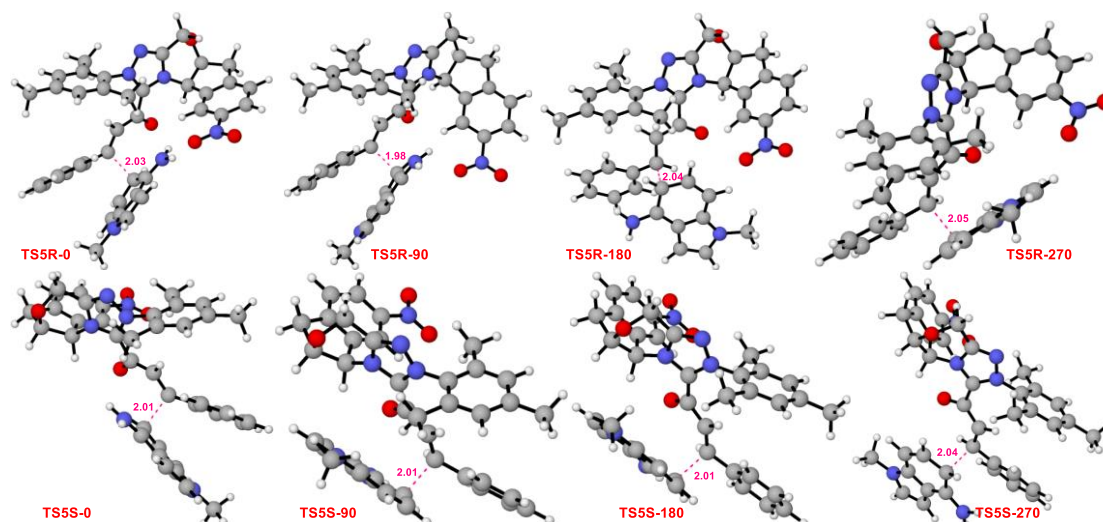


Figure S3. 3D structures for transition states TS5R and TS5S

Part 8: Structures and energy barriers of transition states involving α -protonation process

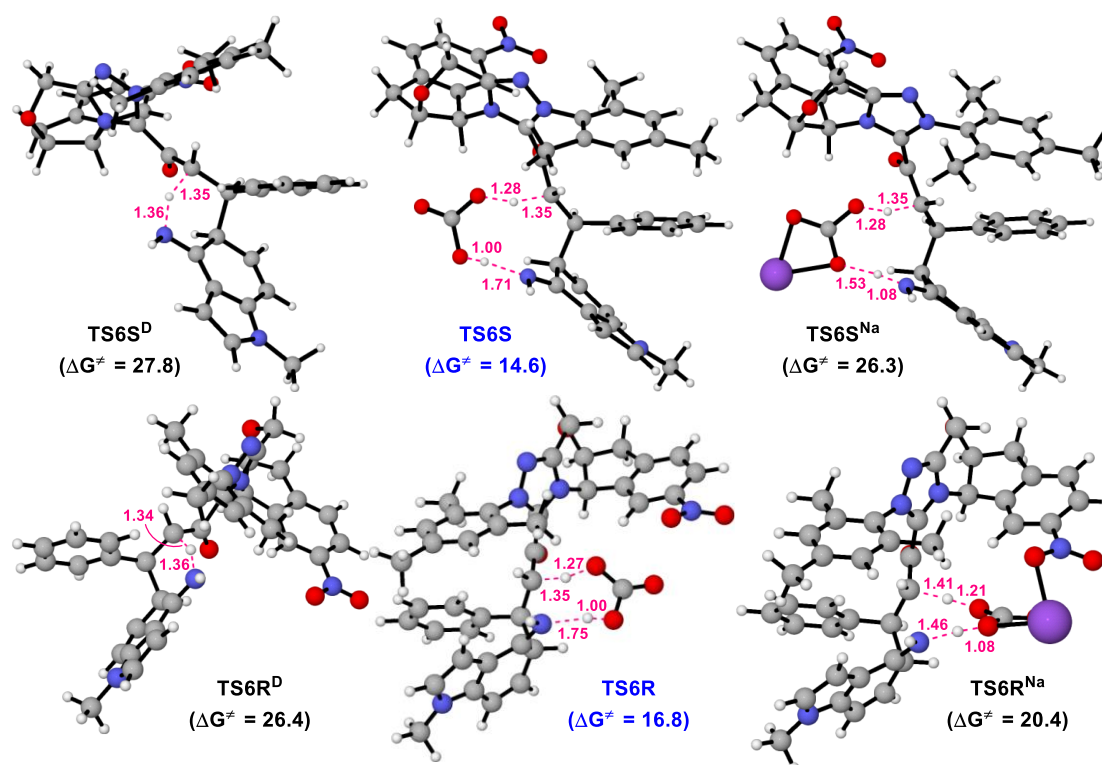


Figure S4. 3D structures and energy barriers for the transition states involving α -protonation process

Part 9: POCV results of intermediate M4 and 4-aminoindole

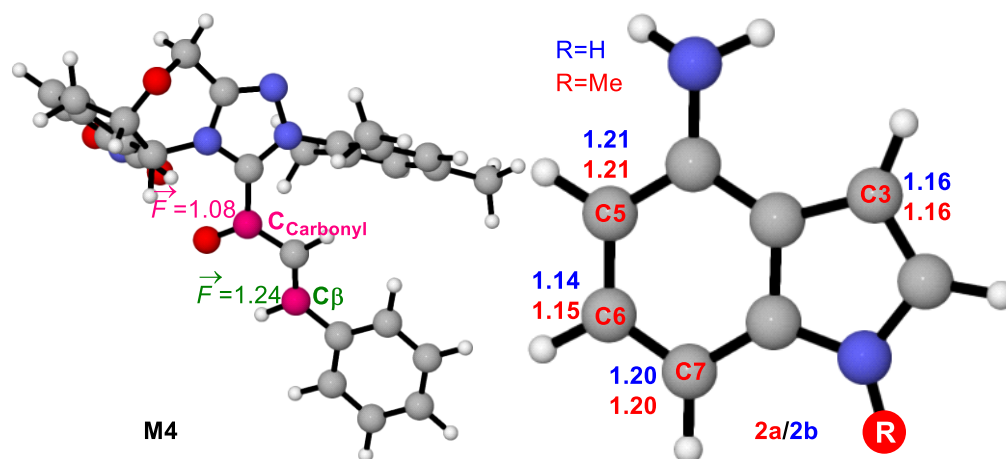


Figure S5. POCV results of intermediate M4 and 4-aminoindole

Part 10: POCV results of intermediate M4 and 4-hydroxyindole

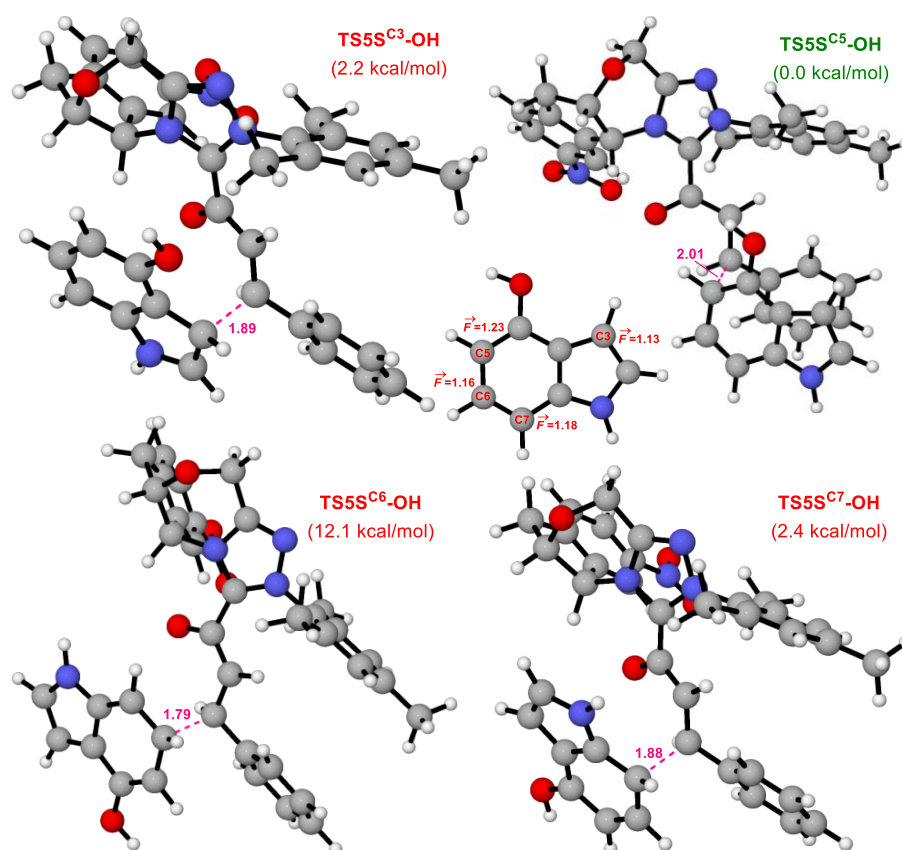


Figure S6. POCV results of intermediate M4 and 4-hydroxyindole

Part 11: Energy information for all stationary points

Table S3. Energy information for all stationary points

Species	Gibbs free energy (au)	Correction to Gibbs free energy (au)	Imaginary frequency (cm ⁻¹)
1a	-2993.888237	0.099798	/
2a	-458.176695	0.141646	/
NHC	-1256.034546	0.333134	/
NaHCO₃	-426.646485	0.000216	/
HCO₃⁻	-588.375133	0.001312	/
HBr	-2572.386749	-0.013143	/
H₂CO₃	-264.89686	0.013913	/
Re-TS1	-4249.910353	0.457995	104.83 <i>i</i>
Si-TS1	-4249.910293	0.458329	100.88 <i>i</i>
Re-M1	-4249.923585	0.459119	/
Si-M1	-4249.921117	0.460525	/
Re-TS2	-4676.567627	0.476698	1319.47 <i>i</i>
Si-TS2	-4676.563444	0.478062	1297.32 <i>i</i>

<i>Re</i>-TS2^C	-4514.327766	0.477413	1348.03 <i>i</i>
<i>Si</i>-TS2^C	-4514.315762	0.481437	1338.31 <i>i</i>
(<i>E,Z</i>)-M2	-4249.92775	0.458877	/
(<i>Z,Z</i>)-M2	-4249.927435	0.456535	/
(<i>E,Z</i>)-TS3	-4249.922398	0.458264	176.93 <i>i</i>
M3	-4249.951889	0.458115	/
TS4	-4676.565955	0.473877	1261.44 <i>i</i>
M4	-1678.00611	0.461751	/
TS5R	-2136.151705	0.630366	424.51 <i>i</i>
TS5S	-2136.154886	0.62586	393.24 <i>i</i>
TS5S^{C3}	-2136.145423	0.627833	438.48 <i>i</i>
M5R	-2136.16139	0.630837	/
M5S	-2136.163229	0.629862	/
TS6S^D	-2136.142164	0.624952	1337.25 <i>i</i>
TS6S	-2400.589914	0.64906	1231.37 <i>i</i>
TS6S^{Na}	-2562.793729	0.645139	1247.97 <i>i</i>
TS6R^D	-2136.14466	0.626358	1351.96 <i>i</i>
TS6R	-2400.586011	0.649421	1184.27 <i>i</i>
TS6R^{Na}	-2562.806827	0.648612	1120.63 <i>i</i>
M6R	-2136.156377	0.630392	/
M6S	-2136.151643	0.630968	/
TS7R	-2136.149216	0.636031	152.49 <i>i</i>
TS7S	-2136.155138	0.629655	199.99 <i>i</i>
M7R	-2136.154031	0.638305	/
M7S	-2136.15722	0.630904	/
TS8R	-2400.571913	0.655057	36.55 <i>i</i>
TS8S	-2400.576744	0.653769	15.23 <i>i</i>
M8R	-2135.733244	0.619679	/
M8S	-2135.735226	0.62	/
TS9R	-2135.731136	0.619493	205.74 <i>i</i>
TS9S	-2135.727363	0.616753	210.17 <i>i</i>
PR	-879.739443	0.260617	/
PS	-879.739434	0.260626	/
TS5S^{C6}	-2136.127799	0.627599	331.71 <i>i</i>
TS5S^{C7}	-2136.149078	0.626021	425.87 <i>i</i>
2b	-418.910912	0.116383	/
TS5S^{C3}-NH	-2096.876468	0.602322	406.97 <i>i</i>
TS5S^{C5}-NH	-2096.887385	0.601440	377.26 <i>i</i>
TS5S^{C6}-NH	-2096.859671	0.601022	259.69 <i>i</i>
TS5S^{C7}-NH	-2096.884349	0.599592	420.76 <i>i</i>
2b-OH	-438.783190	0.104081	/
TS5S^{C3}-OH	-2116.746678	0.589852	402.54 <i>i</i>
TS5S^{C5}-OH	-2116.750116	0.591548	346.05 <i>i</i>
TS5S^{C6}-OH	-2116.730795	0.588521	268.21 <i>i</i>
TS5S^{C7}-OH	-2116.746281	0.588320	390.10 <i>i</i>

Part 12: Cartesian coordinates for all stationary points

1a

C	2.47848800	1.50147400	0.00020900
O	2.36384600	2.70563900	-0.00046300
H	3.47000500	1.01308800	0.00079100
C	1.31452500	0.57323200	0.00022200
C	0.06504200	1.06427300	0.00020200
H	0.07073100	2.15555700	0.00032600
Br	1.82131500	-1.25086400	-0.00002400
C	-1.27199100	0.47465900	0.00008700
C	-1.56237800	-0.90058500	-0.00003500
C	-2.34483600	1.38368400	0.00009100
C	-2.88125400	-1.33814400	-0.00010800
H	-0.76608900	-1.63200000	-0.00009900
C	-3.66094200	0.94269600	0.00001800
H	-2.13186400	2.44908700	0.00016100
C	-3.93306000	-0.42374600	-0.00007600
H	-3.08856700	-2.40348500	-0.00020000
H	-4.47258600	1.66313100	0.00003000
H	-4.95997100	-0.77551300	-0.00013900

2a

C	0.37779200	-0.62387900	0.00866300
C	-0.57539800	0.41877900	-0.00319800
C	-0.22295900	1.77751700	-0.00477300
C	1.13170800	2.05939800	0.00340500
C	2.10710900	1.04409700	0.00655700
C	1.75416100	-0.30251000	0.00779200
C	-0.35109500	-1.86002600	0.01575800
C	-1.67788000	-1.52716900	0.00596000
H	-0.97173300	2.56241000	-0.01119900
H	1.46048000	3.09455600	0.00180500
H	3.16043700	1.31134900	0.00755000
H	0.04933700	-2.86336400	0.03880400
H	-2.55628500	-2.15820500	0.01030100
N	2.70495200	-1.31947400	0.06798500

H	2.41365800	-2.18302400	-0.37293700
H	3.62473400	-1.04194000	-0.25077500
N	-1.82209800	-0.15834300	-0.00706400
C	-3.07116000	0.57293500	-0.00980300
H	-3.15348400	1.19945800	0.88338200
H	-3.14397300	1.20808000	-0.89756800
H	-3.89680800	-0.13946100	-0.01798400

NHC

C	-3.79438200	-0.81793300	-0.10354500
C	-2.59280800	-0.33426300	-0.61899400
C	-2.27399100	1.01406600	-0.58114700
C	-3.21963700	1.86433300	-0.02293400
C	-4.44033500	1.42034500	0.48136800
C	-4.72981200	0.06096600	0.44230500
C	-3.86098100	-2.31762700	-0.22244300
C	-2.43707700	-2.76184500	-0.64041700
C	-1.71587100	-1.45543100	-1.13394300
H	-1.32931300	1.39480500	-0.95441900
H	-5.66770800	-0.30604300	0.84660500
H	-4.15388600	-2.80704500	0.71156400
H	-2.47317800	-3.49540000	-1.44641500
H	-4.58989500	-2.61069700	-0.98537200
H	-1.64030200	-1.43608000	-2.22346900
N	-0.37311100	-1.34943700	-0.59655200
O	-1.74414300	-3.42571200	0.40576400
C	0.68536700	-0.66296000	-1.12901100
C	-0.09594200	-1.78088400	0.67258800
N	1.55040500	-0.74964500	-0.09636300
N	1.10329900	-1.43594100	1.01987300
C	-1.14499400	-2.57935600	1.37407400
H	-1.88474700	-1.91920300	1.84979900
H	-0.70263900	-3.21549600	2.14149000
C	2.84717700	-0.14455700	-0.04712200
C	3.97731700	-0.96665400	-0.04577500
C	2.93429300	1.25120900	0.01985900
C	5.22924200	-0.35233500	0.01104500

C	4.20631500	1.81844400	0.07045700
C	5.36270900	1.03470600	0.06563400
H	6.12010600	-0.97585200	0.00987400
H	4.29649000	2.90126900	0.12355300
H	-5.13556700	2.13424900	0.90559400
C	3.84295700	-2.46406100	-0.10988800
H	3.19569800	-2.76407000	-0.93994400
H	3.39504000	-2.85803300	0.80720100
H	4.81990700	-2.93242200	-0.24672400
C	1.70024200	2.11494700	0.03042700
H	0.95929000	1.74189200	0.74472600
H	1.22558800	2.13086900	-0.95540800
H	1.95487500	3.14129400	0.30274700
C	6.72111500	1.68519900	0.10186400
H	6.76576900	2.46132900	0.87138500
H	6.94847900	2.16405800	-0.85649100
H	7.50709600	0.95448900	0.30596400
N	-2.90483900	3.29506700	0.05465800
O	-1.79725400	3.65512300	-0.30621800
O	-3.76445300	4.04782800	0.47920600

NaHCO₃

C	-0.56647800	0.03796400	-0.00044600
O	-0.03112300	-1.10475700	-0.00122000
O	-1.92407000	0.09602600	0.00129100
H	-2.23706900	-0.81997200	0.00082300
O	0.03580000	1.13698600	-0.00116400
Na	1.90828100	-0.03944100	0.00096300

HCO₃⁻

C	0.14159500	0.06492800	0.00001500
O	-0.11092400	1.28826000	-0.00001000
O	-0.99770500	-0.77150100	-0.00002100
H	-1.73754100	-0.15127300	0.00013100
O	1.21962500	-0.54654700	0.00000400

HBr

H	0.00000000	0.00000000	-1.37378400
Br	0.00000000	0.00000000	0.03925100

H₂CO₃

C	-0.05227700	0.12678000	0.00004400
O	-0.53341100	-1.12451900	0.00000300
O	1.27774100	0.13384900	0.00002600
H	1.61730000	-0.77504700	0.00004500
O	-0.71946200	1.12634600	-0.00006100
H	-1.50257500	-1.07103900	-0.00005300

Re-TS1

C	-5.04655700	-0.82103500	-0.17253200
C	-3.72618300	-0.45052900	-0.42874100
C	-3.40138500	0.81894500	-0.89338500
C	-4.46431400	1.69127900	-1.09850100
C	-5.79411000	1.35217800	-0.86022500
C	-6.08853900	0.07953300	-0.38840200
C	-5.12745600	-2.23029900	0.34856900
C	-3.66494700	-2.66060100	0.61109500
C	-2.76937200	-1.57934600	-0.10030800
H	-2.37770500	1.14689100	-1.07607300
H	-7.11675300	-0.20093100	-0.18325700
H	-5.71597900	-2.30831700	1.26810200
H	-3.45939400	-3.64312200	0.18604300
H	-5.59301200	-2.88934700	-0.39128000
H	-2.30336100	-1.99374200	-0.99820300
N	-1.70153300	-1.13252700	0.77857400
O	-3.37840600	-2.81170500	1.99251400
C	-0.48912200	-0.63207300	0.43473300
C	-1.88323400	-1.02267500	2.13202900
N	-0.00889700	-0.24128000	1.62106600
N	-0.84488200	-0.48265200	2.69217200
C	-3.13571500	-1.60547700	2.69903200
H	-3.97376900	-0.90022800	2.60567800
H	-3.00477000	-1.85636000	3.75217800
C	1.23435000	0.44689700	1.82252600

C	1.20988800	1.84353600	1.88758400
C	2.41224200	-0.29731200	1.89513300
C	2.43217600	2.50003000	2.02263100
C	3.61056300	0.40438500	2.02687000
C	3.63859100	1.79756800	2.08960400
H	2.44282800	3.58695000	2.06774800
H	4.54489100	-0.15183200	2.05870300
H	-6.57226400	2.08470100	-1.03511100
C	-0.08838700	2.59681400	1.78298700
H	-0.81062100	2.24539800	2.52638900
H	-0.52530000	2.45505800	0.78827000
H	0.07486100	3.66498300	1.93987500
C	2.38899700	-1.79704000	1.78538800
H	2.07930700	-2.10873100	0.78271000
H	1.68177900	-2.23600500	2.49654300
H	3.38052000	-2.21149800	1.97900500
C	4.94431200	2.53639600	2.22348300
H	5.04534600	2.97355900	3.22272500
H	5.00876000	3.35789400	1.50312900
H	5.79336200	1.86867600	2.05951400
N	-4.17193800	3.04620700	-1.58542300
O	-3.00579300	3.35167900	-1.75307100
O	-5.11407000	3.79225400	-1.79627100
C	0.03680900	0.26932000	-1.43928400
O	-0.11667200	1.48297200	-1.29311200
H	-0.73108900	-0.35772400	-1.93187700
C	1.41432400	-0.34218500	-1.52369200
C	2.51192100	0.40232800	-1.37427200
H	2.25165700	1.44611400	-1.18837600
Br	1.33998600	-2.20672000	-1.84670100
C	3.95227500	0.12496600	-1.36029000
C	4.54767100	-1.13236500	-1.54758700
C	4.78995300	1.22283600	-1.09945300
C	5.92948700	-1.27649000	-1.46601700
H	3.93827000	-1.99991100	-1.76153800
C	6.16871700	1.07740900	-1.01995700
H	4.33881300	2.20013800	-0.94836500

C	6.74527700	-0.17889900	-1.20050400
H	6.37146300	-2.25722900	-1.61252900
H	6.79141100	1.94281200	-0.81388000
H	7.82210900	-0.30138500	-1.13788800

Si-TS1

C	-2.74682700	-2.26241200	-1.26325700
C	-1.78991000	-1.47812400	-0.62068700
C	-1.74032500	-1.36935400	0.76205100
C	-2.72471300	-2.05107400	1.46781100
C	-3.70176500	-2.83724100	0.86133100
C	-3.70929900	-2.94826600	-0.52373400
C	-2.55408800	-2.23650000	-2.75569400
C	-1.21603000	-1.49426100	-2.98921400
C	-0.87661100	-0.80407800	-1.61842600
H	-0.96483100	-0.80694100	1.27973000
H	-4.45748200	-3.56082500	-1.01653400
H	-2.51318300	-3.23844000	-3.19444000
H	-1.31573000	-0.73640700	-3.76641300
H	-3.37690800	-1.70254800	-3.24182600
H	-1.07290800	0.27019100	-1.67260800
N	0.52597800	-0.96734100	-1.27906400
O	-0.18945300	-2.35154700	-3.46577800
C	1.33229600	-0.13305400	-0.57597300
C	1.21269000	-2.10520200	-1.61355000
N	2.47247400	-0.83247600	-0.53110800
N	2.43279300	-2.05132800	-1.17642900
C	0.49831600	-3.09645800	-2.47196600
H	-0.19056300	-3.70869300	-1.87297300
H	1.20468500	-3.75465400	-2.97844500
C	3.69034600	-0.38789300	0.08100600
C	4.42686300	0.61334800	-0.55543200
C	4.07838600	-0.96395800	1.29490200
C	5.61185300	1.02742500	0.05513100
C	5.27181600	-0.52260000	1.86135600
C	6.05037100	0.46744600	1.25501800

H	6.20492300	1.80348800	-0.42272200
H	5.59890700	-0.95485000	2.80451200
H	-4.43642900	-3.34541800	1.47430600
C	3.94994700	1.22748300	-1.84436000
H	3.01377600	1.77806000	-1.69697600
H	3.75737300	0.45900500	-2.60024600
H	4.69647800	1.91979500	-2.23824800
C	3.20875000	-1.99321400	1.96334600
H	3.07153100	-2.87367900	1.32816400
H	2.22093400	-1.56410200	2.16483000
H	3.64906500	-2.31332900	2.90965600
C	7.32807900	0.92811000	1.90593300
H	7.89653100	1.58701400	1.24571600
H	7.96286000	0.07721300	2.17042000
H	7.11797700	1.47625400	2.83030900
N	-2.75074400	-1.91287700	2.92578600
O	-2.10654700	-1.00208400	3.42071300
O	-3.42049000	-2.70483900	3.56600200
C	0.97555300	1.23305700	1.04252500
O	0.86650100	0.52766000	2.04792100
H	1.91853500	1.74956400	0.78923400
C	-0.24552700	1.89247700	0.44324100
C	-1.42982100	1.82228500	1.05707400
H	-1.36882500	1.25213800	1.98619600
Br	0.09743100	2.77560700	-1.19773700
C	-2.78111300	2.27941200	0.71212700
C	-3.08894900	3.29017200	-0.21064400
C	-3.83751300	1.63610400	1.37849000
C	-4.41446500	3.63034400	-0.46191600
H	-2.29765900	3.82539700	-0.71900200
C	-5.16020600	1.96995600	1.11652500
H	-3.60114300	0.86622600	2.10984900
C	-5.45317900	2.97024300	0.19158700
H	-4.63544200	4.42218200	-1.17104200
H	-5.96106400	1.45611000	1.63879200
H	-6.48465100	3.24058600	-0.01219200

Re-M1

C	-5.17093500	-0.22428400	-0.67429700
C	-3.83092000	0.15833500	-0.63052000
C	-3.43298500	1.37819800	-0.09894300
C	-4.44470400	2.19328200	0.39053200
C	-5.79541200	1.85082500	0.35535900
C	-6.16300700	0.62515100	-0.18538900
C	-5.32671300	-1.58609000	-1.29486000
C	-3.89640600	-2.16330400	-1.36746100
C	-2.94140300	-0.92119700	-1.21666500
H	-2.38379900	1.66803300	-0.10386200
H	-7.20800000	0.33377500	-0.21486600
H	-5.97636700	-2.25241700	-0.71972600
H	-3.70972500	-2.66840500	-2.31528100
H	-5.75273900	-1.50039000	-2.29997700
H	-2.51660200	-0.61976600	-2.17597000
N	-1.83887800	-1.25622500	-0.31896600
O	-3.66945600	-3.16412300	-0.38384000
C	-0.56056500	-0.83295200	-0.30932800
C	-2.04967800	-1.99643400	0.80984600
N	-0.06290000	-1.30224400	0.83760400
N	-0.97779100	-2.04886400	1.53898300
C	-3.36812200	-2.69097700	0.91809100
H	-4.14228700	-2.01680200	1.30756900
H	-3.28844800	-3.55446200	1.57904400
C	1.23528700	-1.07811400	1.41744600
C	1.51404000	0.19441900	1.92848300
C	2.13034900	-2.14604500	1.47487500
C	2.78455200	0.39567100	2.46099600
C	3.38516700	-1.89446100	2.03258100
C	3.73107900	-0.63233700	2.51391700
H	3.04344800	1.37980200	2.84475400
H	4.10973800	-2.70370800	2.07944800
H	-6.53264100	2.53706000	0.75383100
C	0.47743200	1.28424200	1.90886100
H	-0.40599400	0.98067800	2.48357800

H	0.14102300	1.51319400	0.88960600
H	0.87722600	2.19571800	2.35732300
C	1.75874600	-3.51113900	0.96498400
H	1.25531300	-3.44801900	-0.00345000
H	1.08157000	-4.01607700	1.66126800
H	2.65224000	-4.12778000	0.84649100
C	5.10315000	-0.36085100	3.07007100
H	5.73680000	-1.24925800	3.02220600
H	5.04740400	-0.03672800	4.11414100
H	5.59209000	0.44133200	2.50756600
N	-4.06926600	3.48391000	0.98134700
O	-2.88352000	3.72361600	1.12278400
O	-4.96550400	4.24655600	1.30353400
C	-0.05224500	0.16745300	-1.38526000
O	-0.68224800	1.31535400	-1.20754000
H	-0.28164400	-0.38115200	-2.33730300
C	1.47990200	0.23779100	-1.36571200
C	2.13149200	1.38058400	-1.16610800
H	1.44210100	2.21439400	-1.02620900
Br	2.30923000	-1.41648500	-1.82082600
C	3.56889300	1.68542400	-1.11528800
C	4.53270500	0.77436400	-0.65855400
C	3.98553300	2.97319300	-1.48140300
C	5.87511700	1.13754500	-0.60332700
H	4.22654100	-0.21398000	-0.33416600
C	5.32808600	3.33198600	-1.43177100
H	3.24283100	3.69313700	-1.81509000
C	6.27953500	2.41288000	-0.99439400
H	6.60808200	0.42033000	-0.24541200
H	5.63051000	4.33142300	-1.72901800
H	7.32813800	2.69083400	-0.95044900

Si-M1

C	-2.62406100	2.52676700	1.51705400
C	-1.77687200	1.78021700	0.69988700
C	-1.55767200	2.09970900	-0.63451200

C	-2.23507900	3.21666400	-1.10776600
C	-3.09669000	3.98537600	-0.32686000
C	-3.29531500	3.63524700	1.00295700
C	-2.67075300	1.96408400	2.91190500
C	-1.55476900	0.89340900	2.96593600
C	-1.15272000	0.63597100	1.46574500
H	-0.88640400	1.49873400	-1.25961600
H	-3.95652800	4.22578100	1.62886100
H	-2.50670700	2.72185500	3.68440400
H	-1.91289500	-0.03612200	3.40881100
H	-3.64482100	1.50494600	3.10850000
H	-1.53011700	-0.33074500	1.13222000
N	0.30280300	0.62700900	1.31083500
O	-0.46852300	1.27978000	3.79243700
C	1.09548900	-0.00835700	0.42587900
C	1.10314500	1.43188800	2.07753400
N	2.32289700	0.43203100	0.69261600
N	2.34892400	1.32803100	1.72823300
C	0.45163700	2.17567300	3.19525900
H	-0.03919900	3.08508000	2.82200800
H	1.18973800	2.45411400	3.94765500
C	3.53182200	0.11697600	-0.02079900
C	4.28959200	-0.97683100	0.40119600
C	3.88679100	0.93764900	-1.09410200
C	5.46361600	-1.24500500	-0.30015700
C	5.07112000	0.62733300	-1.76120300
C	5.86593700	-0.45613600	-1.38079400
H	6.07635600	-2.08984400	0.00423400
H	5.37672400	1.24572900	-2.60145300
H	-3.59113700	4.84385600	-0.76456100
C	3.83928700	-1.82578600	1.55806400
H	2.87050900	-2.29320400	1.34809400
H	3.72000500	-1.22652700	2.46673400
H	4.56303000	-2.61775000	1.75857600
C	3.00683500	2.08442900	-1.50795200
H	2.86598400	2.79076500	-0.68279200
H	2.02219400	1.69950500	-1.80317600

H	3.44925900	2.62267700	-2.34819900
C	7.12152500	-0.78784600	-2.14294900
H	7.57344700	0.11012500	-2.57126400
H	6.89989500	-1.47202100	-2.96914900
H	7.85913700	-1.27418400	-1.49985900
N	-2.02415200	3.61886500	-2.50496300
O	-1.24331600	2.96753900	-3.17370300
O	-2.64030400	4.58747700	-2.91977300
C	0.70893500	-0.80245500	-0.83920900
O	0.43096600	0.06103600	-1.80312300
H	1.59557600	-1.46427500	-1.00496800
C	-0.43255800	-1.77509300	-0.48390900
C	-1.53779300	-1.84548100	-1.22500500
H	-1.48278500	-1.11345700	-2.03357700
Br	-0.03753800	-2.82649700	1.06252100
C	-2.76310600	-2.65626000	-1.18813700
C	-3.05862300	-3.64993500	-0.24098200
C	-3.71402900	-2.39749900	-2.18983100
C	-4.26022100	-4.34840900	-0.29935700
H	-2.35586400	-3.88638300	0.54587700
C	-4.91351600	-3.09661100	-2.24679800
H	-3.49921100	-1.63307500	-2.93159700
C	-5.19263300	-4.07782200	-1.29798200
H	-4.46529900	-5.11332700	0.44341900
H	-5.62920200	-2.87641700	-3.03281500
H	-6.12766000	-4.62785800	-1.33702500

Re-TS2

C	-4.95863100	-0.41640900	-0.10186300
C	-3.60866200	-0.28517500	0.22320400
C	-3.11367900	-0.68073000	1.45720800
C	-4.03055500	-1.21927200	2.35092900
C	-5.38713100	-1.35710300	2.06569600
C	-5.85699800	-0.94763300	0.82294000
C	-5.22406200	0.07751700	-1.49927800
C	-3.82863200	0.24737900	-2.14306400

C	-2.82611400	0.29610200	-0.93596400
H	-2.06656900	-0.55930700	1.71516200
H	-6.90862300	-1.05535800	0.57729300
H	-5.83764700	-0.60725700	-2.09188100
H	-3.75330500	1.16852000	-2.72115300
H	-5.74462600	1.04066900	-1.46841800
H	-2.50007100	1.31829100	-0.73636900
N	-1.64644500	-0.51086400	-1.22780500
O	-3.54104700	-0.78406200	-3.07798400
C	-0.35937600	-0.36365800	-0.83325100
C	-1.74757300	-1.69658800	-1.89857800
N	0.24542900	-1.48808100	-1.25127600
N	-0.60820300	-2.31441900	-1.94458500
C	-3.06916600	-1.99976600	-2.52444700
H	-3.76580600	-2.41636000	-1.78418700
H	-2.94901900	-2.71610200	-3.33765000
C	1.53619500	-1.98269400	-0.86173300
C	1.75303400	-2.23848500	0.49810500
C	2.49549900	-2.21557500	-1.84799200
C	3.01942900	-2.68762600	0.86492100
C	3.74315400	-2.67813000	-1.42831500
C	4.02633400	-2.90146000	-0.08055500
H	3.22341000	-2.88021500	1.91552700
H	4.51442500	-2.85344500	-2.17412400
H	-6.05044400	-1.78629700	2.80661800
C	0.66236500	-2.06058100	1.52300200
H	-0.26969700	-2.53101500	1.18955400
H	0.45146500	-1.00384700	1.72051700
H	0.95478900	-2.52435900	2.46710500
C	2.19636400	-1.97767700	-3.30191500
H	1.68787100	-1.02051700	-3.44587500
H	1.54742600	-2.76310000	-3.70148300
H	3.12076500	-1.96776400	-3.88298200
C	5.39628700	-3.33935800	0.36386000
H	5.89762500	-2.52791100	0.90284600
H	6.02159200	-3.61885400	-0.48698100
H	5.33731800	-4.19268300	1.04568900

N	-3.53690600	-1.67711900	3.65468600
O	-2.33417200	-1.64742200	3.85149100
O	-4.35445400	-2.06941900	4.46990000
C	0.12161400	0.84431200	-0.15414400
O	-0.62016600	1.04023000	1.02596500
H	-0.28031100	1.82067800	-0.99705500
C	1.59142400	0.96077200	0.03124900
C	2.20861100	1.11901200	1.20641600
H	1.52688900	1.12620500	2.05606400
Br	2.50401500	1.10644700	-1.63809900
C	3.63774300	1.29075600	1.51251600
C	4.64952200	0.62497500	0.80401000
C	4.00167100	2.08764100	2.60717100
C	5.98463600	0.78765700	1.16128600
H	4.38344800	-0.02501900	-0.02288500
C	5.33665200	2.25086100	2.96114500
H	3.22301100	2.58833000	3.17673900
C	6.33477600	1.60301700	2.23597600
H	6.75619300	0.26754100	0.60105500
H	5.59794600	2.87964900	3.80684000
H	7.37772800	1.72587000	2.51131900
C	-1.44259500	3.59289700	-0.88679500
O	-0.83106600	2.75625900	-1.66667200
O	-1.62024200	3.27519500	0.37327200
H	-1.03990200	1.95822600	0.89726000
O	-1.88269700	4.69593800	-1.32166600
Na	-2.47778100	5.25632200	0.70844500

Si-TS2

C	-3.55019100	-2.66020900	-0.56643800
C	-2.51786500	-1.80913000	-0.17552300
C	-2.07491300	-1.73933200	1.13876900
C	-2.72766100	-2.56185500	2.04832400
C	-3.77135300	-3.41659100	1.69982700
C	-4.18761400	-3.46703800	0.37501300
C	-3.81725800	-2.55258100	-2.04385200

C	-2.69039100	-1.65343400	-2.60955700
C	-1.97933100	-1.03092700	-1.35219600
H	-1.25695600	-1.09013500	1.45381900
H	-4.99361700	-4.13219100	0.08247500
H	-3.81705300	-3.52518600	-2.54655900
H	-3.09356300	-0.85083500	-3.22717400
H	-4.79478100	-2.09569800	-2.22657100
H	-2.21239400	0.03011000	-1.27657000
N	-0.52519200	-1.17837500	-1.44672000
O	-1.80889100	-2.34819800	-3.47586800
C	0.46703400	-0.50310000	-0.81566600
C	0.03300800	-2.27658000	-2.04019200
N	1.56486100	-1.22066000	-1.06919100
N	1.31338900	-2.32629400	-1.83069600
C	-0.86654000	-3.17574500	-2.82274900
H	-1.34921900	-3.90833400	-2.16025700
H	-0.29915700	-3.71084100	-3.58510600
C	2.91215600	-0.94315100	-0.65173400
C	3.66755000	-0.04606800	-1.41470800
C	3.40422900	-1.61663800	0.46236100
C	4.98299600	0.16947100	-1.01887000
C	4.74046400	-1.38583700	0.80559400
C	5.53702200	-0.49792300	0.07836300
H	5.59115600	0.87713600	-1.57615300
H	5.16581000	-1.92470100	1.65194800
H	-4.23550500	-4.03132900	2.46145200
C	3.06414900	0.66214700	-2.59400400
H	2.30814700	1.38150700	-2.26040700
H	2.58764900	-0.04490500	-3.28128300
H	3.83242200	1.21205700	-3.14043600
C	2.51457300	-2.51543400	1.27400000
H	2.07683200	-3.30759300	0.65814000
H	1.69279500	-1.92732000	1.69891700
H	3.07198400	-2.98302000	2.08797000
C	6.97039800	-0.23785700	0.46811900
H	7.24444900	-0.77506400	1.38106800
H	7.14580200	0.83303000	0.61869700

H	7.65422500	-0.56234700	-0.32231900
N	-2.28502200	-2.53520900	3.44824800
O	-1.33198600	-1.83126400	3.72972300
O	-2.89263300	-3.22153300	4.25261500
C	0.42888400	0.67981900	0.07723800
O	0.47491300	0.23265000	1.40910800
H	1.49915000	1.49594300	-0.05237300
C	-0.70335900	1.60072500	-0.20180600
C	-1.54501700	2.08562300	0.72034900
H	-1.35823200	1.62990600	1.69266000
Br	-0.68455400	2.11996100	-2.04861100
C	-2.63454000	3.07134800	0.71459100
C	-3.03132600	3.86511100	-0.37490500
C	-3.33574000	3.22634500	1.92379800
C	-4.08349900	4.76686900	-0.25103600
H	-2.51897000	3.78987100	-1.32349600
C	-4.38811100	4.12488900	2.04441600
H	-3.04094500	2.62658400	2.78073200
C	-4.76920300	4.90316700	0.95341200
H	-4.36538900	5.37155500	-1.10781200
H	-4.90735600	4.22071800	2.99313200
H	-5.58750900	5.61081500	1.04197700
C	3.19293700	1.99596800	1.08050500
O	2.44509500	2.32810900	0.07437500
O	2.74108500	1.12566700	1.94975300
H	1.38089800	0.59248900	1.75097300
O	4.35164200	2.48449200	1.23139000
Na	4.79815900	0.84465500	2.61500300

Re-TS2^C

C	5.02285200	0.02174200	-0.01585900
C	3.66205800	-0.27172800	-0.08810300
C	3.15348700	-1.49691000	0.31924400
C	4.07093600	-2.40720400	0.82866100
C	5.43855000	-2.15144600	0.91528900
C	5.92103200	-0.92247000	0.48164200

C	5.30029600	1.40702700	-0.53718900
C	3.91430900	2.08313900	-0.65275000
C	2.87911200	0.90317900	-0.63375300
H	2.09530500	-1.71999300	0.20068300
H	6.98226100	-0.70289300	0.54175300
H	5.95881800	1.99239400	0.11163000
H	3.80967100	2.64715700	-1.57969800
H	5.77462100	1.35033400	-1.52266100
H	2.48675900	0.70569800	-1.63093300
N	1.75404500	1.23381400	0.23475400
O	3.70470100	3.04579100	0.37496900
C	0.45052800	0.86133700	0.16296300
C	1.93440000	1.92083900	1.40017900
N	-0.07869100	1.31050900	1.31817100
N	0.83670700	2.00084400	2.08507500
C	3.28300800	2.52259300	1.62111600
H	3.98474100	1.77385900	2.01436100
H	3.21878600	3.34908900	2.32972700
C	-1.33065100	0.92331000	1.90081400
C	-1.54588300	-0.43878000	2.14896500
C	-2.26638100	1.91136500	2.20850100
C	-2.78848800	-0.80104500	2.66523800
C	-3.48715600	1.49733100	2.74189000
C	-3.77135700	0.14858900	2.95613600
H	-2.99230400	-1.85332500	2.84961400
H	-4.23899900	2.24758100	2.97491400
H	6.10071900	-2.90653400	1.32077900
C	-0.47648300	-1.47005000	1.89457800
H	0.46712400	-1.17285400	2.36774200
H	-0.27960000	-1.61386000	0.82551200
H	-0.77469600	-2.43202500	2.31697400
C	-1.97306700	3.36352900	1.95385500
H	-1.57666500	3.50322000	0.94383000
H	-1.22716800	3.74490500	2.65775900
H	-2.88224600	3.95993700	2.05575700
C	-5.11838300	-0.29206100	3.46528700
H	-5.71827700	0.55878700	3.79643200

H	-5.01748000	-0.99035700	4.30138300
H	-5.67183900	-0.81113500	2.67481300
N	3.57225100	-3.69911800	1.31182000
O	2.36606300	-3.86619000	1.35902700
O	4.39068800	-4.53885200	1.65192600
C	-0.08562200	0.13443600	-0.99409100
O	0.64264800	-1.01292800	-1.22881400
H	0.24378900	0.93442200	-1.98966800
C	-1.56477300	-0.03081600	-1.02384300
C	-2.18589700	-1.20433900	-1.19184000
H	-1.48547000	-2.03559200	-1.26523500
Br	-2.49993400	1.63894700	-1.09049200
C	-3.61624200	-1.52465500	-1.30207500
C	-4.61127200	-0.83316700	-0.59242300
C	-4.00333000	-2.61950900	-2.08941500
C	-5.94798900	-1.20445700	-0.70328900
H	-4.32929100	-0.00523300	0.04915300
C	-5.33958400	-2.98876400	-2.19968100
H	-3.23950800	-3.17533500	-2.62678500
C	-6.32015500	-2.27926300	-1.50876800
H	-6.70370600	-0.65433700	-0.14953400
H	-5.61527100	-3.83345600	-2.82399400
H	-7.36427800	-2.56568300	-1.59118700
C	1.37627000	0.68153200	-3.87322300
O	0.83064100	1.50467800	-3.01787600
O	1.53750500	-0.58843000	-3.48281000
H	1.13542900	-0.80430900	-2.51075500
O	1.76794400	1.02647700	-4.99045000

Si-TS2^C

C	-3.63982700	-2.27725400	-0.87162700
C	-2.54739600	-1.61008600	-0.32026700
C	-2.23727500	-1.68306800	1.03407900
C	-3.09249500	-2.46075800	1.80695600
C	-4.19933700	-3.13621900	1.29466100
C	-4.47694200	-3.04397000	-0.06239200

C	-3.74603000	-2.03645900	-2.35273700
C	-2.48189600	-1.23115500	-2.73844000
C	-1.80464200	-0.82344500	-1.37641100
H	-1.36614400	-1.16505700	1.45704600
H	-5.33068100	-3.56618600	-0.48252600
H	-3.78947600	-2.96757900	-2.92758700
H	-2.73929100	-0.32776300	-3.29176300
H	-4.65026200	-1.46800300	-2.59094700
H	-1.90167200	0.25000600	-1.21146300
N	-0.37996800	-1.14121800	-1.39363100
O	-1.62719400	-1.94391700	-3.61745300
C	0.64426200	-0.58269000	-0.69993900
C	0.11450200	-2.20639000	-2.09091400
N	1.69819000	-1.34026900	-1.02018600
N	1.38932700	-2.35177400	-1.88644800
C	-0.82762800	-2.93191400	-2.99247500
H	-1.43539400	-3.65115000	-2.42488800
H	-0.28150100	-3.46720700	-3.76963700
C	3.05092700	-1.11769000	-0.58885400
C	3.85112000	-0.28534500	-1.37171500
C	3.46717300	-1.67746600	0.61957300
C	5.12419100	0.00782600	-0.89315800
C	4.74535600	-1.34492400	1.05959400
C	5.56945100	-0.48337500	0.33479300
H	5.75925600	0.68073300	-1.46444700
H	5.08229900	-1.72007700	2.02268600
H	-4.82043800	-3.72464100	1.95843700
C	3.31607500	0.33125300	-2.63421100
H	2.52352100	1.05146400	-2.39833100
H	2.88863700	-0.42130300	-3.30483400
H	4.10712200	0.86127100	-3.16848300
C	2.54922200	-2.55694200	1.42104500
H	2.23955100	-3.43540700	0.84375300
H	1.65374700	-1.99124800	1.70086400
H	3.04645300	-2.89787000	2.33122100
C	6.86437600	-0.00356300	0.92720900
H	7.56520500	0.33190700	0.15822500

H	7.34722000	-0.77810600	1.52936700
H	6.63270600	0.84234300	1.58430200
N	-2.81954200	-2.58730000	3.24529700
O	-1.83331500	-2.03272500	3.69073000
O	-3.59801300	-3.24568700	3.91836500
C	0.62975700	0.48507600	0.33808800
O	0.40163900	-0.09371200	1.57451500
H	1.84750500	1.10638900	0.49570500
C	-0.30127600	1.58253300	0.00940200
C	-1.16811600	2.14106500	0.86969900
H	-1.21499700	1.58558000	1.80618100
Br	-0.09036600	2.22994200	-1.79528900
C	-2.04838900	3.30750100	0.74145300
C	-1.71608300	4.46581500	0.02015300
C	-3.28086100	3.28454800	1.41531000
C	-2.60124200	5.53644200	-0.05407900
H	-0.75176000	4.53066500	-0.47006000
C	-4.16406400	4.35549400	1.34136500
H	-3.54238800	2.40501700	1.99806000
C	-3.83144200	5.48759300	0.59905400
H	-2.32028600	6.42254300	-0.61595400
H	-5.11321600	4.30757200	1.86734700
H	-4.51788300	6.32662500	0.54015800
C	3.30764900	1.22188600	2.08089600
O	2.86776200	1.66582600	0.93464100
O	2.52235600	0.38015500	2.75742200
H	1.59002400	0.19707700	2.28082600
O	4.39479000	1.55661900	2.56302700

(E,Z)-M2

C	-5.06635300	0.26979700	-0.59129600
C	-3.69023400	0.48880700	-0.64354000
C	-3.09954400	1.53975500	0.04535000
C	-3.94314800	2.35327700	0.79050800
C	-5.32202600	2.16604400	0.86016800
C	-5.88982100	1.11083300	0.15721700

C	-5.45917700	-0.92836900	-1.41096700
C	-4.12944700	-1.58250400	-1.86270800
C	-2.98868800	-0.56030400	-1.48162600
H	-2.03360600	1.73121400	0.00112400
H	-6.96095400	0.94172900	0.20222000
H	-6.06198800	-1.64619800	-0.84501200
H	-4.11894400	-1.74514000	-2.94054400
H	-6.05284600	-0.62570700	-2.27913800
H	-2.55420800	-0.12442600	-2.38055500
N	-1.92312300	-1.22158700	-0.74404000
O	-3.94744500	-2.87447500	-1.31267500
C	-0.58037400	-0.88852700	-0.60306800
C	-2.17242300	-2.28158400	0.09259800
N	-0.12571700	-1.78204400	0.35479400
N	-1.13502800	-2.66381400	0.74987300
C	-3.54247000	-2.87054400	0.04486200
H	-4.23725800	-2.29387000	0.67229300
H	-3.52509800	-3.90202800	0.39751200
C	0.95303500	-1.56000400	1.26566900
C	1.89710400	-2.58276700	1.43189900
C	1.02797000	-0.36081400	1.98888000
C	2.96074000	-2.36211600	2.30292300
C	2.12732900	-0.17724400	2.82989400
C	3.10644800	-1.15662300	2.99264600
H	3.70374100	-3.14563500	2.43447400
H	2.20642800	0.75355100	3.38764700
H	-5.92474000	2.83481200	1.46229100
C	1.75093800	-3.88242500	0.69089600
H	1.50735900	-3.69746600	-0.35909500
H	0.93826700	-4.48366100	1.11090700
H	2.67449200	-4.46312900	0.74379500
C	-0.03685500	0.70171100	1.90992700
H	-1.03229600	0.26290300	1.78659900
H	0.13522100	1.38092100	1.06735500
H	-0.03981600	1.29814400	2.82516300
C	4.30397500	-0.90729600	3.87148400
H	4.04721000	-0.27069400	4.72238400

H	5.09535700	-0.39890900	3.30922400
H	4.71918100	-1.84308500	4.25437600
N	-3.34742700	3.45906900	1.54830200
O	-2.13240800	3.56161800	1.54848000
O	-4.09727400	4.21554700	2.14161600
C	0.10995400	0.10935000	-1.23213100
O	-0.64361800	1.15758600	-1.76608800
H	-0.34848900	1.31023900	-2.67606100
C	1.54629300	0.29688900	-1.17546300
C	2.13940100	1.49934900	-1.05776000
H	1.43543400	2.32140300	-0.92506200
Br	2.56460800	-1.27944700	-1.57426400
C	3.55544200	1.88908100	-1.10604700
C	4.59472000	1.09212500	-0.60140400
C	3.87740600	3.15816200	-1.61170000
C	5.91160200	1.53891800	-0.64294900
H	4.36641600	0.12754700	-0.16382000
C	5.19432800	3.60090400	-1.65622200
H	3.07887900	3.79770100	-1.97893200
C	6.21987900	2.78846600	-1.17639900
H	6.70106500	0.90882500	-0.24430100
H	5.41952200	4.58255400	-2.06208000
H	7.24939900	3.13139600	-1.20655100

(Z,Z)-M2

C	1.77058800	3.70489600	-1.01158700
C	1.20300800	2.60319500	-0.36930600
C	0.86114900	2.64392200	0.97514500
C	1.11359600	3.83395800	1.64740800
C	1.68741300	4.94815500	1.03996900
C	2.02067000	4.88154900	-0.30777800
C	2.03399400	3.40717100	-2.46460300
C	1.31728600	2.06609800	-2.74486400
C	1.02680700	1.44838100	-1.33228500
H	0.41398400	1.80048200	1.49074100
H	2.45965900	5.74214100	-0.80241400

H	1.66077000	4.18815700	-3.13420900
H	1.94032600	1.38671200	-3.32738700
H	3.10966400	3.30835000	-2.64419700
H	1.73736300	0.64795800	-1.13326600
N	-0.31785600	0.89145700	-1.30601900
O	0.14479700	2.22803200	-3.52906300
C	-0.87175500	0.02115500	-0.38205200
C	-1.35422900	1.64462100	-1.81999100
N	-2.21433900	0.31708200	-0.41422800
N	-2.50178300	1.31357400	-1.34178700
C	-0.98490100	2.69550900	-2.81783600
H	-0.78259100	3.65259300	-2.31598600
H	-1.79507400	2.84680500	-3.53253900
C	-3.25257800	-0.57146100	0.00529000
C	-3.97334900	-0.26487800	1.16339100
C	-3.49620200	-1.72123400	-0.75101500
C	-4.97646200	-1.14650700	1.55639900
C	-4.50593000	-2.58262200	-0.31387300
C	-5.25327000	-2.31029500	0.83169600
H	-5.55183300	-0.92734200	2.45344400
H	-4.71458600	-3.48282200	-0.88725000
H	1.85822100	5.84630100	1.62081900
C	-3.63415600	0.96647000	1.95491100
H	-3.69813900	1.86645500	1.33550600
H	-2.60696300	0.89869500	2.32890800
H	-4.30828800	1.08002300	2.80636100
C	-2.70438500	-2.00805700	-2.00039800
H	-1.63943000	-2.15809100	-1.78686000
H	-2.77631500	-1.17358900	-2.70597100
H	-3.08137100	-2.90563100	-2.49508700
C	-6.34603800	-3.24216700	1.28693100
H	-6.38668600	-4.14104400	0.66763000
H	-7.32366200	-2.75216400	1.23754500
H	-6.19119400	-3.55180100	2.32532700
N	0.75286800	3.92036500	3.06720000
O	0.22398900	2.94984700	3.58109200
O	0.99706600	4.95927500	3.65660100

C	-0.26560600	-0.91886700	0.41996800
O	-0.92426600	-1.22379200	1.60728400
H	-1.20964600	-2.14999400	1.57932100
C	0.99108300	-1.57325700	0.17678000
C	1.79428000	-2.06712800	1.14202800
H	1.52232600	-1.72328000	2.14000100
Br	1.39282400	-1.88689700	-1.69261800
C	2.95840100	-2.95849400	1.08740400
C	3.95125200	-2.79956700	2.06884800
C	3.11301500	-3.99822700	0.15658700
C	5.07576400	-3.61577500	2.09526000
H	3.83430100	-2.01563500	2.81270500
C	4.23872400	-4.81453400	0.18490100
H	2.34302500	-4.17560200	-0.58432000
C	5.22842300	-4.62612400	1.14757400
H	5.83274600	-3.46515000	2.85894300
H	4.33578300	-5.61358800	-0.54422400
H	6.10433500	-5.26708800	1.16521400

(E,Z)-TS3

C	5.11715500	-0.19760800	-0.04628300
C	3.80398000	0.12969500	0.29299200
C	3.25910500	1.36647700	-0.02921300
C	4.08082700	2.25046900	-0.71623700
C	5.39614200	1.95626700	-1.06909700
C	5.92034500	0.71688200	-0.72682100
C	5.48224900	-1.57864100	0.42130800
C	4.19555000	-2.16043700	1.05746400
C	3.11984100	-1.00655800	1.01894400
H	2.24853300	1.64957900	0.24494600
H	6.94305100	0.46726500	-0.99057100
H	5.82674800	-2.21763200	-0.39892700
H	4.36755100	-2.43428000	2.09820800
H	6.29195000	-1.54068400	1.15584800
H	2.82497000	-0.72082400	2.02573100
N	1.90398500	-1.44684500	0.31968000

O	3.77502100	-3.36424500	0.44373500
C	0.63856400	-0.92639400	0.33124200
C	1.92984100	-2.42874300	-0.63718400
N	-0.03323600	-1.65717400	-0.59015600
N	0.77661300	-2.58978700	-1.19674200
C	3.20229900	-3.18061100	-0.83527500
H	3.87471300	-2.63176900	-1.50997500
H	2.99884400	-4.16193800	-1.26481500
C	-1.43263100	-1.66405400	-0.90116500
C	-2.33831900	-2.15265100	0.04316100
C	-1.82447100	-1.19870900	-2.16178600
C	-3.68827400	-2.16369700	-0.31452300
C	-3.18258800	-1.22557800	-2.46586500
C	-4.12810100	-1.70317600	-1.55402800
H	-4.41403000	-2.53320100	0.40630500
H	-3.51397900	-0.85072100	-3.43169500
H	5.98473200	2.69342900	-1.60129900
C	-1.90228100	-2.61137000	1.40765900
H	-1.77530000	-1.75174500	2.07803400
H	-0.95749300	-3.16156500	1.36744700
H	-2.65893800	-3.26686500	1.84467700
C	-0.81024900	-0.66991300	-3.13913400
H	-0.19346600	-1.47877800	-3.54378100
H	-0.13213700	0.04441600	-2.65994800
H	-1.30675600	-0.16715800	-3.97136400
C	-5.59209200	-1.69600700	-1.90518200
H	-5.90443500	-0.69926200	-2.23108600
H	-6.20650500	-1.98183500	-1.04821900
H	-5.80385400	-2.39225600	-2.72353600
N	3.53584400	3.56190400	-1.08693500
O	2.36091800	3.77921500	-0.84803400
O	4.28674700	4.36175700	-1.61804900
C	0.20820200	0.19204600	1.09208500
O	1.02183200	0.53580700	2.15403600
H	0.39448700	0.76555400	2.87285100
C	-0.98843200	0.80961500	0.89103100
C	-1.72157800	1.38070400	-0.05895600

H	-1.11749800	1.77790500	-0.87794500
Br	-1.90306100	0.86833300	3.11972000
C	-3.16546500	1.57720900	-0.22218300
C	-4.13935500	0.97133500	0.58546400
C	-3.59007800	2.37291700	-1.29781300
C	-5.49101800	1.18070200	0.33290000
H	-3.83325500	0.33942400	1.40924100
C	-4.94139000	2.57755600	-1.55086800
H	-2.84412300	2.83340700	-1.94080100
C	-5.89958900	1.98337800	-0.73129200
H	-6.23189300	0.70490000	0.96894100
H	-5.24579800	3.19955700	-2.38698000
H	-6.95670600	2.13983600	-0.92396300

M3

C	-4.84741100	-0.81607600	0.17450900
C	-3.64790100	-0.22400500	-0.22097600
C	-3.59416600	1.08151500	-0.68301100
C	-4.79633000	1.77757000	-0.72210900
C	-6.01190600	1.22133300	-0.33140300
C	-6.03767400	-0.09287100	0.12126900
C	-4.62667600	-2.24006000	0.61218400
C	-3.09134000	-2.42023800	0.69239400
C	-2.50124600	-1.19535900	-0.09447300
H	-2.66924200	1.54987100	-1.00344700
H	-6.97514300	-0.54178200	0.43328000
H	-5.08608600	-2.46618600	1.57914700
H	-2.74797500	-3.33530400	0.20929400
H	-5.05191700	-2.93283100	-0.12115200
H	-2.14187500	-1.53759300	-1.06012700
N	-1.36522400	-0.60362500	0.61804900
O	-2.63484400	-2.53316300	2.03022500
C	-0.21178200	-0.04753900	0.19325900
C	-1.32953200	-0.61246700	1.98475200
N	0.45788800	0.26208900	1.31008900
N	-0.22652400	-0.09502400	2.43401800

C	-2.43825600	-1.30567100	2.70285300
H	-3.34640400	-0.68768400	2.71770300
H	-2.14007100	-1.52333600	3.72870900
C	1.79012000	0.79239600	1.44039900
C	2.83823500	-0.11832900	1.57603300
C	1.96214600	2.17917000	1.42690400
C	4.12684000	0.41355300	1.66846400
C	3.26539900	2.65615700	1.51858800
C	4.35720500	1.78660700	1.63104700
H	4.96907600	-0.26961200	1.74555100
H	3.43633300	3.73005500	1.49484400
H	-6.91386500	1.81893100	-0.38132700
C	2.59148000	-1.60074000	1.63304500
H	1.92488800	-1.95255500	0.83619400
H	2.12581400	-1.87313900	2.58730300
H	3.53641900	-2.14193900	1.55059100
C	0.78699600	3.10046000	1.25290000
H	-0.03347700	2.83576200	1.92698900
H	0.40365000	3.04652300	0.22648200
H	1.07411500	4.13476300	1.45068200
C	5.75710600	2.33653300	1.69132400
H	5.90063800	2.94515800	2.59016600
H	5.96005400	2.97915600	0.82856200
H	6.49816900	1.53405600	1.70006000
N	-4.78155200	3.16566100	-1.19749100
O	-3.70405600	3.65489200	-1.49021400
O	-5.84486700	3.75601100	-1.27309500
C	0.21254400	0.16719300	-1.20071500
O	-0.57989600	-0.38524400	-2.16429100
H	-0.36588200	-1.36861800	-2.11171500
C	1.32384400	0.81291700	-1.48412300
C	2.48491200	1.33854700	-1.77503000
H	2.56075900	2.40242800	-2.00029000
Br	0.23116300	-3.08272300	-1.06433700
C	3.73653300	0.55585400	-1.71483900
C	3.71686400	-0.84071200	-1.59044700
C	4.95792400	1.23437600	-1.69815600

C	4.90843100	-1.53539800	-1.42326700
H	2.77023800	-1.38121000	-1.61253600
C	6.14849200	0.53338500	-1.52647600
H	4.96837200	2.31712100	-1.79644100
C	6.12540200	-0.85210500	-1.38281800
H	4.88710800	-2.61632400	-1.32273900
H	7.09232900	1.06979400	-1.50277500
H	7.05294900	-1.39984400	-1.24736700

TS4

C	4.82917900	-0.70741500	-1.12977900
C	3.74052300	-0.41770200	-0.30201800
C	3.87235500	-0.32018700	1.07264100
C	5.14904500	-0.51807900	1.58934000
C	6.25475300	-0.81387700	0.79778300
C	6.09162900	-0.91326100	-0.58068300
C	4.39081500	-0.76533000	-2.57201600
C	3.02203000	-0.05630100	-2.58786000
C	2.49154500	-0.27697600	-1.13903400
H	3.03800100	-0.09922500	1.72948600
H	6.94384800	-1.13865200	-1.21354500
H	5.08658800	-0.28213100	-3.26184500
H	2.30426500	-0.47797500	-3.29133800
H	4.27653400	-1.80987900	-2.88440900
H	1.86023300	-1.16783300	-1.13370200
N	1.65149100	0.84369000	-0.73069100
O	3.17340100	1.31007600	-2.96743100
C	0.44399000	0.88392600	-0.15624800
C	1.92826500	2.10913200	-1.14578700
N	0.06077100	2.15837400	-0.18851200
N	0.97339600	2.93750900	-0.81188200
C	3.16204300	2.29931000	-1.95986400
H	4.04744200	2.25014500	-1.31148400
H	3.13585300	3.27222500	-2.45151300
C	-1.13053900	2.71494600	0.39990000
C	-2.12848700	3.19102700	-0.45832800

C	-1.23031400	2.72388600	1.79352600
C	-3.29356700	3.66020200	0.14408900
C	-2.41869600	3.20822600	2.33849000
C	-3.45947100	3.66898600	1.53160200
H	-4.09599000	4.02670800	-0.49175700
H	-2.52971000	3.22634900	3.41936700
H	7.22238300	-0.95428600	1.26364700
C	-1.94975000	3.21314300	-1.95073900
H	-1.45632500	2.31132100	-2.33011200
H	-1.33759100	4.07368000	-2.24251900
H	-2.92169500	3.31212400	-2.43895800
C	-0.11846000	2.22851300	2.68091900
H	0.85926700	2.57810200	2.33525700
H	-0.08837600	1.13307600	2.73022300
H	-0.26422500	2.59183300	3.69970800
C	-4.73614200	4.18858200	2.13628600
H	-4.74716100	4.05171500	3.21959400
H	-5.60434800	3.67310500	1.71514000
H	-4.85798200	5.25582200	1.92590100
N	5.33894700	-0.39837300	3.03897400
O	4.37013200	-0.10218100	3.71750300
O	6.45412500	-0.59609300	3.48817800
C	-0.35400500	-0.23982100	0.38117800
O	0.36026000	-1.17549500	0.91538800
H	-0.16023000	-2.08312100	0.93238100
C	-1.73389700	-0.24060600	0.17892900
C	-2.61107700	-0.84940500	1.01567300
H	-2.31926400	-1.06479300	2.04637600
Br	-1.15200600	-3.75242700	0.59530500
C	-3.97013300	-1.22649700	0.64401700
C	-4.56756300	-0.76613700	-0.54315200
C	-4.66575700	-2.13259700	1.45915000
C	-5.82804700	-1.22240700	-0.90776700
H	-4.05166300	-0.04142200	-1.16672000
C	-5.92270300	-2.59048700	1.08448100
H	-4.20228900	-2.49005000	2.37458900
C	-6.50417500	-2.13689900	-0.09926800

H	-6.28728100	-0.85776000	-1.82097400
H	-6.45082500	-3.29958300	1.71367000
H	-7.48909400	-2.48951600	-0.38929000
C	-0.64249900	-0.22737200	-2.59520900
O	-0.05446300	0.74204900	-3.11362200
O	-1.97880700	-0.19667700	-2.39093900
H	-1.98435600	-0.02936600	-1.06685100
O	-0.04707200	-1.27510600	-2.13207900
Na	-1.87854400	-2.41707300	-1.67806200

M4

C	4.82690000	-0.09173700	-0.93566700
C	3.49132500	-0.42314100	-0.70758900
C	3.12602000	-1.34569300	0.26195800
C	4.15450400	-1.91945300	0.99569200
C	5.49910000	-1.62129500	0.78921500
C	5.83857700	-0.69637200	-0.19060600
C	4.95855600	0.93182500	-2.02930400
C	3.51714400	1.39397300	-2.34506900
C	2.57424100	0.35120300	-1.62844500
H	2.09498900	-1.62197900	0.44830800
H	6.87986100	-0.44536100	-0.36411400
H	5.57567900	1.78795600	-1.74020200
H	3.31625300	1.38476600	-3.41592400
H	5.41767400	0.48805700	-2.91799200
H	2.07033900	-0.29328100	-2.34872300
N	1.53540400	1.05267700	-0.85447800
O	3.27583600	2.73437900	-1.95200700
C	0.27883700	0.70867100	-0.52794200
C	1.79180900	2.24635500	-0.24303100
N	-0.16623400	1.67759700	0.27094800
N	0.76330900	2.64819200	0.45150400
C	3.08758900	2.91614500	-0.56190300
H	3.90706500	2.48820900	0.03110500
H	3.01891400	3.98499600	-0.35953100
C	-1.42677700	1.73974000	0.96876600

C	-2.36606300	2.67959500	0.53359400
C	-1.64333900	0.84869300	2.02295800
C	-3.59687800	2.68484200	1.18634000
C	-2.89231600	0.90003100	2.64025000
C	-3.87950300	1.79772100	2.22932100
H	-4.35333000	3.39877100	0.87069100
H	-3.09602800	0.22172100	3.46482700
H	6.25490500	-2.10695900	1.39466200
C	-2.06457300	3.62787000	-0.59482400
H	-1.74138600	3.09206600	-1.49409700
H	-1.26488500	4.32286700	-0.32200700
H	-2.95183800	4.20943700	-0.84852500
C	-0.59383700	-0.13455300	2.46917800
H	0.40997800	0.30043500	2.43852500
H	-0.59746400	-1.03416900	1.84167400
H	-0.79135600	-0.45450200	3.49361800
C	-5.23362900	1.79222000	2.88398100
H	-5.15706700	1.55844000	3.94853700
H	-5.87350700	1.03062900	2.42450900
H	-5.73153700	2.75790900	2.77258600
N	3.79953000	-2.88157000	2.04634100
O	2.61529100	-3.07327200	2.26362700
O	4.70587200	-3.42985400	2.64603100
C	-0.40707900	-0.56972700	-0.96167400
O	0.33249500	-1.50399500	-1.22292200
C	-1.85897500	-0.57319100	-1.03567800
C	-2.49609200	-1.74639800	-1.24125100
H	-1.87792600	-2.63757100	-1.34872800
C	-3.93476500	-1.95321000	-1.32478900
C	-4.86575300	-0.91919500	-1.12360100
C	-4.40071400	-3.24483500	-1.61268600
C	-6.22476800	-1.17786400	-1.21678600
H	-4.52761700	0.08492800	-0.88461300
C	-5.76343100	-3.50019200	-1.70857900
H	-3.68175100	-4.04539800	-1.76338600
C	-6.67601700	-2.46695400	-1.51116600
H	-6.93985600	-0.37718900	-1.05876500

H	-6.11249800	-4.50222400	-1.93481900
H	-7.74117100	-2.66363900	-1.58218100
H	-2.38699700	0.36429100	-0.90746100

TS5R

C	5.21282500	-1.50357400	-0.59935000
C	3.88361000	-1.08601600	-0.54489900
C	2.97028800	-1.66764400	0.31629000
C	3.42662500	-2.72004800	1.09910900
C	4.73779400	-3.18768900	1.04913000
C	5.64244800	-2.56758700	0.19291200
C	6.00064100	-0.64570400	-1.55395700
C	5.06512400	0.53337000	-1.92106800
C	3.63115300	0.06435100	-1.48975500
H	1.95446300	-1.29938800	0.40970100
H	6.67336600	-2.90403200	0.15957000
H	6.93222800	-0.27131600	-1.11898600
H	5.08071900	0.73551400	-2.99155600
H	6.26469100	-1.21175300	-2.45301000
H	3.02546200	-0.22765500	-2.34576100
N	2.91070600	1.13261000	-0.78774300
O	5.45896800	1.75956600	-1.32651000
C	1.59010000	1.35407800	-0.61538900
C	3.58363800	1.97282300	0.05337800
N	1.52487900	2.31891900	0.30924800
N	2.75896600	2.71719800	0.72931500
C	5.07774300	1.93149300	0.02391000
H	5.45161200	1.12397000	0.66882800
H	5.48736000	2.87915500	0.37413100
C	0.36247600	2.92473100	0.90855800
C	-0.17029300	4.07075400	0.32095700
C	-0.17456000	2.31257300	2.04534600
C	-1.30993600	4.61317000	0.91521900
C	-1.31248800	2.89308600	2.59777600
C	-1.89524900	4.03690700	2.04250900
H	-1.75276700	5.50467500	0.47900600

H	-1.76047900	2.43733600	3.47752900
H	5.03858300	-4.01250000	1.68374100
C	0.42993400	4.65977100	-0.92528800
H	0.25280500	3.99953700	-1.78200900
H	1.51077000	4.79743000	-0.82589900
H	-0.02226500	5.62782700	-1.14719000
C	0.40709700	1.03371000	2.58524100
H	1.48725800	1.11252100	2.74363100
H	0.22934100	0.20870900	1.88099600
H	-0.06088600	0.76904400	3.53491900
C	-3.15325900	4.60949900	2.63723800
H	-3.11010600	4.60796100	3.72957400
H	-4.02013100	4.00883900	2.34112700
H	-3.32407400	5.63316700	2.29728100
N	2.48514400	-3.34334600	2.03171400
O	1.32402600	-2.94846700	2.02096400
O	2.89705700	-4.20915400	2.77470700
C	0.49692200	0.65887200	-1.40273700
O	0.88756400	0.00777600	-2.40563000
C	-0.81277900	0.78822100	-0.95617100
C	-1.91218300	0.37063300	-1.76406000
H	-1.77904300	0.52981500	-2.83317700
C	-3.27489200	0.68235900	-1.26548100
C	-3.60782600	0.52656400	0.08571400
C	-4.25926900	1.11949200	-2.15820300
C	-4.89615200	0.80718400	0.53223700
H	-2.86055800	0.16495300	0.78804400
C	-5.54373000	1.41117400	-1.71120900
H	-4.00984600	1.23491900	-3.21013000
C	-5.86651400	1.25156000	-0.36459500
H	-5.14259400	0.67430100	1.58143700
H	-6.29359400	1.76132300	-2.41365400
H	-6.87039600	1.47375800	-0.01587400
H	-1.02226400	1.19957300	0.01965400
C	-2.51319800	-2.65522700	0.00931800
C	-3.82533200	-2.74098300	-0.49302600
C	-4.18598500	-2.41115200	-1.83425600

C	-3.20499700	-1.90560700	-2.62696100
C	-1.87913200	-1.62592700	-2.11761700
C	-1.49709700	-2.16688700	-0.84427900
C	-2.54634600	-3.09195100	1.37215800
C	-3.85157700	-3.40508700	1.63741500
H	-5.19726900	-2.56304300	-2.19546000
H	-3.42233500	-1.62530000	-3.65315000
H	-1.06855400	-1.54012100	-2.83697800
H	-1.72012500	-3.16025800	2.06620500
H	-4.31476700	-3.76700100	2.54429400
N	-0.21865100	-2.08845400	-0.46753600
H	0.46980900	-1.80515900	-1.15868800
H	0.10264400	-2.52976200	0.38658300
N	-4.62003900	-3.19482700	0.50972500
C	-6.05527600	-3.39517900	0.40797600
H	-6.54437700	-2.46051100	0.12250600
H	-6.28166900	-4.16633000	-0.33225200
H	-6.43305200	-3.71337000	1.37916400

TS5S

C	5.57221300	-1.46458400	-0.83073900
C	4.25992100	-1.25608200	-0.40897700
C	3.88949300	-1.41447500	0.91959600
C	4.89101500	-1.78565300	1.80548200
C	6.21035200	-2.01030600	1.41874800
C	6.55373000	-1.84887700	0.08253600
C	5.72176100	-1.22955400	-2.30787000
C	4.34776100	-0.70576500	-2.79174700
C	3.36841500	-0.85232000	-1.56298300
H	2.86537900	-1.28220000	1.24828900
H	7.57675200	-2.01412900	-0.23975500
H	6.50833200	-0.50319200	-2.53796600
H	3.96650000	-1.30395200	-3.61895200
H	5.98237800	-2.15675200	-2.82645500
H	2.58839600	-1.58835200	-1.74656700
N	2.69447500	0.42928300	-1.28226800

O	4.41604700	0.61004100	-3.31369000
C	1.52401300	0.69987700	-0.66831100
C	3.29808600	1.62666100	-1.54844700
N	1.47913500	2.03202000	-0.57669000
N	2.57372700	2.62276900	-1.13026500
C	4.57053100	1.61185300	-2.32765400
H	5.42788000	1.41721800	-1.66913000
H	4.71649700	2.56973300	-2.82742000
C	0.48806800	2.85456300	0.06913400
C	0.51970100	2.95107100	1.45986800
C	-0.46593600	3.48550700	-0.73308200
C	-0.47910000	3.71776600	2.06089700
C	-1.43966600	4.23857800	-0.08367800
C	-1.46598800	4.35643900	1.30996000
H	-0.48732800	3.80954000	3.14374500
H	-2.20209800	4.73758700	-0.67688200
H	6.94468000	-2.30170100	2.15984700
C	1.55267600	2.22204700	2.27368500
H	2.55478400	2.33281100	1.84768400
H	1.32004500	1.15132700	2.32055800
H	1.57062900	2.60301300	3.29609700
C	-0.47217400	3.28942000	-2.22440000
H	-0.67935500	2.23968100	-2.46860400
H	0.49154400	3.55152600	-2.67046100
H	-1.24565100	3.90409600	-2.68820800
C	-2.56343100	5.13577100	1.98275200
H	-3.48655600	4.54635700	2.00764100
H	-2.77879100	6.06194400	1.44338900
H	-2.29944400	5.38605300	3.01242900
N	4.53883800	-1.94582500	3.22158500
O	3.40973600	-1.64096500	3.56505600
O	5.39515400	-2.36910600	3.97763000
C	0.54660300	-0.34909800	-0.18806000
O	1.01251100	-1.51157600	-0.09572300
C	-0.75915200	0.05247900	0.07649600
C	-1.67049100	-0.88681600	0.64677300
H	-1.19483500	-1.64828800	1.26304800

C	-2.96848200	-0.39732100	1.16633100
C	-3.64487600	0.66397100	0.54677700
C	-3.55467000	-1.01002000	2.27851100
C	-4.87018300	1.10313900	1.03162600
H	-3.22074500	1.12937800	-0.33992100
C	-4.77890100	-0.56371100	2.77286200
H	-3.04283000	-1.83902100	2.76054400
C	-5.43929400	0.49196900	2.14968800
H	-5.38533600	1.91924100	0.53432100
H	-5.21592400	-1.04124600	3.64433800
H	-6.39409400	0.83968400	2.53196900
H	-1.08701000	1.05793800	-0.13831300
C	-4.19221400	-1.46837800	-1.70095300
C	-4.85737100	-2.34846500	-0.82587200
C	-4.18796300	-3.30031500	-0.00051900
C	-2.82925000	-3.27335200	-0.01575500
C	-2.08981300	-2.26671000	-0.74822100
C	-2.77965300	-1.46900100	-1.72204300
C	-5.19328100	-0.69021500	-2.36444700
C	-6.39489400	-1.11330900	-1.86767700
H	-4.74579100	-4.00971900	0.60118200
H	-2.25958400	-3.96492000	0.59751200
H	-1.03403600	-2.46386600	-0.93129100
H	-5.04955300	0.08661400	-3.10198000
H	-7.40099200	-0.78863700	-2.09260500
N	-2.08877900	-0.65342200	-2.53032300
H	-2.56161200	-0.08117400	-3.21503400
H	-1.08859400	-0.75051800	-2.61314400
N	-6.18961400	-2.11585400	-0.94254100
C	-7.23024800	-2.79711500	-0.19216000
H	-7.18633900	-3.87352700	-0.37288500
H	-7.11610500	-2.60022800	0.87672000
H	-8.19710900	-2.42030200	-0.52518500

TS5S^{C3}

C	-4.97729500	-0.01767100	-0.08275500
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C	-3.63085100	-0.00640400	0.27859000
C	-3.22867000	-0.16651200	1.59751600
C	-4.23513800	-0.34934200	2.53624300
C	-5.59034900	-0.36487700	2.21243300
C	-5.96545500	-0.19387900	0.88587300
C	-5.15081000	0.18578400	-1.56326700
C	-3.72133700	0.17278400	-2.15697700
C	-2.74157300	0.20369900	-0.92538900
H	-2.18341900	-0.12778700	1.88338100
H	-7.01549100	-0.20392400	0.61220700
H	-5.76181000	-0.59575200	-2.02685000
H	-3.53639000	1.05275700	-2.77408000
H	-5.64370100	1.14101000	-1.76822400
H	-2.18919500	1.14144300	-0.86356900
N	-1.74402100	-0.86885100	-1.04186400
O	-3.50339700	-0.92180700	-3.03302500
C	-0.48372000	-0.94679300	-0.57780500
C	-2.03195400	-2.06160100	-1.64332500
N	-0.07274300	-2.17956700	-0.88789600
N	-1.02592100	-2.88225500	-1.56536400
C	-3.32760900	-2.16519900	-2.37791700
H	-4.15499600	-2.39220400	-1.69224300
H	-3.27019500	-2.94745300	-3.13546700
C	1.17963600	-2.80891700	-0.55653300
C	1.40560900	-3.18807200	0.76860000
C	2.11383100	-2.98304200	-1.58103700
C	2.65067800	-3.74056700	1.06390000
C	3.34197300	-3.54138300	-1.23140500
C	3.63085200	-3.91241000	0.08409300
H	2.85948000	-4.03988700	2.08793600
H	4.09250200	-3.68301200	-2.00488400
H	-6.32667200	-0.51006100	2.99325100
C	0.36957200	-2.98552300	1.84046700
H	-0.62935200	-3.27150700	1.49718600
H	0.33368000	-1.93602700	2.15503900
H	0.61334300	-3.58538300	2.71898800
C	1.81187300	-2.54713900	-2.98891600

H	1.51260900	-1.49213400	-3.01451000
H	0.99191800	-3.13173500	-3.41729100
H	2.69077000	-2.67524900	-3.62344000
C	4.98460000	-4.46060900	0.44698000
H	5.47909700	-4.90526100	-0.41974800
H	4.90837800	-5.21875700	1.23046400
H	5.62935400	-3.66006000	0.82645900
N	-3.84857400	-0.53771100	3.93997700
O	-2.65899000	-0.56902000	4.20327800
O	-4.73697900	-0.65634900	4.76553100
C	0.22328400	0.19069500	0.12035400
O	-0.53314000	1.01465500	0.69085100
C	1.60983500	0.21057900	0.02760900
C	2.31393800	1.29747900	0.63170300
H	1.70937500	1.80232800	1.38499100
C	3.73838800	1.10875700	1.03942400
C	4.61655800	0.31672900	0.28952900
C	4.21230500	1.72728000	2.19968700
C	5.93518800	0.14618200	0.69577600
H	4.26805900	-0.17159000	-0.61712900
C	5.53197000	1.55378900	2.61002000
H	3.53505800	2.33782700	2.79268600
C	6.39728700	0.76396800	1.85771700
H	6.60433500	-0.47142900	0.10454600
H	5.88230100	2.03252700	3.51911600
H	7.42660800	0.62854100	2.17422700
H	2.13379200	-0.52775000	-0.56275000
C	1.14018900	2.83122300	-1.37099900
C	0.41530700	3.85266500	-0.74705500
C	-0.89480500	4.18626800	-1.06446900
C	-1.46480900	3.45437400	-2.10329200
C	-0.76051500	2.44981700	-2.77381200
C	0.55607500	2.11128800	-2.42361200
C	2.42820600	2.72030500	-0.67880000
C	2.43897000	3.84380800	0.20123500
H	-1.43323300	4.97591200	-0.55333700
H	-2.48050400	3.67987200	-2.41459600

H	-1.23246500	1.92058800	-3.59819700
H	3.33891400	2.40272200	-1.17450200
H	3.22665400	4.16046000	0.87462000
N	1.23278000	1.08985100	-3.07884400
H	2.24153900	1.13591700	-3.00504800
H	0.94001800	0.94538800	-4.03768800
N	1.25720400	4.44212500	0.21349200
C	0.84055500	5.51986900	1.09804000
H	0.50928500	6.37090300	0.49953900
H	0.02106800	5.17525300	1.73238100
H	1.68749100	5.81411100	1.71641300

TS5S^{C6}

C	-5.14338900	0.29253500	-0.29296900
C	-3.76803400	0.24956300	-0.06621800
C	-3.22632700	0.51815200	1.18359800
C	-4.12468400	0.82325700	2.19679400
C	-5.50390100	0.87735700	2.00744500
C	-6.01891800	0.60969600	0.74521500
C	-5.47199800	-0.02400000	-1.72605300
C	-4.14528400	-0.50128100	-2.36197900
C	-3.01733600	-0.12228700	-1.32709900
H	-2.15531500	0.51551400	1.35300700
H	-7.09025100	0.64122500	0.57620400
H	-6.23979800	-0.79735100	-1.82670200
H	-3.95192800	0.00366400	-3.30821500
H	-5.84327300	0.86779800	-2.24075600
H	-2.39296900	0.69525900	-1.68585300
N	-2.13252100	-1.27095700	-1.09148000
O	-4.16977200	-1.87775900	-2.69960000
C	-0.83434600	-1.32912300	-0.73814300
C	-2.60570600	-2.55330500	-1.12172500
N	-0.58395800	-2.62805800	-0.54886600
N	-1.67746500	-3.40437400	-0.79852300
C	-4.00334100	-2.75820200	-1.60378300
H	-4.72693300	-2.56565000	-0.79962800

H	-4.13487500	-3.77888400	-1.96318700
C	0.62243400	-3.23750200	-0.05019300
C	1.40516400	-3.96991600	-0.94425100
C	0.95212900	-3.04820600	1.29522800
C	2.58615800	-4.52139300	-0.44794000
C	2.14550700	-3.61484900	1.73608900
C	2.97377300	-4.34688700	0.88154500
H	3.21861400	-5.09753000	-1.11857800
H	2.43426300	-3.48196000	2.77592200
H	-6.14992200	1.12079100	2.84211700
C	0.99851700	-4.13294000	-2.38384300
H	0.82760400	-3.16071400	-2.85962800
H	0.07119400	-4.70688400	-2.47167900
H	1.77890800	-4.65251300	-2.94220000
C	0.08264000	-2.24325700	2.22303200
H	-0.98139400	-2.43674500	2.05527200
H	0.25828600	-1.16930500	2.08813100
H	0.31158100	-2.48690500	3.26206300
C	4.27025800	-4.91728000	1.38998600
H	5.00729500	-4.12014800	1.53360600
H	4.68752000	-5.64165400	0.68728100
H	4.13110000	-5.41179400	2.35523100
N	-3.58986700	1.10238200	3.53555500
O	-2.39531100	0.94181600	3.71543800
O	-4.36911700	1.47655600	4.39429900
C	0.05039700	-0.13152400	-0.51172700
O	-0.55910000	0.93672100	-0.20887400
C	1.41060000	-0.32002800	-0.63556700
C	2.32465500	0.72751400	-0.21743300
H	1.88008000	1.39434500	0.52403000
C	3.67778000	0.23682600	0.21083500
C	4.42006200	-0.65382400	-0.57072800
C	4.20628900	0.67662700	1.42699700
C	5.66393900	-1.10379500	-0.13643300
H	4.02734200	-0.99681400	-1.52536500
C	5.44623300	0.22013100	1.86613800
H	3.63820500	1.37971800	2.03055600

C	6.17825200	-0.67123400	1.08543600
H	6.23320000	-1.79352400	-0.75214700
H	5.84001300	0.56430300	2.81743600
H	7.14685000	-1.02491000	1.42462000
H	1.80864400	-1.26664500	-0.97634000
C	2.05994300	4.52880300	-0.57981600
C	1.06286100	3.71367100	-1.19537300
C	1.32012000	2.47817500	-1.72677700
C	2.64404400	1.94091800	-1.53796100
C	3.68981400	2.83901600	-1.05489000
C	3.42397500	4.08010000	-0.54579000
C	1.41989200	5.68017800	-0.10475100
C	0.07287000	5.54358300	-0.43488900
H	0.54197700	1.87601700	-2.18108200
H	2.97024700	1.23936800	-2.30528400
H	4.70629400	2.45784400	-1.02543400
H	1.85561900	6.51278700	0.42737000
H	-0.75118600	6.21555100	-0.23349400
N	4.37118800	4.89725200	0.05121700
H	4.22342900	5.88885700	-0.09135400
H	5.33049900	4.63255400	-0.13478300
N	-0.14394900	4.38238900	-1.08280400
C	-1.42095800	3.84430000	-1.51784700
H	-1.44503500	3.76494400	-2.60752600
H	-1.55459700	2.85683000	-1.06636500
H	-2.21340900	4.51604300	-1.18798800

TS5S^{C7}

C	-5.03830700	-0.02874600	-0.16169900
C	-3.68262000	0.03918300	0.15868000
C	-3.24456600	0.03594700	1.47568400
C	-4.22368800	-0.05942700	2.45547500
C	-5.58614500	-0.13074200	2.17264700
C	-5.99817500	-0.11124500	0.84613800
C	-5.25139200	0.00218100	-1.65007900
C	-3.84176900	-0.12476500	-2.27445800
C	-2.82744700	0.09347900	-1.08830700

H	-2.19395800	0.12231200	1.72971900
H	-7.05426400	-0.16763700	0.60341400
H	-5.89838700	-0.80629500	-2.00488300
H	-3.67497600	0.63610700	-3.03727200
H	-5.71931800	0.94427300	-1.95206300
H	-2.28624100	1.03650400	-1.17303600
N	-1.82412800	-0.98350800	-1.07550200
O	-3.65946200	-1.35333400	-2.95875100
C	-0.55171200	-1.00161400	-0.63571200
C	-2.14137700	-2.25844500	-1.45509000
N	-0.16249400	-2.27463700	-0.74484900
N	-1.14035400	-3.06746700	-1.26756700
C	-3.46524500	-2.47048800	-2.11141300
H	-4.26343600	-2.57129700	-1.36384800
H	-3.44269300	-3.36938600	-2.72746400
C	1.08277100	-2.86417700	-0.32636900
C	1.97512400	-3.27628200	-1.31780400
C	1.34148400	-2.96931100	1.04358900
C	3.19686600	-3.79784500	-0.89365800
C	2.57855300	-3.49372800	1.41108200
C	3.51692900	-3.90429400	0.46090100
H	3.91529700	-4.12625800	-1.64041400
H	2.81480900	-3.58375400	2.46863900
H	-6.29912100	-0.20336800	2.98497000
C	1.63862600	-3.14014300	-2.77807300
H	1.28822000	-2.12886600	-3.01256900
H	0.84333800	-3.83422000	-3.06675600
H	2.51521500	-3.35064700	-3.39296800
C	0.35216900	-2.50518500	2.07839400
H	-0.67771200	-2.74165800	1.79307700
H	0.42310700	-1.42097800	2.22677800
H	0.55613100	-2.98320200	3.03827500
C	4.85432600	-4.43750100	0.89943400
H	4.73836300	-5.20330300	1.67149100
H	5.46559400	-3.63548800	1.32615900
H	5.40245400	-4.87332000	0.06133700
N	-3.79764900	-0.08849100	3.86022300

O	-2.60124200	-0.11838200	4.09096400
O	-4.66250700	-0.08620500	4.71835800
C	0.17908700	0.21456200	-0.10715500
O	-0.56139600	1.11207200	0.34858600
C	1.57384500	0.19040300	-0.17481800
C	2.31787700	1.24820800	0.41075900
H	1.74476300	1.84467200	1.12040000
C	3.72730200	0.98442300	0.81308700
C	4.57993000	0.19876700	0.02736500
C	4.21377500	1.51611600	2.01212600
C	5.88196900	-0.06086100	0.44028500
H	4.22603100	-0.20842800	-0.91693200
C	5.51563500	1.25137400	2.42883400
H	3.56082300	2.13488000	2.62283600
C	6.35292100	0.46097100	1.64481000
H	6.53137800	-0.67178600	-0.17919900
H	5.87573300	1.66126100	3.36729200
H	7.36883900	0.25501500	1.96684400
H	2.08049200	-0.64351900	-0.64186400
C	0.26953600	3.82799300	-1.00324900
C	1.22129300	2.90677600	-1.47312200
C	2.52854200	2.75454600	-0.90694900
C	2.90176000	3.82175400	-0.02297800
C	2.00007800	4.73075200	0.45917000
C	0.64215700	4.74561200	0.00572200
C	-0.93607100	3.60662800	-1.74544000
C	-0.66401700	2.59669900	-2.62411300
H	3.30995100	2.28888200	-1.50053300
H	3.92362900	3.84863200	0.34332500
H	2.30429800	5.47230000	1.19119400
H	-1.87471700	4.13513000	-1.65643400
H	-1.27508400	2.15332500	-3.39865800
N	-0.22747200	5.62729000	0.51191500
H	-1.19352000	5.63409100	0.22114400
H	0.05431100	6.28108300	1.22724700
N	0.63812200	2.16102500	-2.44528100
C	1.32650900	1.24312700	-3.33858500

H	1.80582400	1.78772500	-4.15730700
H	2.08058400	0.68332700	-2.78427200
H	0.59973200	0.54296900	-3.75416900

M5R

C	-5.60563100	1.21324400	-1.09108500
C	-4.25405700	1.08351200	-0.77557100
C	-3.67926200	1.77731100	0.27990300
C	-4.52375500	2.59744700	1.01513200
C	-5.87741900	2.75919800	0.72593100
C	-6.42377000	2.06068700	-0.34371800
C	-5.97634500	0.35081700	-2.26669000
C	-4.73843000	-0.53680800	-2.53804400
C	-3.56687900	0.09915500	-1.69730100
H	-2.61876700	1.69515700	0.49488300
H	-7.47703800	2.16775600	-0.58203600
H	-6.85518300	-0.27300100	-2.07489900
H	-4.46881900	-0.53614700	-3.59368900
H	-6.20318500	0.96753900	-3.14189000
H	-2.81952900	0.58371800	-2.32622200
N	-2.87713000	-0.94086300	-0.92285000
O	-4.97356700	-1.90414300	-2.23869000
C	-1.60392300	-1.00849800	-0.49722700
C	-3.53838500	-2.02574100	-0.41493900
N	-1.54969200	-2.10229800	0.26480000
N	-2.74999600	-2.75699000	0.31566700
C	-4.94847700	-2.23027700	-0.86185600
H	-5.63887900	-1.61220800	-0.27186000
H	-5.23251600	-3.27751600	-0.75492200
C	-0.47348000	-2.52946200	1.11750200
C	0.27428100	-3.64906900	0.74144700
C	-0.26040200	-1.82069600	2.30243900
C	1.30238400	-4.04130200	1.59514600
C	0.77718800	-2.26102500	3.12766800
C	1.56614500	-3.36254300	2.78970100
H	1.90688000	-4.90360100	1.32484400

H	0.96552400	-1.73136000	4.05866200
H	-6.48152000	3.41671100	1.33921800
C	-0.03022800	-4.38690200	-0.53285300
H	-0.07011600	-3.70469800	-1.38842100
H	-1.00286500	-4.88500500	-0.46747000
H	0.73086800	-5.14374900	-0.72921700
C	-1.07613000	-0.60151900	2.64676900
H	-2.14670800	-0.78165000	2.50784000
H	-0.79821300	0.25446400	2.01680400
H	-0.91023700	-0.31411100	3.68620200
C	2.66265100	-3.83663700	3.70591000
H	2.93793900	-3.06686600	4.43063200
H	3.55463100	-4.11956200	3.14062900
H	2.33789600	-4.72012900	4.26524400
N	-3.96002000	3.32123700	2.16072800
O	-2.79951200	3.09687500	2.46042400
O	-4.68231900	4.10092500	2.75645600
C	-0.54284000	-0.00219400	-0.84071200
O	-0.94395400	1.20443100	-0.89430100
C	0.71052300	-0.48921000	-1.10742400
C	1.75022100	0.48432100	-1.57236200
H	1.30130900	1.10795800	-2.35644600
C	3.01342100	-0.14538000	-2.11811700
C	3.60002000	-1.26723200	-1.52152500
C	3.63677300	0.41921300	-3.23408400
C	4.77888900	-1.80705900	-2.03062100
H	3.13254000	-1.72642100	-0.65323800
C	4.81420400	-0.11895100	-3.74648900
H	3.18694300	1.28717300	-3.71007300
C	5.38918100	-1.23526300	-3.14477100
H	5.22005100	-2.67957500	-1.55825800
H	5.27776800	0.33062400	-4.61926700
H	6.30480900	-1.66010300	-3.54416100
H	0.91816600	-1.55234900	-1.07670100
C	4.16470000	1.31483200	0.95332900
C	4.73175700	2.36925500	0.21606800
C	4.03309500	3.11973900	-0.79594500

C	2.77519100	2.74458600	-1.07691600
C	2.09153000	1.57892700	-0.44009700
C	2.83240700	0.93871300	0.69072700
C	5.16768000	0.84402700	1.86232800
C	6.27273500	1.61176600	1.63784000
H	4.51727700	3.95195300	-1.29553100
H	2.19922400	3.26850600	-1.83452700
H	1.09277200	1.88917600	-0.09968700
H	5.08695800	0.03983500	2.57943500
H	7.25024200	1.59225200	2.09743100
N	2.21494400	0.00429600	1.38319800
H	1.30006400	-0.31943300	1.07887400
H	2.68871200	-0.51937900	2.10962100
N	5.99776300	2.53624600	0.64184700
C	6.93340500	3.52793700	0.13123900
H	7.14200000	3.34171400	-0.92423300
H	6.52053000	4.53089800	0.25492500
H	7.86038100	3.45182600	0.69827600

M5S

C	4.98125100	1.99453300	0.11549800
C	3.79502900	1.34592400	-0.22486200
C	3.72485000	0.46378400	-1.29391700
C	4.90307300	0.24755100	-1.99562400
C	6.10607800	0.87977300	-1.68775000
C	6.14410200	1.76771100	-0.61981100
C	4.78999400	2.88910900	1.30933900
C	3.38440700	2.55134200	1.85950300
C	2.67785600	1.71362300	0.72694500
H	2.79419100	-0.01509000	-1.57983100
H	7.07142300	2.26784200	-0.35990500
H	5.54848500	2.73731100	2.08342900
H	2.80695500	3.45370500	2.05983900
H	4.83832600	3.94132900	1.01138000
H	1.88459100	2.27174200	0.23144700
N	2.07028100	0.50300500	1.29340100

O	3.43393900	1.88466400	3.11085900
C	0.99821900	-0.21027100	0.90237800
C	2.64246700	-0.16035900	2.34352700
N	0.97878700	-1.28052000	1.70415600
N	1.99113700	-1.25017100	2.62105100
C	3.77719900	0.51272400	3.04218600
H	4.72417200	0.34566400	2.51124300
H	3.86995900	0.13319900	4.05999600
C	0.11971700	-2.43784600	1.65469200
C	0.31164200	-3.37010600	0.63220200
C	-0.84156200	-2.58306200	2.65994000
C	-0.51465100	-4.49558100	0.63863500
C	-1.64112300	-3.72318300	2.61736600
C	-1.48500300	-4.69266600	1.62169300
H	-0.39213300	-5.23513600	-0.14857800
H	-2.40048400	-3.85965400	3.38354100
H	6.98946800	0.66423700	-2.27645500
C	1.32860100	-3.15987400	-0.45577700
H	2.28236900	-2.79980900	-0.05784700
H	0.96449600	-2.42676700	-1.18584200
H	1.51391900	-4.09436400	-0.98821900
C	-1.01008500	-1.53913200	3.73104100
H	-1.13390400	-0.53995000	3.29921600
H	-0.13603300	-1.50435800	4.38885600
H	-1.88780600	-1.75910000	4.34113900
C	-2.34276700	-5.93062900	1.62453900
H	-3.37563300	-5.69616200	1.89603900
H	-1.97003700	-6.65437700	2.35722700
H	-2.34034900	-6.41811700	0.64695600
N	4.87785600	-0.70124900	-3.11620000
O	3.83276800	-1.28503800	-3.34398800
O	5.90419800	-0.85691900	-3.75420300
C	0.10439200	0.13232300	-0.23410500
O	0.67548000	0.80748200	-1.19118900
C	-1.19146500	-0.25853600	-0.16231900
C	-2.08946900	-0.08539800	-1.35201300
H	-1.44284700	0.13691400	-2.20985500

C	-2.87316300	-1.34480500	-1.71375600
C	-2.96211200	-2.44587600	-0.86016200
C	-3.52791000	-1.40627800	-2.94967600
C	-3.69066200	-3.57680600	-1.22907600
H	-2.45206600	-2.44300200	0.09809400
C	-4.25750700	-2.53138200	-3.31887700
H	-3.45516500	-0.56673000	-3.63832100
C	-4.34344600	-3.62342300	-2.45601600
H	-3.73923400	-4.42325300	-0.54953900
H	-4.75341100	-2.55944800	-4.28430900
H	-4.91009100	-4.50357200	-2.74303400
H	-1.57185400	-0.72169200	0.73992000
C	-3.15761100	3.54999100	-0.63525300
C	-4.33597300	3.27078900	0.07200100
C	-4.82963400	1.93907200	0.33500600
C	-4.18498100	0.91634600	-0.24529400
C	-3.04967900	1.12390900	-1.21267100
C	-2.35540200	2.46255200	-1.09314200
C	-2.95677300	4.96371200	-0.58699200
C	-4.01623200	5.47618100	0.10971900
H	-5.68334500	1.78488600	0.98641800
H	-4.52174700	-0.10619600	-0.10486800
H	-3.55606300	1.23848000	-2.19200400
H	-2.15748600	5.53384100	-1.03876200
H	-4.27160500	6.49738700	0.35301800
N	-1.11590400	2.61013200	-1.46777100
H	-0.74035900	3.55363500	-1.44566500
H	-0.37336200	1.80503900	-1.53685800
N	-4.84161500	4.44417200	0.51263700
C	-6.04449200	4.59812400	1.31903800
H	-6.89130300	4.12059600	0.82333000
H	-5.89960000	4.15655000	2.30746700
H	-6.25037800	5.66218700	1.42964100

TS6S^D

C	5.37269300	-2.00267800	-0.59265700
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C	4.12363700	-1.53762200	-0.18205400
C	3.84513200	-1.28251200	1.15329800
C	4.87261600	-1.50953500	2.05839200
C	6.12887600	-1.98261700	1.68638700
C	6.38090500	-2.23210900	0.34289700
C	5.42288900	-2.18965100	-2.08409800
C	4.11025500	-1.57601400	-2.62605400
C	3.19682900	-1.34857100	-1.36220200
H	2.87555600	-0.93297200	1.48825700
H	7.35516300	-2.59211600	0.02894400
H	6.28810500	-1.70350300	-2.54564200
H	3.60830600	-2.25391600	-3.31608300
H	5.47714500	-3.25325300	-2.33648600
H	2.35665200	-2.04102200	-1.34004100
N	2.64716000	0.01731500	-1.36370900
O	4.32628100	-0.39925200	-3.38658300
C	1.51953100	0.52023800	-0.83056400
C	3.36030300	1.06931500	-1.86521400
N	1.60155800	1.83964000	-1.00709300
N	2.73945200	2.19592800	-1.66052900
C	4.60840200	0.75798300	-2.62424300
H	5.45586600	0.61378100	-1.94093900
H	4.84407500	1.57048800	-3.31176000
C	0.70300100	2.85668200	-0.52229700
C	0.66459200	3.09866000	0.85454800
C	-0.10563100	3.51485800	-1.45025100
C	-0.26770000	4.03132700	1.30266200
C	-1.02211600	4.43684800	-0.94545000
C	-1.12556800	4.69601600	0.42260200
H	-0.32936300	4.23816500	2.36827700
H	-1.67514400	4.95860800	-1.64014800
H	6.88842700	-2.13951300	2.44241700
C	1.55308400	2.35747200	1.81828600
H	2.56661000	2.23329700	1.42455400
H	1.14899900	1.36279100	2.04478900
H	1.62059900	2.90141700	2.76203700
C	-0.00824800	3.22715300	-2.92355300

H	-0.12210300	2.15788800	-3.13253900
H	0.96224600	3.53754300	-3.32221400
H	-0.78863800	3.76400800	-3.46527100
C	-2.15458300	5.65735200	0.95303500
H	-1.70932200	6.35903800	1.66359200
H	-2.94480900	5.11399300	1.48157200
H	-2.61860700	6.22925900	0.14680200
N	4.61893000	-1.22870300	3.47694900
O	3.55643200	-0.70873400	3.77247200
O	5.48528200	-1.52473000	4.27980600
C	0.45019100	-0.31365300	-0.14123800
O	0.84218300	-1.39268600	0.30877100
C	-0.89387000	0.15884700	-0.16883200
C	-1.84624000	-0.53641100	0.79821600
H	-1.30012700	-0.81821100	1.70715700
C	-3.01249300	0.34811400	1.19221800
C	-3.62347700	1.21360100	0.27800100
C	-3.51006400	0.29864000	2.49753700
C	-4.70258600	2.00689400	0.66104300
H	-3.25567100	1.27420800	-0.74326900
C	-4.58764400	1.09111800	2.88406600
H	-3.04116500	-0.36556100	3.21952300
C	-5.18766100	1.94909000	1.96540600
H	-5.16186900	2.67452700	-0.06170200
H	-4.95449500	1.04161800	3.90468000
H	-6.02650400	2.56994000	2.26400000
H	-1.02144300	1.23268100	-0.25954700
C	-4.37712300	-2.04321600	-1.30180400
C	-5.03113800	-2.70542400	-0.25753600
C	-4.41627800	-3.04651500	1.00600900
C	-3.14132100	-2.67948700	1.19865100
C	-2.33789500	-1.91837100	0.18931000
C	-3.00792600	-1.65968500	-1.14378000
C	-5.31601900	-1.89683900	-2.36744000
C	-6.48248500	-2.46541900	-1.93155300
H	-4.97802700	-3.58571300	1.76202400
H	-2.63490600	-2.91314400	2.13139400

H	-1.40882200	-2.47097400	-0.00408500
H	-5.15811200	-1.43228200	-3.33035400
H	-7.44123300	-2.57249900	-2.41785200
N	-2.27190500	-1.05281800	-2.02848900
H	-1.36391700	-0.32697200	-1.33225800
H	-2.76101400	-0.76802200	-2.87651600
N	-6.30121800	-2.95534700	-0.65338800
C	-7.31255600	-3.64832000	0.13008000
H	-7.00454100	-4.67810500	0.32455100
H	-7.47883000	-3.13085400	1.07712000
H	-8.24222400	-3.65688600	-0.43788000

TS6S

C	5.66909400	-1.33580100	-0.09571500
C	4.46291300	-0.78577100	0.34002300
C	4.35510100	-0.13221400	1.55907700
C	5.51442300	-0.04752900	2.32112400
C	6.73490700	-0.58560800	1.91937300
C	6.81157400	-1.24160300	0.69671400
C	5.50828000	-1.99970700	-1.43654800
C	4.11568300	-1.56859300	-1.94888400
C	3.37100600	-1.02201600	-0.67785500
H	3.41387800	0.27957500	1.90885900
H	7.75357100	-1.66563400	0.36427400
H	6.28578600	-1.71789200	-2.15281600
H	3.53638700	-2.40272900	-2.34479700
H	5.54436900	-3.08830100	-1.32306000
H	2.62830400	-1.75583700	-0.35607800
N	2.65961000	0.21177000	-1.00749300
O	4.20443900	-0.63005600	-3.01551800
C	1.45493500	0.64420800	-0.62595700
C	3.13900300	1.10855900	-1.91964400
N	1.25037700	1.77932400	-1.28267400
N	2.29591200	2.08526600	-2.10552900
C	4.39017400	0.72076200	-2.63693900
H	5.27183200	0.86011100	-1.99693000

H	4.50749400	1.31514500	-3.54325800
C	0.07102700	2.60303000	-1.23130300
C	-0.17228900	3.36434400	-0.08573300
C	-0.79517400	2.54641500	-2.32610800
C	-1.34842100	4.11212600	-0.06578800
C	-1.95221200	3.32091700	-2.25694000
C	-2.23957500	4.10968400	-1.14085400
H	-1.57603800	4.70722700	0.81529700
H	-2.65055700	3.29511700	-3.08986700
H	7.60140200	-0.48481700	2.56113400
C	0.77705200	3.35595700	1.08267100
H	1.81671700	3.45050400	0.75364600
H	0.69084900	2.42648800	1.65649000
H	0.55372500	4.18402400	1.75738200
C	-0.50364100	1.65211700	-3.50064600
H	-0.28368200	0.62770300	-3.17542700
H	0.36381200	2.00782600	-4.06506800
H	-1.36141000	1.61962700	-4.17459300
C	-3.48608700	4.95180700	-1.09010900
H	-3.24855000	6.00324700	-1.28434600
H	-3.95441200	4.89578300	-0.10360700
H	-4.21357200	4.63112000	-1.83956700
N	5.45167400	0.65075500	3.60990000
O	4.39081100	1.15487600	3.93472300
O	6.46498100	0.69443300	4.28671700
C	0.56907400	-0.02868000	0.40778000
O	1.12806900	-0.28860900	1.47267700
C	-0.71584700	-0.42507500	-0.07167800
C	-1.72652900	-0.80139400	0.99962000
H	-1.16493500	-0.91955700	1.93369700
C	-2.74070500	0.31045800	1.22023300
C	-3.42309700	0.89951300	0.14910000
C	-3.01796700	0.76594300	2.51123900
C	-4.36647800	1.89902800	0.36463800
H	-3.22555900	0.56672400	-0.86730100
C	-3.95586900	1.77358800	2.73279500
H	-2.49373100	0.32070700	3.35356700

C	-4.63643000	2.34145500	1.65914000
H	-4.88979200	2.33469700	-0.48205700
H	-4.15325500	2.11288000	3.74546500
H	-5.37168700	3.12293000	1.82739100
H	-1.08734800	0.21723200	-0.87135400
C	-4.65291300	-1.98773700	-0.35553600
C	-5.23436500	-2.07978500	0.90531700
C	-4.51234100	-2.43853100	2.10974200
C	-3.17879700	-2.54473400	2.02678400
C	-2.41021700	-2.20808700	0.77555500
C	-3.22778000	-2.22200600	-0.50556600
C	-5.68571100	-1.65550400	-1.27686200
C	-6.84136400	-1.54788200	-0.54240000
H	-5.04749300	-2.62350900	3.03613300
H	-2.58958800	-2.80127800	2.90312100
H	-1.58221400	-2.91345700	0.64284500
H	-5.59254700	-1.49251100	-2.34163700
H	-7.84945500	-1.29966500	-0.84181400
N	-2.60455500	-2.40232100	-1.61610000
H	-1.14746100	-3.29208800	-1.60787700
H	-3.23978700	-2.35560700	-2.41493300
N	-6.56158900	-1.81418100	0.77870200
C	-7.52566400	-1.79634900	1.86523500
H	-7.63787900	-2.79299700	2.29909100
H	-7.20731300	-1.09480300	2.63961400
H	-8.48800500	-1.47270100	1.46872000
C	0.77840500	-3.22062900	-1.57479800
O	1.85081000	-3.81838300	-1.55100200
O	0.65179200	-1.92901300	-1.67354300
H	-0.17138500	-1.36495800	-0.86490200
O	-0.36834600	-3.91358200	-1.48466100

TS6S^{Na}

C	-5.67494200	1.03692900	0.04411000
C	-4.44575700	0.48260100	0.40202700
C	-4.32044100	-0.38660700	1.47583300

C	-5.48522100	-0.68275200	2.17287800
C	-6.72909900	-0.14776700	1.84652500
C	-6.82400000	0.72634700	0.77022500
C	-5.53370700	1.94489900	-1.14803400
C	-4.09811400	1.72012300	-1.67730500
C	-3.34969400	0.96348300	-0.52099300
H	-3.36372500	-0.80631100	1.76962400
H	-7.78470300	1.15106000	0.49739600
H	-6.26742900	1.73668000	-1.93270400
H	-3.56706600	2.65341400	-1.86488100
H	-5.66598100	2.98949400	-0.84707400
H	-2.64535000	1.64455500	-0.03974700
N	-2.57914500	-0.15326400	-1.06832200
O	-4.08405800	1.02994400	-2.92003400
C	-1.38199900	-0.63448200	-0.72097100
C	-2.99918100	-0.86830900	-2.15424100
N	-1.12649300	-1.62506100	-1.56726600
N	-2.12928000	-1.78332600	-2.47885000
C	-4.23054800	-0.37557800	-2.84251300
H	-5.13546900	-0.67452300	-2.29683700
H	-4.27972500	-0.76933600	-3.85786800
C	0.03280800	-2.47892400	-1.57753400
C	0.17194600	-3.43198300	-0.56407900
C	0.96874800	-2.28908800	-2.59754500
C	1.31641600	-4.22607700	-0.59930000
C	2.09107700	-3.11643100	-2.58870200
C	2.27723100	-4.08843800	-1.60331000
H	1.45786400	-4.97415000	0.17703900
H	2.83907200	-2.99221300	-3.36786500
H	-7.59904500	-0.42162300	2.43095300
C	-0.85638300	-3.59092100	0.52394600
H	-1.87455100	-3.53685000	0.12618300
H	-0.75310200	-2.81198000	1.28777100
H	-0.73475000	-4.55580800	1.01898600
C	0.77780400	-1.21976800	-3.63955100
H	0.56170700	-0.24865600	-3.17796700
H	-0.06019200	-1.45703300	-4.30187500

H	1.67792700	-1.11849400	-4.24860700
C	3.48845200	-4.98178200	-1.61194800
H	3.21243400	-6.00221900	-1.89791900
H	3.93987200	-5.03188900	-0.61675100
H	4.24139100	-4.62687500	-2.31932900
N	-5.39926200	-1.61017100	3.30726000
O	-4.31142800	-2.09533200	3.56483500
O	-6.41994500	-1.84795400	3.92903400
C	-0.53118300	-0.12566300	0.42985700
O	-1.09930200	-0.05820300	1.51649800
C	0.74950300	0.38980600	0.04084300
C	1.73653500	0.57148600	1.18154500
H	1.15225200	0.58750900	2.10796000
C	2.69530000	-0.60508900	1.27358900
C	3.41861100	-1.05335900	0.16307900
C	2.86268400	-1.27466900	2.48859500
C	4.30827400	-2.11826900	0.27210100
H	3.29168200	-0.56749600	-0.80152600
C	3.74053700	-2.35089400	2.59989700
H	2.29664900	-0.94759900	3.35766300
C	4.47492000	-2.76973500	1.49313800
H	4.86521600	-2.44446800	-0.60206300
H	3.85281300	-2.85823300	3.55326300
H	5.16781400	-3.60147900	1.57910600
H	1.15473600	-0.11148100	-0.84049300
C	4.58645800	1.90892300	-0.15516000
C	5.27844700	1.70388300	1.04655100
C	4.68466100	1.82551500	2.35917500
C	3.35716700	2.00624000	2.42147200
C	2.47999600	1.98466100	1.20274700
C	3.20368800	2.22974700	-0.09312100
C	5.52999500	1.78188500	-1.22028500
C	6.72913700	1.48807100	-0.63177000
H	5.30305000	1.77813900	3.24920500
H	2.85099300	2.07799000	3.37976100
H	1.67199300	2.72040400	1.28189900
H	5.34459200	1.86331300	-2.28179600

H	7.69950800	1.29728300	-1.06690200
N	2.51454300	2.69460700	-1.09778500
H	1.55235700	3.15071000	-0.91565900
H	2.98103700	2.83365600	-1.98791700
N	6.56933200	1.45204800	0.74161500
C	7.63291800	1.20319400	1.70432600
H	7.85908500	2.11088000	2.26834400
H	7.33473400	0.40708100	2.38889700
H	8.52315700	0.88901200	1.16061600
C	-0.75630900	3.34424200	-0.83641200
O	-1.86815900	3.94750000	-0.80234600
O	-0.66137900	2.12444200	-1.27295400
H	0.17336300	1.43121600	-0.58569500
O	0.33088200	3.93331700	-0.42337400
Na	-0.87048900	5.74273500	-0.01374100

M6S

C	5.44655900	-1.80786900	-0.93081700
C	4.21055500	-1.42237000	-0.41125600
C	3.92847900	-1.52352400	0.94359200
C	4.93883500	-2.02124000	1.75498500
C	6.18102600	-2.42301200	1.27054300
C	6.43652300	-2.31627200	-0.09089500
C	5.50884400	-1.59429300	-2.41765300
C	4.21918400	-0.82563600	-2.78465700
C	3.29967300	-0.90820800	-1.50436900
H	2.97201300	-1.24045600	1.36691800
H	7.39916400	-2.61953000	-0.48929200
H	6.39052800	-1.02424800	-2.72589900
H	3.70284000	-1.28714900	-3.62556300
H	5.54339400	-2.55279500	-2.94461800
H	2.44676600	-1.56505400	-1.67631900
N	2.77042100	0.42588900	-1.17308900
O	4.47548200	0.50029100	-3.21345100
C	1.61184600	0.81076400	-0.61287500
C	3.49539100	1.55974700	-1.40394100

N	1.68368000	2.13659700	-0.50540300
N	2.84995700	2.61892000	-0.99815800
C	4.76629200	1.41712600	-2.17586900
H	5.58531000	1.07668100	-1.52806200
H	5.04058800	2.37032400	-2.62782900
C	0.70547600	3.02461500	0.07347200
C	0.52981500	2.99796400	1.45964900
C	-0.06022000	3.80399900	-0.79797200
C	-0.50616600	3.77443500	1.97450000
C	-1.08166200	4.56032200	-0.22717800
C	-1.32664100	4.54683900	1.14840700
H	-0.68248800	3.76660400	3.04697600
H	-1.70886100	5.16560200	-0.87624700
H	6.92535000	-2.80571600	1.95825000
C	1.37457700	2.12901000	2.35409300
H	2.42385700	2.12540300	2.04478300
H	1.01668600	1.09180200	2.35983000
H	1.32496800	2.49047600	3.38255700
C	0.18955600	3.80514100	-2.28123900
H	0.21125000	2.78861500	-2.68862500
H	1.15084200	4.27256600	-2.51541600
H	-0.59654500	4.35973300	-2.79564500
C	-2.44104300	5.36752600	1.73768700
H	-3.19387900	5.60937400	0.98428200
H	-2.05288900	6.30966300	2.13885800
H	-2.92969300	4.83530600	2.55761100
N	4.68127900	-2.12113000	3.19712000
O	3.60733100	-1.71924500	3.61059200
O	5.55509200	-2.59403700	3.90043100
C	0.51293900	-0.14329800	-0.17171600
O	0.88398500	-1.24237000	0.17463800
C	-0.90530900	0.31352700	-0.25053700
C	-1.88418800	-0.61749400	0.47130000
H	-1.40248600	-0.95901700	1.39546100
C	-3.15699900	0.11962200	0.84474800
C	-3.69931100	1.09902900	0.00430200
C	-3.82930700	-0.18948300	2.03020200

C	-4.88840000	1.74190000	0.33373800
H	-3.19805600	1.35301300	-0.92610200
C	-5.02165600	0.45086800	2.36084100
H	-3.41504200	-0.94006200	2.69811200
C	-5.55550800	1.41804500	1.51290200
H	-5.29502600	2.49495900	-0.33435000
H	-5.53068100	0.19897000	3.28625800
H	-6.48257200	1.92048500	1.77069300
H	-0.98501500	1.32962600	0.14266400
C	-4.44762100	-1.90670600	-1.49086600
C	-4.90580300	-2.72809900	-0.46690900
C	-4.05233600	-3.31611300	0.54551600
C	-2.76229700	-2.95487300	0.56299100
C	-2.18298400	-1.91928300	-0.36667600
C	-3.03401200	-1.57299900	-1.58577000
C	-5.57331000	-1.55702300	-2.28835100
C	-6.66183700	-2.17004000	-1.71648400
H	-4.45467200	-4.03355700	1.25433400
H	-2.08325000	-3.36483100	1.30619100
H	-1.21314300	-2.27503100	-0.73053600
H	-5.58993300	-0.92394300	-3.16459100
H	-7.70583200	-2.16015200	-1.99483500
N	-2.45866900	-0.97872200	-2.56868500
H	-1.14547200	0.37184400	-1.32568900
H	-3.15064500	-0.76020800	-3.29154200
N	-6.24935500	-2.88345100	-0.61530700
C	-7.11376500	-3.65739600	0.25968200
H	-6.81576600	-4.70844300	0.26132100
H	-7.07235900	-3.26527900	1.27869200
H	-8.13672900	-3.58090700	-0.10837600

TS6R^D

C	5.68276000	-1.10429700	-1.04910600
C	4.31498500	-1.00883700	-0.79541900
C	3.69052800	-1.80451000	0.15367900
C	4.49742000	-2.69928400	0.84259500

C	5.86433200	-2.83179000	0.60886700
C	6.46375300	-2.02474700	-0.35043300
C	6.11170300	-0.12585700	-2.10788200
C	4.87729500	0.76642500	-2.37932600
C	3.67108700	0.05335100	-1.65815200
H	2.62495800	-1.74991700	0.34457800
H	7.52862400	-2.10707700	-0.54216700
H	6.96332600	0.48769200	-1.79707300
H	4.66477000	0.83824300	-3.44552500
H	6.40949300	-0.65043100	-3.02082800
H	2.96708400	-0.36870400	-2.37403600
N	2.93053000	1.01254800	-0.82282800
O	5.06983600	2.11030800	-1.97097200
C	1.64784300	1.03002500	-0.42128400
C	3.55934900	2.05610200	-0.20357900
N	1.55237200	2.05350700	0.42731800
N	2.73689800	2.70875800	0.56652400
C	4.97985400	2.32837400	-0.57649700
H	5.66230200	1.68405500	-0.00546600
H	5.22734200	3.37100100	-0.37624600
C	0.43259400	2.43449800	1.25294700
C	-0.28772000	3.57824300	0.89791600
C	0.14189800	1.64756800	2.36895400
C	-1.36756600	3.92070900	1.70787000
C	-0.94607200	2.04070000	3.15009700
C	-1.70932300	3.16623900	2.83509400
H	-1.95456500	4.79948000	1.45390900
H	-1.19851300	1.45177700	4.02889400
H	6.43745600	-3.55276700	1.17915500
C	0.08257900	4.38494800	-0.31601800
H	0.12735900	3.75662100	-1.21215500
H	1.06490500	4.85154200	-0.19308700
H	-0.65228600	5.17265200	-0.48901900
C	0.93238200	0.40895000	2.69497000
H	2.00903900	0.57190000	2.58428800
H	0.63877900	-0.42418700	2.04428600
H	0.74200300	0.09969400	3.72398800

C	-2.85991700	3.58405800	3.71059400
H	-3.64812200	4.06327100	3.12504700
H	-2.52394000	4.30502300	4.46347100
H	-3.28893100	2.72955900	4.23919200
N	3.87436700	-3.54122000	1.87129200
O	2.69792400	-3.34805300	2.12638500
O	4.56688000	-4.38074000	2.41751000
C	0.58240700	0.06138200	-0.90130600
O	0.98739500	-1.04960100	-1.24712600
C	-0.76836700	0.51747900	-0.85870100
C	-1.77745800	-0.31260700	-1.64317500
H	-1.32339400	-0.66909900	-2.57620300
C	-3.02954400	0.47535200	-1.97941000
C	-3.55477600	1.42869400	-1.09914300
C	-3.70627600	0.23162500	-3.17805100
C	-4.72425800	2.11746100	-1.41036700
H	-3.04820800	1.63856600	-0.16036100
C	-4.87539100	0.91959700	-3.49228800
H	-3.30781500	-0.50250800	-3.87385900
C	-5.38866800	1.86554100	-2.60788900
H	-5.11526500	2.85352400	-0.71449400
H	-5.38276200	0.72059400	-4.43132200
H	-6.29735100	2.40659600	-2.85245000
H	-0.88792600	1.59807100	-0.91489900
C	-4.04752700	-1.66080900	0.81826000
C	-4.74509200	-2.46822700	-0.08461400
C	-4.20754700	-2.94344000	-1.33959400
C	-2.96978200	-2.55354900	-1.67673600
C	-2.13412900	-1.63531900	-0.83720100
C	-2.71515400	-1.24189700	0.50512500
C	-4.91080600	-1.42032500	1.92909400
C	-6.07965900	-2.07974200	1.65700400
H	-4.79521700	-3.60076600	-1.97226800
H	-2.52151200	-2.89035700	-2.60779900
H	-1.16326800	-2.11584000	-0.65797000
H	-4.69926400	-0.83851900	2.81496400
H	-6.99490700	-2.15897300	2.22545000

N	-1.95400600	-0.48893300	1.24273400
H	-1.14589600	0.19324500	0.38467600
H	-2.38980100	-0.11915500	2.08706500
N	-5.97190900	-2.71096900	0.43382700
C	-7.00491000	-3.52733600	-0.18485100
H	-7.16646700	-3.20549400	-1.21543300
H	-6.72168700	-4.58238500	-0.17063600
H	-7.93134500	-3.39657300	0.37362100

TS6R

C	-0.37562700	-0.62636600	-1.18950300
O	-0.66492400	-0.84902400	-2.36353300
C	0.58677900	0.27355000	-0.64711800
C	1.67088000	0.74153400	-1.59652800
H	1.20371900	0.94518800	-2.56688700
C	2.71730600	-0.34017600	-1.82233500
C	3.30561600	-1.01673400	-0.74849600
C	3.11318600	-0.68075500	-3.11801600
C	4.28142900	-1.98642700	-0.96393400
H	3.00567200	-0.78083900	0.27012000
C	4.08277200	-1.65723400	-3.33999800
H	2.65307900	-0.17326600	-3.96270000
C	4.67666300	-2.30818500	-2.26147400
H	4.73368200	-2.49078000	-0.11413300
H	4.37241500	-1.90894800	-4.35596300
H	5.43519000	-3.06681400	-2.42938700
H	0.93692900	0.00326200	0.34634300
C	4.14616300	1.80170200	0.53867800
C	5.04875900	1.93449000	-0.51120700
C	4.68472200	2.36176600	-1.84778100
C	3.37984000	2.48989200	-2.12802100
C	2.29740400	2.12244000	-1.14694200
C	2.74093700	2.08775200	0.30809100
C	4.88592200	1.40551300	1.68888100
C	6.19683000	1.29759500	1.28902900
H	5.45391700	2.56709600	-2.58588600

H	3.05587200	2.78916900	-3.12122400
H	1.47367100	2.84242000	-1.20924700
H	4.50717100	1.21320300	2.68346500
H	7.08297100	1.01738300	1.84039600
N	1.85246000	2.29280500	1.21472700
H	0.41140100	3.17739000	0.76223200
H	2.25144800	2.21932300	2.15261900
N	6.28868500	1.62963000	-0.04336500
C	7.50710100	1.62520900	-0.83429700
H	7.67064000	2.60638700	-1.28565000
H	7.44801000	0.86791900	-1.62003700
H	8.34697100	1.39511800	-0.17908700
C	-1.41026000	3.09240600	0.12776300
O	-2.42492700	3.67910400	-0.21294300
O	-1.30605700	1.79477200	0.26255700
H	-0.30010900	1.19813900	-0.23332100
O	-0.28817900	3.78785800	0.39431100
C	-5.81159500	-0.35392000	-1.27498400
C	-4.51507600	-0.06828500	-0.84333000
C	-4.23342700	1.01793000	-0.02992800
C	-5.31062700	1.82872800	0.30084800
C	-6.60822800	1.60878600	-0.14860500
C	-6.86538200	0.49136800	-0.93836000
C	-5.83528800	-1.63396600	-2.07197000
C	-4.48458200	-2.30498400	-1.75691200
C	-3.55041800	-1.11361800	-1.36705700
H	-3.22978900	1.25320000	0.31816100
H	-7.87692400	0.27831400	-1.26878500
H	-6.66397100	-2.29657400	-1.80943700
H	-4.08121500	-2.84826600	-2.61237800
H	-5.90405000	-1.41979400	-3.14435300
H	-2.97573700	-0.76276900	-2.22608600
N	-2.59594200	-1.55129000	-0.34802900
O	-4.59927400	-3.28212600	-0.72469300
C	-1.28559100	-1.31886000	-0.17547200
C	-3.01688400	-2.32423600	0.69633300
N	-0.96622700	-1.93630900	0.96134600

N	-2.03491200	-2.58267100	1.51198900
C	-4.41508000	-2.84695700	0.61340200
H	-5.14054400	-2.08087300	0.91227700
H	-4.52787300	-3.71671300	1.26113900
C	0.33301100	-2.05567100	1.57851700
C	1.19182500	-3.05242600	1.11517700
C	0.66040600	-1.15948900	2.60081200
C	2.43928500	-3.14986300	1.73278000
C	1.92904600	-1.28402200	3.16363700
C	2.82776800	-2.27040600	2.74309100
H	3.12915400	-3.91920200	1.39520800
H	2.22024300	-0.59712400	3.95498600
H	-7.39922300	2.28977500	0.14311500
C	0.81652700	-3.93842000	-0.04033500
H	0.82891900	-3.37011800	-0.97828000
H	-0.18287000	-4.36658100	0.08283500
H	1.53190400	-4.75652500	-0.14063500
C	-0.30125200	-0.08476500	3.02734200
H	-1.25229800	-0.51472100	3.35849200
H	-0.52181400	0.60510400	2.20208300
H	0.11784500	0.49461500	3.85190100
C	4.21015900	-2.34178500	3.33451100
H	4.19813200	-2.11208700	4.40318700
H	4.86690200	-1.61130100	2.84757900
H	4.65164500	-3.33155700	3.19656600
N	-5.07043000	2.95374700	1.20973400
O	-4.15096500	2.85499800	1.99804100
O	-5.82975500	3.90714200	1.14354000

TS6R^{Na}

C	-0.38382700	-0.98569200	-1.26404100
O	-0.61560100	-1.39440100	-2.40170800
C	0.50163800	0.03810600	-0.83929800
C	1.65800900	0.34641200	-1.77540500
H	1.25497100	0.40553700	-2.79317900
C	2.71118100	-0.74984400	-1.76639400

C	3.20430900	-1.26997100	-0.56541500
C	3.21015400	-1.25776500	-2.96796000
C	4.18679300	-2.25632000	-0.56692900
H	2.82035800	-0.89832900	0.38228500
C	4.18798100	-2.25037900	-2.97484100
H	2.82646200	-0.86899500	-3.90824500
C	4.68408500	-2.74894200	-1.77277400
H	4.56370500	-2.64035800	0.37680900
H	4.56018600	-2.63485400	-3.91964600
H	5.44756400	-3.52126400	-1.77481900
H	0.74568200	0.01919400	0.21700600
C	4.05302000	1.70665600	0.27254700
C	4.99671800	1.70615700	-0.75309200
C	4.68103200	1.94320300	-2.14690400
C	3.38615600	2.01367100	-2.48671800
C	2.27050300	1.78253800	-1.50240800
C	2.66450400	1.93128300	-0.04571600
C	4.74687200	1.46506100	1.49326700
C	6.06966800	1.31455500	1.16010300
H	5.47419400	2.05537700	-2.87922900
H	3.09394600	2.16460900	-3.52222600
H	1.45147400	2.48346100	-1.70036100
H	4.32966900	1.38596600	2.48786000
H	6.93390900	1.10478200	1.77393100
N	1.74212300	2.20338100	0.81683600
H	0.40519000	2.70927300	0.53675500
H	2.09669900	2.24077600	1.77311000
N	6.21399500	1.47222200	-0.20149100
C	7.46821500	1.38208300	-0.93179400
H	7.69557100	2.33280000	-1.41936700
H	7.41067300	0.59019400	-1.68202700
H	8.26389100	1.14673200	-0.22550800
C	-1.30267300	3.03716900	-0.61605900
O	-2.26024300	3.81026100	-0.78168200
O	-1.03343700	2.06248400	-1.41322500
H	-0.34289600	1.14706000	-1.02139800
O	-0.53802400	3.23000000	0.46458000

C	-5.65303100	-0.49994700	-1.12357400
C	-4.28597400	-0.34086800	-0.89445700
C	-3.78502500	0.74090000	-0.19458300
C	-4.70925100	1.69186200	0.21822700
C	-6.07236800	1.60957900	-0.05120200
C	-6.55174300	0.48659900	-0.71910700
C	-5.92224300	-1.82521900	-1.78809500
C	-4.60214900	-2.62002600	-1.65155700
C	-3.50660400	-1.52760100	-1.41628600
H	-2.72846200	0.86069100	0.02396000
H	-7.61594600	0.37625900	-0.89895400
H	-6.74973100	-2.37480600	-1.33112600
H	-4.37971400	-3.19327900	-2.55121700
H	-6.16438300	-1.68223100	-2.84653800
H	-2.94624500	-1.30786600	-2.32656900
N	-2.55469600	-1.96389900	-0.39483300
O	-4.64143000	-3.59095300	-0.61380800
C	-1.27513000	-1.61194800	-0.19101200
C	-2.99073000	-2.60893700	0.72619400
N	-0.98521200	-2.04536200	1.03460200
N	-2.04374600	-2.68314000	1.61708200
C	-4.39348100	-3.13088900	0.70142800
H	-5.10047200	-2.35090500	1.01509100
H	-4.49047800	-3.98230500	1.37607000
C	0.25809700	-1.93307600	1.75800800
C	1.19675000	-2.95701900	1.61781800
C	0.44258000	-0.81348500	2.57242900
C	2.37551400	-2.83641900	2.35064900
C	1.65472900	-0.72668700	3.25809500
C	2.62685800	-1.72624700	3.16053300
H	3.12228400	-3.62267100	2.27179400
H	1.83548000	0.13411000	3.89799000
H	-6.73990200	2.39181000	0.29200100
C	0.96405000	-4.10342600	0.67433900
H	0.99689400	-3.75405800	-0.36447900
H	-0.01033200	-4.57355600	0.84016900
H	1.74000700	-4.86084800	0.79630900

C	-0.60229100	0.26683400	2.66761400
H	-1.59670400	-0.15334300	2.84788000
H	-0.64689500	0.85899000	1.74430200
H	-0.36851800	0.95104400	3.48595800
C	3.93778600	-1.60311600	3.89003300
H	3.89985400	-0.81698800	4.64768800
H	4.74418600	-1.35936500	3.18942900
H	4.20400800	-2.54282200	4.38157400
N	-4.20404000	2.81661200	0.98822600
O	-3.18286600	2.63775700	1.64920400
O	-4.78701100	3.88227000	0.93922600
Na	-2.12275900	4.69173500	1.26811800

M6R

C	5.62827500	-1.37685600	-0.94533200
C	4.27245200	-1.18212500	-0.68045700
C	3.60722500	-1.92119500	0.28738500
C	4.35812500	-2.86077800	0.98030800
C	5.71052400	-3.08720400	0.73773600
C	6.35256700	-2.33569100	-0.23828200
C	6.11688900	-0.45694800	-2.02923800
C	4.93947900	0.49894700	-2.33138800
C	3.69398700	-0.10804000	-1.57423800
H	2.55310900	-1.79350300	0.50328000
H	7.40681700	-2.49362600	-0.44060900
H	7.00137000	0.11431100	-1.73008000
H	4.72026300	0.53724300	-3.39788400
H	6.38706200	-1.02331700	-2.92539500
H	2.96548800	-0.50874300	-2.27772400
N	3.01471300	0.93542200	-0.78293700
O	5.21814600	1.84319000	-1.98270800
C	1.72683000	1.08987900	-0.42384800
C	3.70622900	1.97491900	-0.23236100
N	1.68929400	2.18966400	0.32629500
N	2.91378900	2.75456300	0.45123900
C	5.14621400	2.12279300	-0.59857300
H	5.77562300	1.45216200	0.00177300
H	5.46876500	3.15189800	-0.43883600

C	0.55390300	2.79411700	0.98246600
C	0.00377600	3.93632000	0.39275200
C	0.07357700	2.20803000	2.15430100
C	-1.11037400	4.48846700	1.01739400
C	-1.04747100	2.80242900	2.73474900
C	-1.64863400	3.93498000	2.18417000
H	-1.57039000	5.37202200	0.58200500
H	-1.45596800	2.36586400	3.64230400
H	6.23923200	-3.83942600	1.31037000
C	0.59138200	4.53673600	-0.85545800
H	0.73388400	3.78568500	-1.64017900
H	1.56879500	4.98511300	-0.65095400
H	-0.06534400	5.31494100	-1.24722900
C	0.70394600	0.97377600	2.73756200
H	1.79449500	1.05886800	2.77592500
H	0.43408000	0.08740300	2.15187600
H	0.33668700	0.80684700	3.75152200
C	-2.84325700	4.57071500	2.84274200
H	-3.30695500	3.89249600	3.56206400
H	-3.59341800	4.85950400	2.10180000
H	-2.54666900	5.47786000	3.37951800
N	3.68807300	-3.65292700	2.01932700
O	2.51645900	-3.40935500	2.25049900
O	4.33968600	-4.50545600	2.59428600
C	0.61145500	0.14248000	-0.82398400
O	0.96782300	-0.95853700	-1.18260600
C	-0.80499600	0.62208300	-0.78933200
C	-1.77471600	-0.43173600	-1.33062800
H	-1.30606900	-0.90463300	-2.20113700
C	-3.08899400	0.17059700	-1.78445200
C	-3.70743700	1.21556600	-1.08890500
C	-3.72871400	-0.35720600	-2.90880300
C	-4.94167000	1.70920700	-1.50450700
H	-3.23102900	1.63640100	-0.20636800
C	-4.96391900	0.13258600	-3.32452600
H	-3.25297300	-1.16558100	-3.45803200
C	-5.57465500	1.16758300	-2.62127800

H	-5.41216800	2.51758700	-0.95304300
H	-5.44511300	-0.29170300	-4.20052300
H	-6.53678300	1.55271900	-2.94456300
H	-0.85617600	1.56240500	-1.35634200
C	-4.20523500	-1.50306400	0.94626600
C	-4.65704100	-2.51275400	0.10396400
C	-3.82126900	-3.20743200	-0.85373300
C	-2.55969000	-2.78347400	-1.00698600
C	-1.99375500	-1.58908600	-0.28212200
C	-2.81079500	-1.08730200	0.90736400
C	-5.30897300	-1.09517600	1.74695300
C	-6.37860600	-1.86512300	1.35813700
H	-4.21381600	-4.04863700	-1.41703000
H	-1.89609700	-3.26957800	-1.71769000
H	-0.99952400	-1.85422100	0.09534200
H	-5.32620900	-0.32535100	2.50603000
H	-7.40383400	-1.87359900	1.69882800
N	-2.22421200	-0.31864900	1.75295600
H	-1.05636700	0.87274300	0.25109800
H	-2.88896400	-0.02013000	2.47229700
N	-5.97474100	-2.72684700	0.36539700
C	-6.82195800	-3.69687800	-0.30687800
H	-6.89229400	-3.46755600	-1.37291500
H	-6.42468800	-4.70625900	-0.17709300
H	-7.81822700	-3.65035400	0.13225800

TS7S

C	4.95273400	-1.99786200	-0.15031900
C	3.83299300	-1.26777000	0.24717700
C	3.88066100	-0.38463400	1.31661000
C	5.10186300	-0.26044000	1.96508600
C	6.23819000	-0.98037000	1.60258600
C	6.16157500	-1.86083400	0.53059300
C	4.64267400	-2.87381500	-1.33311300
C	3.23075300	-2.45267400	-1.80279700
C	2.64186300	-1.58007900	-0.63094900

H	3.00722900	0.16627100	1.64486500
H	7.03671300	-2.42632300	0.22758100
H	5.36410700	-2.76029500	-2.14822200
H	2.58993800	-3.31885700	-1.96885400
H	4.64732700	-3.92873800	-1.04169300
H	1.86002600	-2.10631400	-0.08269900
N	2.04507500	-0.34997000	-1.16874300
O	3.24661900	-1.78507900	-3.05560300
C	1.01492300	0.39199700	-0.73052100
C	2.57118700	0.28739900	-2.25765700
N	0.95948400	1.43998200	-1.54573400
N	1.92372900	1.38647100	-2.51383600
C	3.64499300	-0.42682500	-3.01091900
H	4.62274200	-0.29190000	-2.53013500
H	3.69748300	-0.05408600	-4.03407800
C	0.07074300	2.57389800	-1.49699400
C	0.42869400	3.65011200	-0.68584600
C	-1.08960100	2.53637600	-2.27485800
C	-0.44081500	4.74145800	-0.66641200
C	-1.92511000	3.64735100	-2.21523400
C	-1.61477800	4.75643700	-1.42075500
H	-0.18979800	5.59983600	-0.04888600
H	-2.83867900	3.65006700	-2.80465600
H	7.16096300	-0.83815300	2.15157400
C	1.68696700	3.61802700	0.13975700
H	2.56476400	3.41330300	-0.48169500
H	1.63848600	2.83789400	0.90919900
H	1.83857700	4.57417700	0.64280700
C	-1.43347900	1.32443200	-3.09718500
H	-1.66439200	0.46914500	-2.44836300
H	-0.60409500	1.03330500	-3.74915900
H	-2.30834200	1.52035800	-3.71902200
C	-2.54738400	5.93686800	-1.37799600
H	-2.08688600	6.78863800	-0.87359500
H	-3.46673900	5.68171700	-0.84095200
H	-2.83342700	6.24523500	-2.38740200
N	5.19838300	0.68240400	3.08616500

O	4.22710300	1.37713700	3.33071900
O	6.24541000	0.72454600	3.70746000
C	0.16679700	-0.02051600	0.47589300
O	0.82297700	-0.55830300	1.38812900
C	-1.04894600	0.83253500	0.80202300
C	-1.97310500	0.10675100	1.79934900
H	-1.54573700	0.22052100	2.79909400
C	-3.33733800	0.76714700	1.79594600
C	-4.19671100	0.64090200	0.69905900
C	-3.74760600	1.53507700	2.88603600
C	-5.43845700	1.26705700	0.69611400
H	-3.89362200	0.04103600	-0.15818700
C	-4.98905700	2.16923900	2.88420700
H	-3.08786100	1.63664000	3.74418100
C	-5.83744100	2.03628400	1.78958500
H	-6.09817600	1.15613700	-0.15907600
H	-5.29109700	2.76422000	3.74061000
H	-6.80584900	2.52667500	1.78639500
H	-0.70698400	1.76984600	1.25661300
C	-2.74583900	-2.75580200	-0.49365200
C	-3.78700800	-3.28340100	0.27680700
C	-4.02893100	-2.95118200	1.66273700
C	-3.20268100	-2.07132700	2.24520200
C	-2.02973200	-1.44339200	1.55089800
C	-1.83191500	-1.82715600	0.09750100
C	-2.85487100	-3.31694300	-1.80269600
C	-3.93880900	-4.15186600	-1.77080000
H	-4.85989300	-3.40030800	2.19657000
H	-3.35185500	-1.77782400	3.28081900
H	-1.12300800	-1.82390400	2.04241700
H	-2.22343100	-3.12810300	-2.65928000
H	-4.37528300	-4.77255800	-2.53979000
N	-0.81089200	-1.30365500	-0.50591700
H	-1.59414700	1.08670000	-0.10913400
H	-0.66275400	-1.58934600	-1.47375800
N	-4.49789200	-4.12561600	-0.50785800
C	-5.66233100	-4.89185200	-0.08842900

H	-5.38455700	-5.61215700	0.68412200
H	-6.43532600	-4.22300400	0.29492000
H	-6.05248200	-5.42721500	-0.95351100

TS7R

C	-5.33905400	0.55694300	-0.48759400
C	-3.96048000	0.45755900	-0.66973500
C	-3.09967300	1.47774800	-0.29222700
C	-3.67850800	2.59990300	0.28283400
C	-5.05186500	2.74175000	0.46918900
C	-5.89189000	1.70640700	0.07711700
C	-6.04718700	-0.67986000	-0.96678100
C	-4.93036500	-1.67450500	-1.36980700
C	-3.57758800	-0.86811000	-1.28257300
H	-2.02731900	1.41636400	-0.44445600
H	-6.96403300	1.79289100	0.22049900
H	-6.69189200	-1.11921000	-0.19864200
H	-5.06263200	-2.01749800	-2.39564200
H	-6.68381000	-0.45404700	-1.82707900
H	-3.11964800	-0.75113000	-2.26121900
N	-2.59588800	-1.56785900	-0.42615900
O	-4.94417200	-2.86292200	-0.59987200
C	-1.25032600	-1.50250000	-0.37481300
C	-3.00028700	-2.39257700	0.58724900
N	-0.90036400	-2.28685400	0.64957600
N	-1.98228100	-2.85377700	1.25185300
C	-4.45445500	-2.70189500	0.71457200
H	-4.97447500	-1.90135900	1.25780300
H	-4.59086200	-3.64103800	1.25109400
C	0.41599100	-2.66158100	1.11183600
C	1.03154500	-3.74756100	0.46805300
C	0.99431000	-1.97864000	2.17837600
C	2.31824000	-4.07908400	0.86879700
C	2.29263000	-2.35633200	2.54353700
C	2.97196700	-3.38197300	1.89398700
H	2.82710500	-4.90199100	0.37328700
H	2.77430400	-1.83063200	3.36482000

H	-5.44248600	3.64628800	0.91941800
C	0.32298600	-4.50707100	-0.62007500
H	0.10630400	-3.86774300	-1.48280600
H	-0.62941200	-4.90945700	-0.26028300
H	0.93829700	-5.33986600	-0.96375000
C	0.28780800	-0.90440300	2.96126300
H	-0.72855100	-0.71890800	2.60635800
H	0.85406500	0.03228300	2.93029700
H	0.21612600	-1.20351700	4.01095900
C	4.37621600	-3.75785500	2.28198000
H	4.76926900	-3.09068000	3.05224600
H	5.04091600	-3.71286100	1.41367600
H	4.41174300	-4.78188100	2.66669600
N	-2.78905900	3.68064200	0.72260700
O	-1.58728100	3.47089500	0.69814300
O	-3.29725400	4.72237400	1.09665200
C	-0.40511800	-0.64441200	-1.34034000
O	-1.05831700	0.01100800	-2.15716000
C	0.98276800	-1.15298900	-1.67712100
C	1.94891800	-0.05487200	-2.18353700
H	1.91737300	-0.03725700	-3.27670100
C	3.37068000	-0.38799700	-1.76179300
C	3.69593800	-0.53150000	-0.40760700
C	4.38082100	-0.53903300	-2.71245900
C	5.00034000	-0.81469600	-0.01594000
H	2.92020100	-0.43108000	0.34999600
C	5.68812000	-0.82920600	-2.32368200
H	4.14135900	-0.43171000	-3.76775800
C	6.00206300	-0.96649900	-0.97482500
H	5.23411300	-0.91817400	1.04007000
H	6.46019500	-0.94840500	-3.07763100
H	7.01976700	-1.19162800	-0.67136900
H	0.85541100	-1.90516100	-2.46448800
C	1.65162800	2.49822700	0.53311400
C	2.61583700	3.36281100	0.00931200
C	3.11527200	3.30717300	-1.34670400
C	2.60946100	2.36915700	-2.15821400

C	1.55187200	1.38763000	-1.74061300
C	1.10732700	1.45811700	-0.29109500
C	1.43704500	2.87382600	1.89339900
C	2.26660000	3.93658000	2.13421400
H	3.87279300	4.00768900	-1.68284800
H	2.95403300	2.28613600	-3.18564800
H	0.64156500	1.62869500	-2.30982800
H	0.74020900	2.44144500	2.59760900
H	2.41577500	4.52841600	3.02570900
N	0.24127800	0.57725000	0.09589800
H	1.42073800	-1.64970000	-0.81538100
H	-0.09936100	0.70670800	1.04786200
N	2.97693400	4.22705100	0.98699100
C	3.96538500	5.28598200	0.85536800
H	4.96184300	4.86299600	0.70913500
H	3.71367700	5.93157700	0.01166400
H	3.95934400	5.87947700	1.76889600

M7S

C	5.13249300	-1.73261800	-0.18442300
C	3.90668100	-1.19532900	0.20703700
C	3.77246700	-0.46090700	1.37792600
C	4.92905600	-0.26480200	2.12000100
C	6.17328400	-0.77405500	1.75339800
C	6.27436700	-1.52281500	0.58774900
C	5.00266700	-2.51961700	-1.45923300
C	3.58374900	-2.21407600	-1.99078200
C	2.82065800	-1.52684200	-0.79452600
H	2.80564500	-0.08848400	1.70013600
H	7.23220800	-1.93251600	0.28409300
H	5.75439300	-2.25425700	-2.20912800
H	3.05922100	-3.12350100	-2.28371500
H	5.11179300	-3.59011700	-1.25904900
H	2.05519300	-2.16571700	-0.35648500
N	2.14878200	-0.30096200	-1.26488500
O	3.61348400	-1.42774900	-3.17223700

C	1.02218100	0.31199800	-0.85403300
C	2.71448900	0.48607400	-2.22912300
N	0.95756000	1.43465700	-1.57090900
N	2.00541400	1.55534200	-2.43878500
C	3.90009500	-0.05852000	-2.95405300
H	4.82249000	0.09004800	-2.37658500
H	4.00629200	0.42839100	-3.92351100
C	-0.00723500	2.50320400	-1.49963000
C	0.27662300	3.57277000	-0.64697900
C	-1.16698600	2.41129900	-2.26847800
C	-0.68446900	4.57570700	-0.55129800
C	-2.09716100	3.44225000	-2.13591000
C	-1.87551500	4.52342400	-1.28108000
H	-0.49922000	5.41662200	0.11238100
H	-3.01743100	3.39654000	-2.71287400
H	7.03655000	-0.57978800	2.37816000
C	1.55505000	3.61825200	0.14490300
H	2.42672700	3.61102400	-0.51711000
H	1.64198800	2.75471400	0.81467300
H	1.59437000	4.52256900	0.75405200
C	-1.42485100	1.22502800	-3.15710100
H	-1.70148400	0.34578800	-2.56172000
H	-0.54047000	0.96682700	-3.74758500
H	-2.24714600	1.43312500	-3.84358300
C	-2.88503200	5.63351200	-1.16775900
H	-3.87285400	5.30567400	-1.49902200
H	-2.58892000	6.48583200	-1.78852500
H	-2.96418100	5.98959700	-0.13760000
N	4.83386200	0.52025100	3.35738600
O	3.75393200	1.00833800	3.64147600
O	5.84103300	0.64597500	4.03196000
C	0.11746600	-0.28806200	0.26513900
O	0.84024400	-0.92288600	1.13038400
C	-0.88483500	0.73311000	0.84215000
C	-1.85935400	0.03739900	1.81752900
H	-1.45683800	0.10420000	2.83094700
C	-3.21715100	0.71367800	1.79920700

C	-3.96820900	0.78527600	0.61977800
C	-3.74949000	1.26397600	2.96536900
C	-5.21722500	1.39629800	0.60838000
H	-3.56938500	0.36413900	-0.30209000
C	-4.99968100	1.88132200	2.95724000
H	-3.17779600	1.21357700	3.88862300
C	-5.73677900	1.94865800	1.77911300
H	-5.78656000	1.44335600	-0.31500400
H	-5.39533600	2.30892100	3.87334500
H	-6.70971500	2.42991000	1.76967900
H	-0.32777800	1.51162900	1.37147500
C	-2.74598800	-2.69459800	-0.56056200
C	-3.79037500	-3.23519600	0.20708200
C	-3.99424300	-2.97134000	1.61108100
C	-3.13477900	-2.13795900	2.21705200
C	-1.97196400	-1.50430800	1.52421900
C	-1.83221300	-1.81065000	0.06041700
C	-2.89924900	-3.18104300	-1.89749500
C	-4.00490200	-3.98287300	-1.88331700
H	-4.81889700	-3.43429500	2.14200700
H	-3.24871200	-1.89702600	3.27030400
H	-1.04425000	-1.91605900	1.95287900
H	-2.28315300	-2.96251800	-2.75801200
H	-4.47746500	-4.54590800	-2.67494800
N	-0.82986500	-1.23650000	-0.55807700
H	-1.45465900	1.20984900	0.04312500
H	-0.65221500	-1.47888600	-1.52934800
N	-4.53946200	-4.00801100	-0.60632800
C	-5.71547800	-4.76725200	-0.20495500
H	-5.42504800	-5.64066700	0.38306400
H	-6.38049400	-4.13324600	0.38360600
H	-6.23942000	-5.09445300	-1.10230800

M7R

C	-5.34703500	0.48613100	-0.46021100
C	-3.96607100	0.48942800	-0.64952200

C	-3.16827600	1.51627200	-0.16695400
C	-3.80561200	2.52121700	0.54556300
C	-5.18263600	2.55295000	0.75617400
C	-5.96248100	1.52498600	0.23995800
C	-5.98416800	-0.71611600	-1.10008300
C	-4.81100900	-1.57229000	-1.64395200
C	-3.49799500	-0.73746600	-1.39349800
H	-2.10519100	1.54728300	-0.37776000
H	-7.03695100	1.53112000	0.39158000
H	-6.59238300	-1.29451500	-0.39693600
H	-4.91375900	-1.73194100	-2.71687200
H	-6.64610800	-0.41504900	-1.91719500
H	-2.97073400	-0.48605800	-2.31073800
N	-2.53459300	-1.49687700	-0.56239800
O	-4.78114400	-2.87879500	-1.09801300
C	-1.20854500	-1.33357300	-0.37713300
C	-2.94428200	-2.48861700	0.28597100
N	-0.87906100	-2.22460100	0.56331700
N	-1.95042900	-2.95671800	0.98051300
C	-4.37172700	-2.92197400	0.25235000
H	-4.98583900	-2.27463300	0.89338100
H	-4.45754200	-3.95004500	0.60573500
C	0.40186400	-2.48629300	1.17238600
C	1.13614000	-3.58306700	0.69670800
C	0.80916800	-1.70716600	2.25427900
C	2.36409800	-3.83414900	1.29692500
C	2.05414600	-2.00088600	2.82050300
C	2.84051700	-3.05146300	2.35578000
H	2.96409600	-4.66741500	0.94028800
H	2.39724000	-1.40128800	3.66036300
H	-5.62228100	3.36995600	1.31572100
C	0.59157800	-4.46778100	-0.39166900
H	0.22683100	-3.88966600	-1.24652600
H	-0.25090500	-5.05821900	-0.01623000
H	1.36055300	-5.15520300	-0.74733000
C	-0.04501100	-0.62507800	2.85879800
H	-0.99561800	-0.49044000	2.33467000

H	0.49382100	0.32754200	2.87621300
H	-0.28156800	-0.87627800	3.89667700
C	4.16242900	-3.37828500	2.99696200
H	4.54847600	-2.53298100	3.57126400
H	4.90374600	-3.65897500	2.24393200
H	4.05508800	-4.22599300	3.68215600
N	-2.97829100	3.59305900	1.10812500
O	-1.76554600	3.46343800	1.04993100
O	-3.54140500	4.54661700	1.61441800
C	-0.33026400	-0.33689900	-1.21057300
O	-1.04945100	0.34913500	-2.04094900
C	0.84755200	-1.11913100	-1.85254400
C	1.99030600	-0.18553900	-2.32289900
H	2.05014800	-0.21076900	-3.41417700
C	3.34577600	-0.59932200	-1.77558600
C	3.53331100	-0.84525400	-0.41062700
C	4.44673200	-0.69249700	-2.62948100
C	4.79471600	-1.16070400	0.08600200
H	2.68830000	-0.79988800	0.27479700
C	5.70839000	-1.01902000	-2.13659300
H	4.31236700	-0.51032100	-3.69303700
C	5.88709700	-1.24890300	-0.77505900
H	4.92141600	-1.33918600	1.15014500
H	6.55020300	-1.09299400	-2.81817300
H	6.86954600	-1.50061400	-0.38789400
H	0.41556600	-1.64766900	-2.70588000
C	1.76720800	2.45912100	0.27801400
C	2.78395100	3.27837200	-0.24499800
C	3.32634700	3.16189500	-1.57660500
C	2.80724400	2.21778300	-2.37590300
C	1.69854600	1.30695100	-1.95938600
C	1.24238900	1.43164400	-0.53503500
C	1.51111000	2.90063900	1.61593800
C	2.36462100	3.94168300	1.84164000
H	4.12105400	3.82273200	-1.90592900
H	3.17473500	2.08902600	-3.39006200
H	0.79250900	1.56849700	-2.53324500

H	0.77349100	2.52605300	2.31002300
H	2.49902500	4.56695000	2.71228100
N	0.33748300	0.56447200	-0.13658800
H	1.25611400	-1.85876600	-1.16258400
H	-0.11318500	0.73152400	0.75903400
N	3.13160100	4.16327500	0.70956800
C	4.14644800	5.19861400	0.57414800
H	5.13506500	4.74915300	0.46019400
H	3.92464900	5.82686400	-0.29056700
H	4.13199000	5.81350300	1.47311100

TS8S

C	5.26388200	-1.57337800	-0.67820500
C	4.00211800	-1.14948200	-0.26403200
C	3.72522100	-0.87222000	1.06829400
C	4.77964200	-1.01263400	1.96030400
C	6.05375800	-1.43390200	1.58340300
C	6.29706300	-1.72236600	0.24670000
C	5.29177200	-1.83612700	-2.15904800
C	3.94573500	-1.29924800	-2.70024600
C	3.04356000	-1.06353900	-1.43163900
H	2.72136800	-0.60581900	1.38357900
H	7.28129400	-2.05304400	-0.06914200
H	6.12718800	-1.34347600	-2.66655200
H	3.46545000	-2.02107500	-3.36104000
H	5.38067500	-2.90938200	-2.35533200
H	2.24379000	-1.79516600	-1.33216600
N	2.40723700	0.26452000	-1.49336700
O	4.11519600	-0.14358600	-3.50812100
C	1.24257100	0.72233200	-0.98759200
C	3.06502600	1.32724700	-2.04777300
N	1.25158600	2.03123600	-1.25624300
N	2.38043600	2.42376600	-1.92122300
C	4.33475300	1.05110700	-2.78220700
H	5.18189500	0.96738800	-2.08814300
H	4.54029900	1.85043500	-3.49465500

C	0.28757800	3.03559300	-0.88597400
C	0.50920200	3.72884500	0.30884400
C	-0.80705400	3.26280100	-1.71799000
C	-0.45514700	4.65445000	0.69313700
C	-1.74342500	4.20632800	-1.28860000
C	-1.59147500	4.89583400	-0.08570400
H	-0.32115100	5.19661000	1.62607000
H	-2.61257400	4.40206100	-1.91175400
H	6.82962400	-1.52972500	2.33293700
C	1.73601200	3.47140400	1.14048600
H	2.64578100	3.70489500	0.57808300
H	1.80014700	2.42302800	1.45068500
H	1.72230000	4.08628900	2.04173000
C	-0.98722000	2.50942000	-3.00781700
H	-1.26877200	1.46854000	-2.81382800
H	-0.06449800	2.50311500	-3.59634400
H	-1.77481800	2.96801100	-3.60822300
C	-2.62525600	5.88696100	0.37794200
H	-3.43310300	5.98983700	-0.34966200
H	-2.17834800	6.87314600	0.53589200
H	-3.06013000	5.56982700	1.33086400
N	4.54079400	-0.70271000	3.37502500
O	3.46703900	-0.21427900	3.67848400
O	5.43458500	-0.94047700	4.17025000
C	0.22495600	-0.22563200	-0.23630900
O	0.87108600	-1.22793300	0.27530500
C	-0.65582500	0.56983200	0.74842200
C	-1.69532100	-0.37225100	1.36531100
H	-1.16306900	-1.12842900	1.94778000
C	-2.59754300	0.40088500	2.30763200
C	-3.36569200	1.47843000	1.85007300
C	-2.66741800	0.05352000	3.65715400
C	-4.17219500	2.19954300	2.72474100
H	-3.33923800	1.74823500	0.79588800
C	-3.47080400	0.77795900	4.53742500
H	-2.10614500	-0.80861700	4.00433600
C	-4.22307100	1.85388100	4.07535500

H	-4.76624500	3.02986500	2.35344400
H	-3.51250400	0.49388900	5.58479300
H	-4.85162600	2.41673600	4.75893400
H	-0.01776100	0.97210000	1.54152100
C	-2.80912100	-1.48503700	-2.16001100
C	-4.13384100	-1.85734400	-1.87520100
C	-4.70720900	-1.80620400	-0.57129700
C	-3.89874500	-1.39224500	0.43660500
C	-2.47518500	-1.10755400	0.24854900
C	-1.97219800	-1.02284500	-1.11072000
C	-2.61960100	-1.62855400	-3.57205800
C	-3.80575800	-2.09014600	-4.07115700
H	-5.74034000	-2.08690200	-0.39897200
H	-4.25481900	-1.37803100	1.46051500
H	-2.11078500	-2.30847800	0.41739900
H	-1.72563100	-1.42478800	-4.14450900
H	-4.09140100	-2.34210000	-5.08261500
N	-0.73055500	-0.59651100	-1.36643800
H	-1.16539100	1.40096400	0.25450900
H	-0.31832600	-0.90911300	-2.24003300
N	-4.71820300	-2.22961300	-3.04440100
C	-6.08857600	-2.69019700	-3.18307400
H	-6.25916100	-3.56601500	-2.55259400
H	-6.78864000	-1.89958000	-2.90171000
H	-6.26050800	-2.96368700	-4.22404600
C	-2.13846100	-3.86097200	2.01854500
O	-1.77935700	-3.73365500	0.79959700
O	-1.94852600	-5.12104100	2.52912100
H	-1.55226400	-5.64337600	1.81815300
O	-2.62275900	-3.01777000	2.77125400

TS8R

C	5.14496800	0.45119000	1.45873800
C	3.93905200	0.25599900	0.77954500
C	3.76807400	0.69267700	-0.52202300
C	4.82996500	1.37799200	-1.10396600

C	6.02979000	1.62003100	-0.44378000
C	6.19098600	1.14130000	0.85350900
C	5.09196900	-0.19787600	2.81734600
C	3.86417900	-1.12958900	2.75428400
C	2.95853900	-0.48568300	1.66051700
H	2.87806100	0.48406400	-1.10609300
H	7.13005300	1.29526600	1.37482400
H	5.99499800	-0.76167800	3.06390100
H	3.33541200	-1.17828200	3.70674900
H	4.94513400	0.55925900	3.59559200
H	2.19810100	0.16523100	2.10666600
N	2.23258000	-1.51614500	0.92980700
O	4.22677400	-2.47869300	2.46585100
C	0.96105100	-1.56017700	0.48926100
C	2.84944400	-2.68175800	0.57995300
N	0.87257300	-2.73637700	-0.13689300
N	2.03786200	-3.45651500	-0.07751700
C	4.23294900	-2.88752800	1.10813000
H	4.96574500	-2.33314500	0.50766600
H	4.48935400	-3.94712100	1.08638800
C	-0.25218800	-3.28153900	-0.85029900
C	-1.04914600	-4.22631900	-0.20182500
C	-0.50345600	-2.81171400	-2.14022700
C	-2.17044300	-4.68605400	-0.88892500
C	-1.63883900	-3.30099100	-2.78380100
C	-2.48739600	-4.22388700	-2.16847900
H	-2.81971000	-5.41293100	-0.40750900
H	-1.86876700	-2.94784100	-3.78603100
H	6.82295900	2.15625900	-0.95020000
C	-0.71957700	-4.69426400	1.18879400
H	-0.68630600	-3.85329100	1.89060100
H	0.25862600	-5.18423500	1.21983000
H	-1.47160400	-5.40121100	1.54289500
C	0.38568600	-1.78163400	-2.78310600
H	1.44389000	-2.04033300	-2.67251200
H	0.23138000	-0.79458000	-2.32908300
H	0.16402700	-1.69604000	-3.84835100

C	-3.74050800	-4.68996000	-2.85930700
H	-4.58719600	-4.05527300	-2.57553000
H	-3.98930200	-5.71675800	-2.58018600
H	-3.63696800	-4.64024700	-3.94585800
N	4.67613600	1.84815400	-2.48388000
O	3.62148300	1.61097100	-3.05316700
O	5.60481100	2.44740700	-2.99233100
C	-0.10756200	-0.48346900	0.94857100
O	0.13280000	-0.16576100	2.17323400
C	-1.54043900	-0.94322100	0.62653500
C	-2.54029300	0.15476000	1.01418300
H	-2.65651900	0.17128000	2.09805000
C	-3.89277600	-0.15969300	0.40358600
C	-4.05811500	-0.23591900	-0.98439400
C	-4.99861600	-0.38628500	1.22389200
C	-5.29491500	-0.54910900	-1.53866100
H	-3.20962300	-0.03877600	-1.63861100
C	-6.23905900	-0.70495800	0.67160300
H	-4.88039000	-0.28194000	2.29861000
C	-6.39036400	-0.79178700	-0.70941800
H	-5.40691400	-0.60187900	-2.61783500
H	-7.08980100	-0.88002900	1.32370700
H	-7.35647300	-1.03757500	-1.13999600
H	-1.76526500	-1.84678700	1.20115800
C	-0.58079900	2.72960400	-1.06091300
C	-1.61231800	3.66727800	-1.22861000
C	-2.88106900	3.60043600	-0.55814100
C	-3.07258700	2.57384700	0.29243300
C	-2.02065900	1.57772900	0.62526600
C	-0.78878200	1.62295600	-0.19804900
C	0.50159700	3.12778600	-1.91153800
C	0.09308800	4.27150000	-2.53645700
H	-3.63890100	4.35757700	-0.72721200
H	-3.98344700	2.48450800	0.87582800
H	-1.66619500	2.01045000	1.62849500
H	1.45905800	2.64240400	-2.04705800
H	0.60112400	4.90269900	-3.25135600

N	0.11139300	0.66711200	-0.06470500
H	-1.64077900	-1.18149200	-0.43557200
H	1.02976200	0.83790500	-0.45883600
N	-1.18788900	4.59158300	-2.12114000
C	-1.95331200	5.74665500	-2.56190700
H	-2.91532300	5.42765700	-2.96859300
H	-2.11910200	6.43541700	-1.73027100
H	-1.39114100	6.25754500	-3.34302200
C	-2.88298200	2.59927100	3.66111800
O	-3.79420500	1.86845100	3.21736300
O	-3.14849800	3.24474000	4.86059500
H	-4.03984000	2.95982200	5.10196000
O	-1.75285400	2.84711300	3.18801300

M8R

C	-5.02779900	-0.54325500	-1.33931500
C	-3.73383100	-0.32722800	-0.85918600
C	-3.49343100	0.50686100	0.22182300
C	-4.59867100	1.13818000	0.78311400
C	-5.89743900	0.96299800	0.31529100
C	-6.11411700	0.10657900	-0.75962100
C	-5.01027200	-1.53845500	-2.46967100
C	-3.61874100	-2.20181400	-2.38726300
C	-2.73319300	-1.15663900	-1.63641500
H	-2.50232600	0.65431700	0.64196000
H	-7.12187600	-0.06042000	-1.12596300
H	-5.80216500	-2.28932700	-2.40096200
H	-3.20594400	-2.40794200	-3.37524300
H	-5.12193400	-1.02280600	-3.42995600
H	-2.10929100	-0.57222600	-2.32351600
N	-1.80417300	-1.82748600	-0.73541800
O	-3.66247000	-3.47226700	-1.74529300
C	-0.54118400	-1.51606600	-0.38390600
C	-2.20570300	-2.90550700	-0.00156600
N	-0.24536900	-2.40796300	0.56871900
N	-1.26786400	-3.29270900	0.80904400
C	-3.54453100	-3.48290100	-0.33220700
H	-4.34815600	-2.91700900	0.15729800

H	-3.59774500	-4.52177900	-0.00508500
C	0.93550000	-2.48284300	1.38595800
C	1.88929100	-3.45694500	1.08994700
C	1.06596300	-1.56709100	2.43354000
C	3.04860200	-3.46751100	1.86462100
C	2.24596200	-1.61587400	3.17401900
C	3.24930300	-2.54699800	2.89516800
H	3.81681600	-4.20615800	1.65027400
H	2.38327700	-0.90694600	3.98688800
H	-6.71622100	1.47967200	0.80076700
C	1.67052800	-4.44090400	-0.02672000
H	1.44581500	-3.92962500	-0.96862800
H	0.82532700	-5.10053600	0.19417300
H	2.55972500	-5.05606500	-0.17567400
C	-0.00810800	-0.55456000	2.72456900
H	-0.99050000	-1.03404400	2.79685800
H	-0.05956900	0.19903400	1.92927300
H	0.19315500	-0.04590900	3.66923200
C	4.53593800	-2.53827000	3.67700400
H	4.36097800	-2.28312000	4.72533200
H	5.22657000	-1.79345100	3.26630100
H	5.03363900	-3.50993100	3.63404300
N	-4.38278700	2.01489500	1.93926600
O	-3.24543500	2.12434000	2.36771100
O	-5.34887700	2.58511500	2.41366200
C	0.30286900	-0.42253700	-1.17779500
O	-0.05267100	-0.47723200	-2.43384500
C	1.80656000	-0.66338000	-0.92107400
C	2.59603200	0.43122900	-1.64385900
H	2.31596400	0.36980100	-2.70349100
C	4.08413600	0.17180600	-1.52463800
C	4.71605000	0.18418500	-0.27467600
C	4.84887300	-0.12180800	-2.65449600
C	6.07425300	-0.09287400	-0.16109700
H	4.13463400	0.42012100	0.61408300
C	6.21131500	-0.40064300	-2.54511400
H	4.36906200	-0.13305500	-3.63008300

C	6.82773300	-0.38804900	-1.29803400
H	6.54904300	-0.07663200	0.81582300
H	6.78871300	-0.62744500	-3.43658200
H	7.88817300	-0.60403500	-1.20970200
H	2.05284000	-0.63068500	0.14444000
C	0.45474500	3.18645000	-0.11372500
C	1.33407000	4.28516000	-0.20581800
C	2.62816800	4.16819700	-0.73444800
C	3.00750600	2.91106700	-1.16591200
C	2.15686500	1.78292300	-1.10050400
C	0.86735700	1.91757600	-0.58033400
C	-0.75642000	3.66594300	0.48734100
C	-0.56730800	5.00114000	0.72500600
H	3.30065900	5.01746700	-0.79781200
H	4.00199200	2.77354600	-1.58147300
H	-1.64128400	3.09684300	0.73677100
H	-1.23100100	5.73034200	1.16955800
N	-0.04298900	0.84890900	-0.46204300
H	-0.95769100	1.15304200	-0.79349300
N	0.68764100	5.38295400	0.31015600
C	1.25388400	6.71159600	0.39522000
H	2.16907200	6.70270800	0.99438900
H	1.48618800	7.09915000	-0.60135300
H	0.52906300	7.37375100	0.87016100
H	2.07486800	-1.64892400	-1.31594800

M8S

C	5.13378800	1.46317600	-0.68162200
C	3.85294600	0.91555900	-0.72047100
C	3.58331000	-0.26971400	-1.39169700
C	4.66545600	-0.89661000	-1.99489000
C	5.96107700	-0.38259800	-1.97340800
C	6.19695200	0.81605100	-1.31223300
C	5.14519600	2.76583200	0.07047700
C	3.74763000	2.87840600	0.72577100
C	2.86257900	1.77871600	0.02810000

H	2.56435400	-0.63946600	-1.46599800
H	7.19759700	1.23540300	-1.28574500
H	5.92643600	2.81386900	0.83570700
H	3.30611400	3.86109900	0.56017300
H	5.31376700	3.60106200	-0.61666500
H	2.11972100	2.19004700	-0.65308500
N	2.13147700	0.99158100	1.03427100
O	3.81092300	2.75637400	2.13941900
C	0.94467700	0.35052600	0.97514400
C	2.69186900	0.72289900	2.25204800
N	0.84712200	-0.27351200	2.15309500
N	1.92663100	-0.04675000	2.96443100
C	3.96033700	1.42692000	2.60148300
H	4.82840400	0.92636700	2.15085400
H	4.09087900	1.45387100	3.68370800
C	-0.19905500	-1.14798500	2.61301800
C	-0.03317700	-2.52182400	2.40961500
C	-1.32711700	-0.58660200	3.20909800
C	-1.09087600	-3.34906700	2.77402900
C	-2.35949000	-1.46021500	3.55745900
C	-2.26602100	-2.83308000	3.33033600
H	-1.00164500	-4.42044400	2.61089100
H	-3.25983200	-1.05253900	4.01006200
H	6.75930000	-0.92113500	-2.46929100
C	1.23304900	-3.06864200	1.80816400
H	2.09911500	-2.82371000	2.43145100
H	1.41885800	-2.64990100	0.81296600
H	1.17328300	-4.15404100	1.71167000
C	-1.43219600	0.89577900	3.43767200
H	-1.51780900	1.42299600	2.48084400
H	-0.54312500	1.27652600	3.95108400
H	-2.30813100	1.12845300	4.04588300
C	-3.40947400	-3.75406600	3.66404900
H	-4.20331500	-3.22652000	4.19713800
H	-3.07501000	-4.59108600	4.28386400
H	-3.83812600	-4.17717500	2.74953900
N	4.43170300	-2.16599500	-2.69289900

O	3.32197400	-2.66262900	-2.61542200
O	5.36188500	-2.66200500	-3.30697600
C	0.00976400	0.41624200	-0.29705200
O	0.75814100	0.62425700	-1.35339400
C	-0.87301100	-0.84887900	-0.38494100
C	-1.79107500	-0.69859600	-1.60185700
H	-1.13500000	-0.58846900	-2.47469100
C	-2.62241400	-1.95316600	-1.78000400
C	-3.59418000	-2.30927800	-0.83631300
C	-2.40268800	-2.80487100	-2.86330900
C	-4.32165800	-3.48673700	-0.97367000
H	-3.78085400	-1.64950500	0.00849800
C	-3.12959300	-3.98707600	-3.00473900
H	-1.64990400	-2.53951200	-3.60176200
C	-4.09098600	-4.33188000	-2.06002900
H	-5.07395600	-3.74597900	-0.23393800
H	-2.94214900	-4.63606700	-3.85524600
H	-4.65894800	-5.25108300	-2.16767300
H	-0.22637500	-1.72355200	-0.51019800
C	-2.87524900	2.80762700	-0.56631200
C	-4.08855500	2.92658100	-1.27462000
C	-4.59303800	1.89212600	-2.07682600
C	-3.83755400	0.73643700	-2.13812300
C	-2.61365900	0.57260500	-1.44862000
C	-2.11879900	1.61623800	-0.66217700
C	-2.68203000	4.03896700	0.14481800
C	-3.75605200	4.83319200	-0.15578700
H	-5.52809300	1.98895600	-2.61855600
H	-4.18979800	-0.09131000	-2.74776200
H	-1.86314500	4.30110500	0.79948800
H	-3.99738800	5.83547900	0.17151100
N	-0.92380700	1.53044400	0.07098200
H	-0.42048100	2.41466700	0.02877700
N	-4.60793600	4.17168200	-1.00976500
C	-5.85268700	4.68085900	-1.54374600
H	-5.81669700	4.72267400	-2.63638200
H	-6.69132700	4.04735600	-1.23989000

H	-6.01506200	5.68785800	-1.15788000
H	-1.48932300	-0.98952200	0.50780900
TS9R			
C	-5.52329600	-0.58994000	-0.43324800
C	-4.16404600	-0.39597500	-0.66829700
C	-3.65802300	0.84142300	-1.03644400
C	-4.56643500	1.88490400	-1.13325500
C	-5.93384300	1.72947500	-0.90974700
C	-6.41743600	0.47417300	-0.56205900
C	-5.81391300	-2.01785500	-0.06150700
C	-4.43272500	-2.72154100	0.00762700
C	-3.36297000	-1.65574300	-0.44311600
H	-2.60769400	0.96007900	-1.27719000
H	-7.47852500	0.33195500	-0.38356600
H	-6.33393700	-2.10080200	0.89898300
H	-4.39426200	-3.56483900	-0.68172400
H	-6.45283200	-2.49526900	-0.81028300
H	-2.82062400	-1.94803900	-1.34248000
N	-2.35100600	-1.44752700	0.60139800
O	-4.17710300	-3.29779700	1.27741400
C	-1.10729700	-0.92394200	0.48004800
C	-2.59873600	-1.69999300	1.92503500
N	-0.67516000	-0.89408500	1.74670800
N	-1.57879600	-1.37910000	2.66152900
C	-3.88984300	-2.35165200	2.29012100
H	-4.68953700	-1.60392000	2.38721900
H	-3.79314000	-2.88572100	3.23605600
C	0.60056000	-0.39936600	2.18363400
C	1.63062900	-1.31209000	2.43264700
C	0.75400300	0.98028100	2.33450600
C	2.88147100	-0.78984000	2.76022600
C	2.02385200	1.45389000	2.66254700
C	3.10065600	0.58706100	2.85242400
H	3.70486400	-1.47690700	2.94308200
H	2.17575700	2.52687300	2.75605600
H	-6.59396100	2.58281800	-1.00677600

C	1.38824800	-2.79758500	2.38608400
H	0.83792000	-3.09853900	1.48948100
H	0.79322800	-3.11433100	3.24934300
H	2.33416400	-3.34313600	2.40659800
C	-0.42108100	1.90433100	2.17214900
H	-1.23691800	1.60993700	2.84134200
H	-0.80351000	1.87209800	1.14747800
H	-0.13672400	2.93269700	2.40248800
C	4.47973800	1.12668200	3.12208400
H	5.04001100	1.20794500	2.18376700
H	5.04509300	0.46962400	3.78828000
H	4.43554800	2.12251800	3.57008500
N	-4.05590400	3.21579400	-1.47681500
O	-2.84660400	3.36581100	-1.53670400
O	-4.86451800	4.10658400	-1.67337000
C	-0.27058900	-0.52648500	-1.19041700
O	-1.17842200	-0.63085300	-2.06358300
C	0.84726700	-1.57741000	-1.12242800
C	2.06757800	-1.15540700	-1.95762700
H	1.73114500	-0.99963700	-2.99280900
C	3.08625300	-2.27575000	-1.95882800
C	3.72813600	-2.65253500	-0.77210100
C	3.36756700	-2.98858200	-3.12467200
C	4.62371200	-3.71625800	-0.75459700
H	3.52754500	-2.09204400	0.13957900
C	4.26454100	-4.05664800	-3.11118000
H	2.87547200	-2.70547700	-4.05187200
C	4.89488400	-4.42383600	-1.92638600
H	5.11476800	-3.99376800	0.17377200
H	4.47044000	-4.59923900	-4.02910900
H	5.59411400	-5.25436300	-1.91345900
H	1.19716600	-1.71370000	-0.09717300
C	2.04332500	2.38973000	-0.61128900
C	3.42366000	2.68301800	-0.58775800
C	4.40114700	1.75231500	-0.96839200
C	3.94675500	0.51252500	-1.38383300
C	2.57838300	0.17014900	-1.41236400

C	1.61855500	1.09875900	-0.99649600
C	1.35575100	3.57051600	-0.17237300
C	2.32115600	4.50144400	0.10405900
H	5.45932300	1.99217500	-0.95153200
H	4.66840100	-0.22868700	-1.71433000
H	0.28910500	3.71819500	-0.08155700
H	2.22850000	5.52064700	0.45394000
N	0.26068000	0.79274500	-0.95816100
H	-0.37000000	1.53469000	-1.23965300
N	3.56930700	3.97275500	-0.13541000
C	4.83691500	4.64978100	0.02815000
H	5.48686900	4.08446600	0.70307700
H	5.34325800	4.76817500	-0.93470100
H	4.65899100	5.63666500	0.45676900
H	0.42227300	-2.51932200	-1.48153200

TS9S

C	-5.00970300	-0.03301700	-0.56533800
C	-3.69650600	-0.14613400	-0.10718500
C	-3.40659600	-0.39027000	1.23051900
C	-4.49808500	-0.50217100	2.08420200
C	-5.82121800	-0.38709600	1.66408600
C	-6.07995400	-0.15163500	0.31966500
C	-5.05197300	0.21301200	-2.04815700
C	-3.59724000	0.03070100	-2.54184000
C	-2.70781900	0.02535900	-1.24217800
H	-2.38298400	-0.48916000	1.59955100
H	-7.10339100	-0.06986400	-0.03237200
H	-5.71933000	-0.47712700	-2.57399700
H	-3.29170100	0.85404500	-3.18796300
H	-5.40319800	1.22798200	-2.26054600
H	-2.15019200	0.95974600	-1.15917600
N	-1.72221200	-1.04895000	-1.28304800
O	-3.44091600	-1.12546000	-3.34869900
C	-0.46899800	-1.10196100	-0.76450700
C	-2.01489400	-2.24466700	-1.88618100

N	-0.08094500	-2.34379200	-1.09000200
N	-1.01695800	-3.06660300	-1.79498800
C	-3.30445900	-2.34102900	-2.63049700
H	-4.14688100	-2.50864700	-1.94502900
H	-3.26913200	-3.15602800	-3.35416800
C	1.18644700	-2.94820800	-0.78855100
C	1.32436600	-3.63259200	0.41949700
C	2.23478600	-2.78098500	-1.69733700
C	2.59047200	-4.13118200	0.73016300
C	3.48042400	-3.29151000	-1.34076900
C	3.67727100	-3.95726500	-0.12778300
H	2.73051700	-4.65595700	1.67197600
H	4.31844500	-3.15961900	-2.02127600
H	-6.62238000	-0.49065100	2.38535800
C	0.16156300	-3.76434800	1.36364200
H	-0.70252900	-4.21498800	0.86428900
H	-0.13621900	-2.77206900	1.72457900
H	0.42964400	-4.38785100	2.21899700
C	2.02339800	-2.04355000	-2.99138100
H	1.77924400	-0.99100100	-2.80926100
H	1.19455600	-2.47554300	-3.56095300
H	2.92418900	-2.08067700	-3.60688900
C	5.04928800	-4.44687100	0.25395900
H	4.99856400	-5.19233900	1.05106800
H	5.66488700	-3.61391000	0.61129600
H	5.56402300	-4.89082400	-0.60252500
N	-4.24397000	-0.75905900	3.50799500
O	-3.09018400	-0.91814000	3.86101300
O	-5.20332100	-0.79781400	4.26137300
C	0.22777600	0.00347200	0.65657600
O	-0.28094900	-0.50634600	1.69233800
C	1.72980000	-0.11722800	0.40490300
C	2.48148100	1.02457900	1.10507100
H	2.23974900	0.96769200	2.17580900
C	3.97276800	0.80318900	0.95659300
C	4.58363200	0.85728000	-0.30224900
C	4.75395800	0.46840800	2.06336400

C	5.93867100	0.57928400	-0.44797900
H	3.98826400	1.12803000	-1.17151000
C	6.11278600	0.18897100	1.92187000
H	4.28988700	0.42021900	3.04521500
C	6.70877200	0.24111400	0.66545600
H	6.39684300	0.62739800	-1.43150400
H	6.70357500	-0.07009500	2.79540900
H	7.76654400	0.02405100	0.55199900
H	2.06295100	-1.08022400	0.79571700
C	0.09208900	3.65824900	-0.21813500
C	0.93663500	4.78838900	-0.27142500
C	2.29437100	4.72913200	0.07264100
C	2.77778600	3.50046600	0.48448600
C	1.96587600	2.34756400	0.56543700
C	0.61758600	2.42056000	0.21066700
C	-1.20781100	4.08540500	-0.64829500
C	-1.10122800	5.41992600	-0.93638000
H	2.93577200	5.60273400	0.02209500
H	3.82200700	3.41204000	0.77010700
H	-2.10705400	3.49074000	-0.72519000
H	-1.84622500	6.11922500	-1.29110200
N	-0.25256400	1.31544300	0.26907100
H	-1.11998900	1.52452300	0.75641400
N	0.18555400	5.85081600	-0.71481000
C	0.68714400	7.19482600	-0.90760300
H	1.06289700	7.60529500	0.03404000
H	1.49349500	7.20199300	-1.64696500
H	-0.12616100	7.82589900	-1.26717300
H	1.94597100	-0.07694100	-0.66821600

PR

C	-0.32281900	2.92821100	0.13145000
O	-0.41586900	4.14394000	0.17737700
C	-1.48583000	1.98685400	0.35171700
C	-1.38912700	0.70488700	-0.49301400
H	-1.46233700	1.00428100	-1.54875800

C	-2.56538600	-0.20306700	-0.19637900
C	-2.69345900	-0.82569700	1.05092100
C	-3.56470800	-0.40083100	-1.14978000
C	-3.79685300	-1.62290000	1.33603600
H	-1.91519900	-0.69033800	1.79839000
C	-4.67352500	-1.19779800	-0.86672200
H	-3.47391800	0.07691100	-2.12213600
C	-4.79234700	-1.81068500	0.37673000
H	-3.88147700	-2.10020100	2.30767900
H	-5.44203800	-1.33917500	-1.62052200
H	-5.65413900	-2.43177000	0.60048800
H	-1.48821800	1.72493700	1.41832200
C	2.36340400	0.38947900	-0.01592800
C	2.52994700	-1.01273400	-0.09364800
C	1.45236400	-1.89071600	-0.26619700
C	0.19145700	-1.32809700	-0.36192300
C	-0.02382600	0.06394000	-0.29231800
C	1.06366700	0.91716200	-0.12188500
C	3.66651700	0.95999600	0.16494300
C	4.54422100	-0.08999500	0.18799200
H	1.59658800	-2.96444000	-0.32457800
H	-0.66839200	-1.97612100	-0.50072000
H	3.92522100	2.00356200	0.27280000
H	5.61919700	-0.09415000	0.30643700
N	0.87713300	2.30715600	-0.08534000
H	1.68704400	2.91187000	-0.15171000
N	3.87083400	-1.27883200	0.03554600
C	4.46165900	-2.60027200	-0.00816400
H	4.02746300	-3.23905600	0.76600200
H	4.30195200	-3.06449500	-0.98567700
H	5.53365300	-2.51213500	0.17007000
H	-2.40635600	2.53410200	0.14047500
PS			
C	0.32269500	2.92825500	0.13134300
O	0.41573500	4.14399200	0.17718700

C	1.48569000	1.98693800	0.35189400
C	1.38913900	0.70502700	-0.49290500
H	1.46234100	1.00452500	-1.54862200
C	2.56540400	-0.20294600	-0.19635000
C	2.69378400	-0.82515100	1.05114700
C	3.56439000	-0.40118300	-1.14998500
C	3.79712000	-1.62243600	1.33618400
H	1.91577900	-0.68939500	1.79880800
C	4.67317800	-1.19824300	-0.86700000
H	3.47338200	0.07625200	-2.12247100
C	4.79228000	-1.81072500	0.37661300
H	3.88199200	-2.09942300	2.30795900
H	5.44144300	-1.33997700	-1.62098500
H	5.65404000	-2.43187600	0.60032100
H	2.40623200	2.53423100	0.14083800
C	-2.36339800	0.38943100	-0.01598600
C	-2.52986700	-1.01280300	-0.09354500
C	-1.45224100	-1.89074200	-0.26601500
C	-0.19135300	-1.32807900	-0.36175500
C	0.02386100	0.06397200	-0.29227400
C	-1.06367800	0.91716100	-0.12195200
C	-3.66653300	0.95989400	0.16486300
C	-4.54419200	-0.09013600	0.18798900
H	-1.59641100	-2.96447700	-0.32435000
H	0.66851400	-1.97608300	-0.50051500
H	-3.92530000	2.00346300	0.27253200
H	-5.61916500	-0.09433400	0.30645600
N	-0.87718900	2.30715700	-0.08554700
H	-1.68708200	2.91185000	-0.15228700
N	-3.87074700	-1.27894900	0.03564300
C	-4.46151700	-2.60041100	-0.00810400
H	-4.30279900	-3.06419700	-0.98598600
H	-4.02643500	-3.23948100	0.76532500
H	-5.53332100	-2.51244700	0.17133300
H	1.48788200	1.72502800	1.41850100

2b-OH

C	0.19889100	-0.52224500	-0.00003300
C	0.69719800	0.79978200	-0.00003600
C	-0.13900300	1.92780200	-0.00004300
C	-1.50059100	1.69201000	-0.00005100
C	-2.03268400	0.38555100	0.00003500
C	-1.19467500	-0.71764800	0.00003500
C	1.32666200	-1.40831600	-0.00004100
C	2.44065900	-0.61604500	-0.00003300
H	0.26661800	2.93369500	-0.00002700
H	-2.18806900	2.53213300	-0.00004100
H	-3.10936500	0.23807900	0.00007800
H	1.30605400	-2.48763900	-0.00012600
H	3.48688500	-0.88607600	-0.00007900
N	2.06640700	0.70852600	0.00011800
H	2.70189400	1.49196800	0.00017900
O	-1.63782600	-2.00253200	0.00001100
H	-2.60499700	-2.00692600	0.00010300

TS5S^{C3}-OH

C	-4.92302300	0.07652100	0.02301100
C	-3.57273800	0.04525000	0.36885600
C	-3.14697800	-0.42484800	1.60387800
C	-4.13323200	-0.87493300	2.47063300
C	-5.49189900	-0.85531400	2.16131700
C	-5.89119600	-0.37052200	0.92202600
C	-5.12292500	0.63352900	-1.35933200
C	-3.70146400	0.81560800	-1.94502500
C	-2.70488200	0.56577400	-0.75342900
H	-2.09944900	-0.41814400	1.88474900
H	-6.94398700	-0.35081100	0.65967400
H	-5.71741200	-0.02664200	-1.99941100
H	-3.55256600	1.82844900	-2.32073600
H	-5.64600800	1.59358200	-1.31772100
H	-2.16354500	1.46765700	-0.46897800
N	-1.69538000	-0.43371200	-1.13590800

O	-3.46111400	-0.01595900	-3.06847800
C	-0.43935300	-0.62611200	-0.69008000
C	-1.97861900	-1.45123400	-2.00373800
N	-0.02738600	-1.75140600	-1.27782500
N	-0.97415500	-2.27013200	-2.11324200
C	-3.27351600	-1.38182800	-2.74342100
H	-4.09722100	-1.77953700	-2.13531000
H	-3.21163400	-1.95014600	-3.67156400
C	1.19558200	-2.47713600	-1.05398600
C	1.36573700	-3.12664700	0.17084000
C	2.14398100	-2.49831600	-2.07994900
C	2.56543600	-3.81235400	0.35902700
C	3.32296700	-3.19980100	-1.84032500
C	3.55080000	-3.85682100	-0.62789200
H	2.72993300	-4.32672100	1.30249100
H	4.08151200	-3.23383000	-2.61842400
H	-6.21178300	-1.22115400	2.88335100
C	0.32302600	-3.06799400	1.25461600
H	-0.68893900	-3.18220700	0.85332500
H	0.37115300	-2.11103300	1.78720900
H	0.49005200	-3.86157900	1.98492700
C	1.90515500	-1.76370500	-3.37071600
H	1.64835500	-0.71682500	-3.17417100
H	1.08167800	-2.21003700	-3.93652800
H	2.80160200	-1.78487700	-3.99281400
C	4.84996600	-4.57526700	-0.37990500
H	5.24824300	-5.00477800	-1.30231000
H	4.72513200	-5.37626000	0.35236700
H	5.60042900	-3.88093000	0.01353800
N	-3.71910100	-1.40167700	3.77713400
O	-2.52470900	-1.51614800	3.99169900
O	-4.59098000	-1.70023500	4.57412600
C	0.26732200	0.32309100	0.24205200
O	-0.48853200	1.01520500	0.97220900
C	1.64985500	0.37308200	0.14872300
C	2.32970500	1.35486700	0.94834700
H	1.71152100	1.66386300	1.79118200

C	3.75770800	1.12153700	1.32719200
C	4.68530600	0.61860200	0.40670200
C	4.17824700	1.39982400	2.62996300
C	6.00294700	0.39317000	0.78817400
H	4.37500100	0.40535200	-0.61369400
C	5.49758400	1.16953100	3.01411200
H	3.46131300	1.78633500	3.35054600
C	6.41261000	0.66721500	2.09335900
H	6.71359300	0.00202000	0.06680100
H	5.80746300	1.38173100	4.03261500
H	7.44171100	0.48847600	2.38876100
H	2.18541900	-0.22244000	-0.57807600
C	1.11563900	3.15991200	-0.75702400
C	0.34605000	4.05662400	-0.01110300
C	-0.95422700	4.42237600	-0.33554300
C	-1.47190800	3.85525500	-1.49614100
C	-0.72629800	2.96635200	-2.28151600
C	0.57395600	2.60792800	-1.91921600
C	2.38857500	2.95387500	-0.05518600
C	2.34267800	3.91384300	1.00557000
H	-1.52466300	5.11898000	0.26750300
H	-2.47633900	4.11986700	-1.81190600
H	-1.15530300	2.55571800	-3.19330400
H	3.31219000	2.77645400	-0.59494800
H	3.09638300	4.11581200	1.75658600
N	1.14896100	4.48072400	1.05986200
H	0.84049400	5.10731500	1.79603400
O	1.35143700	1.77977900	-2.65924900
H	0.91483900	1.59301200	-3.50360200

TS5S^{CS}-OH

C	5.48276900	-1.24190800	-0.86271800
C	4.15129500	-1.10156600	-0.47441700
C	3.74049000	-1.36056900	0.82554200
C	4.72147300	-1.76372200	1.72031900
C	6.05794300	-1.93073400	1.36485000

C	6.44228600	-1.66713100	0.05593200
C	5.67422900	-0.88322300	-2.31009700
C	4.31080500	-0.32791300	-2.78890000
C	3.29090700	-0.63157300	-1.62557800
H	2.70426900	-1.27315300	1.13000900
H	7.48024100	-1.78153300	-0.23925600
H	6.46077600	-0.13594300	-2.45613600
H	3.97488800	-0.83161000	-3.69501300
H	5.95472200	-1.76392100	-2.89516800
H	2.55563500	-1.37844500	-1.91697800
N	2.55013900	0.58732900	-1.25219700
O	4.37105700	1.04080000	-3.15150100
C	1.34243200	0.75271200	-0.67651200
C	3.12078800	1.82460700	-1.35529300
N	1.23918100	2.06424600	-0.44776900
N	2.33719300	2.74587800	-0.87364500
C	4.43477400	1.93273400	-2.05592400
H	5.26195900	1.69535600	-1.37307700
H	4.57303300	2.94237500	-2.44315500
C	0.18656600	2.77731000	0.23247600
C	0.14927500	2.71435200	1.62815800
C	-0.74874700	3.46648600	-0.54016000
C	-0.90463600	3.37062200	2.25923400
C	-1.78198500	4.10851000	0.14272900
C	-1.87958700	4.06200000	1.53473600
H	-0.96859900	3.33710600	3.34400800
H	-2.53115100	4.65034500	-0.42877700
H	6.77445700	-2.25498400	2.10971800
C	1.17109100	1.93131600	2.40614200
H	2.18555200	2.10947000	2.03629600
H	0.96822800	0.85558200	2.33461900
H	1.13843700	2.20551900	3.46184200
C	-0.68054000	3.45958400	-2.04297100
H	-0.92761900	2.46536200	-2.43517000
H	0.31643700	3.72503300	-2.40499500
H	-1.39791300	4.16807300	-2.46008000
C	-3.02736400	4.72083000	2.25071900

H	-3.73089100	3.96555000	2.61704800
H	-3.57238100	5.39857200	1.59031500
H	-2.67757600	5.28761400	3.11770000
N	4.32672100	-2.02070900	3.11052200
O	3.18263600	-1.75202000	3.43541800
O	5.16410600	-2.48178700	3.86513300
C	0.39280200	-0.37650200	-0.34312900
O	0.89603200	-1.52169500	-0.37184200
C	-0.93713800	-0.06283800	-0.04631400
C	-1.77413500	-1.10964400	0.43356100
H	-1.22722600	-1.93333600	0.88907800
C	-3.05258200	-0.79015900	1.10587700
C	-3.81157500	0.33865600	0.76444800
C	-3.51656800	-1.63733700	2.11789900
C	-4.99851000	0.61546500	1.43198400
H	-3.48029400	0.99665100	-0.03517600
C	-4.70162000	-1.35658600	2.79196800
H	-2.93498200	-2.51789700	2.37796600
C	-5.44458100	-0.23003000	2.44862200
H	-5.57953200	1.49029200	1.15753700
H	-5.04316000	-2.01651500	3.58300900
H	-6.36974500	-0.00923300	2.97196800
H	-1.31648400	0.94339600	-0.14123000
C	-4.38176200	-1.46393200	-1.84238200
C	-4.96693800	-2.53962200	-1.13485400
C	-4.21318500	-3.56495500	-0.50266200
C	-2.85673900	-3.44997300	-0.54783500
C	-2.20801800	-2.29764500	-1.12579500
C	-2.98785000	-1.38059000	-1.88227900
C	-5.44571200	-0.64182300	-2.34016800
C	-6.60563600	-1.22986500	-1.92579300
H	-4.70618500	-4.39906800	-0.01582400
H	-2.22663500	-4.20063800	-0.08097400
H	-1.15081200	-2.39474600	-1.37016300
H	-5.35391800	0.26377900	-2.92047100
H	-7.63356000	-0.93777200	-2.08159600
N	-6.30885500	-2.37051200	-1.20483900

H	-6.99402200	-2.98762700	-0.79015500
O	-2.43059400	-0.35700700	-2.52999500
H	-1.46959400	-0.36566800	-2.38841800

TS5S^{C6}-OH

C	-5.14534200	0.62359000	-0.19241400
C	-3.76389000	0.54183000	-0.02246600
C	-3.16517300	0.78002300	1.20722100
C	-4.01277200	1.08841500	2.26193500
C	-5.39690600	1.18017400	2.13012700
C	-5.96940100	0.94729700	0.88576300
C	-5.53994300	0.34150700	-1.61578700
C	-4.24607600	-0.12595300	-2.32461900
C	-3.07079200	0.16850400	-1.31437400
H	-2.08872400	0.75196400	1.33336600
H	-7.04538300	1.01198400	0.76104300
H	-6.31599700	-0.42629600	-1.69834700
H	-4.07357300	0.43128300	-3.24512900
H	-5.93215900	1.24500600	-2.09264500
H	-2.41438100	0.96184700	-1.66669100
N	-2.23643000	-1.03102200	-1.12939700
O	-4.31416400	-1.47797000	-2.74309400
C	-0.94216800	-1.16727000	-0.77419300
C	-2.77325500	-2.28654100	-1.20516100
N	-0.76021500	-2.48527300	-0.63329100
N	-1.89046600	-3.19399500	-0.91188100
C	-4.17693300	-2.41694300	-1.69385800
H	-4.89375600	-2.23986300	-0.88004000
H	-4.34108600	-3.41465400	-2.10162300
C	0.41290600	-3.19406000	-0.18775300
C	1.17944500	-3.85934600	-1.14510400
C	0.72275100	-3.17271000	1.17556500
C	2.32924400	-4.51000400	-0.69713500
C	1.88179600	-3.83660600	1.56834000
C	2.69742800	-4.50204100	0.64886900
H	2.95117100	-5.03171100	-1.41992100

H	2.15692300	-3.83327000	2.62032500
H	-6.00213900	1.42673300	2.99399400
C	0.79396200	-3.84622100	-2.59911500
H	0.74638300	-2.82162500	-2.98473100
H	-0.18939000	-4.30086100	-2.75278300
H	1.52499800	-4.39887100	-3.19142400
C	-0.13579900	-2.43715600	2.16739800
H	-1.19932000	-2.63858400	2.00593500
H	0.02167400	-1.35481500	2.08927200
H	0.11762000	-2.73650900	3.18583400
C	3.95513800	-5.18585900	1.11325500
H	4.45081700	-5.70771700	0.29191000
H	3.73708600	-5.91318400	1.90068900
H	4.65749800	-4.45661000	1.52919700
N	-3.41597400	1.32582500	3.58237000
O	-2.21395100	1.16303800	3.70032100
O	-4.15445700	1.66676700	4.48935900
C	0.00452000	-0.01808100	-0.53289500
O	-0.54650800	1.10677700	-0.34795900
C	1.35532400	-0.29291200	-0.53316600
C	2.29990000	0.73417800	-0.11559700
H	1.84936000	1.45186000	0.57376300
C	3.59572800	0.18340400	0.41467900
C	4.31765300	-0.78184600	-0.29369800
C	4.08931100	0.63596000	1.64057500
C	5.50512200	-1.29421100	0.22086800
H	3.94957400	-1.13823200	-1.25334300
C	5.27417000	0.11923400	2.15950200
H	3.53802100	1.39428000	2.19065500
C	5.98487000	-0.84690900	1.45137400
H	6.05494500	-2.04582400	-0.33746600
H	5.64162500	0.47324400	3.11769800
H	6.90976500	-1.24791900	1.85380200
H	1.72766000	-1.27552400	-0.78531200
C	2.24872800	4.55428500	-0.83310500
C	1.25776500	3.73192000	-1.44816900
C	1.48125700	2.43081200	-1.81261900

C	2.74810100	1.83598900	-1.45152500
C	3.80080200	2.72356900	-0.94692900
C	3.55621300	4.01638900	-0.60720700
C	1.67140100	5.80377800	-0.57784900
C	0.35903100	5.72555000	-1.03473300
H	0.71443900	1.83322900	-2.28993900
H	3.10585500	1.08838400	-2.16034000
H	4.78543500	2.29802600	-0.77732200
H	2.13591300	6.66359500	-0.12050700
H	-0.41591400	6.48007900	-1.01735300
N	0.11688800	4.50364100	-1.55059900
H	-0.77141700	4.18373900	-1.91312700
O	4.45493200	4.87633000	-0.07881200
H	5.29835400	4.42260600	0.06561600

TS5S^{C7}-OH

C	-5.00652700	-0.03456600	-0.09825400
C	-3.64189400	0.04990400	0.17652400
C	-3.15928900	0.07380900	1.47743800
C	-4.10415500	-0.01235500	2.49091500
C	-5.47467900	-0.09928200	2.25467700
C	-5.93135200	-0.10631100	0.94268500
C	-5.26829200	-0.02833200	-1.57891700
C	-3.87843000	-0.15126800	-2.24706700
C	-2.82786100	0.08896200	-1.09745100
H	-2.10133200	0.17535700	1.69211900
H	-6.99444300	-0.17418500	0.73625300
H	-5.91751200	-0.84881100	-1.90047300
H	-3.74200900	0.60190300	-3.02344900
H	-5.75572500	0.90442700	-1.87886400
H	-2.29394200	1.03289700	-1.21124300
N	-1.82010700	-0.98406700	-1.09855100
O	-3.70794300	-1.38657600	-2.92237000
C	-0.53600700	-0.99099700	-0.69414000
C	-2.14159100	-2.26540500	-1.45268400
N	-0.14303100	-2.26319100	-0.79904000

N	-1.13144100	-3.06726900	-1.28390000
C	-3.48310800	-2.49190500	-2.06711400
H	-4.25795000	-2.58678600	-1.29448200
H	-3.47373900	-3.39847400	-2.67220000
C	1.11955600	-2.83983100	-0.41539200
C	1.99169100	-3.23305500	-1.43226300
C	1.41412900	-2.95400600	0.94632200
C	3.22884100	-3.74576900	-1.04436800
C	2.66526500	-3.46930500	1.27781000
C	3.58325200	-3.86242800	0.30101100
H	3.93108400	-4.05924500	-1.81268200
H	2.92872100	-3.56680200	2.32825600
H	-6.15968300	-0.16104700	3.09146000
C	1.61874500	-3.07826200	-2.88174600
H	1.33629400	-2.04376900	-3.10905800
H	0.76661300	-3.71312500	-3.14220900
H	2.45939000	-3.34981000	-3.52220000
C	0.44949800	-2.50633600	2.01099000
H	-0.58679000	-2.74168300	1.74948700
H	0.52179200	-1.42356400	2.16878700
H	0.67950000	-2.99430900	2.95980300
C	4.93498200	-4.38883300	0.70250200
H	4.84238500	-5.16677700	1.46557900
H	5.54770000	-3.58746300	1.12839500
H	5.46902000	-4.80700700	-0.15341600
N	-3.63148300	-0.01446700	3.88106500
O	-2.42772800	-0.01964000	4.07267100
O	-4.46722300	-0.01695100	4.76759200
C	0.20511700	0.23395700	-0.20862000
O	-0.52442700	1.15270800	0.23352500
C	1.59278200	0.22045800	-0.30321300
C	2.31829700	1.32562400	0.25670900
H	1.72289000	1.88011500	0.98302600
C	3.71834000	1.05471800	0.71166900
C	4.60019000	0.29545400	-0.06552600
C	4.15472700	1.54780100	1.94470000
C	5.88690500	0.02478300	0.38699800

H	4.27878200	-0.08524700	-1.03231000
C	5.44170400	1.27280300	2.40089900
H	3.47648200	2.14317100	2.55118100
C	6.31018600	0.50995600	1.62399000
H	6.56033800	-0.56652600	-0.22579800
H	5.76549400	1.65338200	3.36457500
H	7.31380800	0.29626400	1.97792700
H	2.11663700	-0.61378000	-0.74970700
C	0.28934700	3.86757000	-1.25063400
C	1.20450000	2.86318500	-1.62421300
C	2.50213100	2.69129100	-1.02460500
C	2.91477500	3.82437800	-0.22714000
C	2.04782200	4.81172400	0.15272900
C	0.71186700	4.83858000	-0.34031500
C	-0.92086300	3.64453000	-1.99023300
C	-0.69279300	2.55056900	-2.77074700
H	3.27186100	2.21767700	-1.63024700
H	3.93065900	3.83340500	0.15583700
H	2.36913400	5.60438700	0.82190600
H	-1.82177200	4.23866500	-1.95873100
H	-1.31875300	2.07012900	-3.50866800
N	0.59392600	2.08484200	-2.53632200
H	1.02075900	1.29260100	-2.99681200
O	-0.15267400	5.77790900	0.02303300
H	0.25236200	6.40261600	0.64602800

2b

C	0.18036000	-0.51189800	-0.00536100
C	0.71991200	0.79342900	0.00653500
C	-0.07863800	1.94807400	0.00800000
C	-1.44684800	1.74889200	-0.00204300
C	-2.01673400	0.46103800	-0.00685100
C	-1.22319000	-0.68238800	-0.00764700
C	1.28659900	-1.42849200	-0.01360500
C	2.42408100	-0.67009300	-0.00316800
H	0.35778600	2.94092300	0.01530400

H	-2.10949900	2.60922900	-0.00077300
H	-3.09770700	0.35170300	-0.01055400
H	1.24765500	-2.50815300	-0.03679400
H	3.46183900	-0.97092100	-0.00758000
N	-1.76525300	-1.96415400	-0.07265400
H	-1.20044900	-2.67602300	0.37352100
H	-2.72862800	-2.02023200	0.23261700
N	2.08695800	0.66320700	0.01025900
H	2.74382300	1.42872600	0.01586500

TS5S^{C3}-NH

C	-4.92931200	0.07855000	0.03474200
C	-3.57921600	0.06290900	0.38289700
C	-3.15346800	-0.37507800	1.62978000
C	-4.13861700	-0.81337000	2.50402700
C	-5.49644800	-0.81305300	2.19054900
C	-5.89624600	-0.35734500	0.94050000
C	-5.13148000	0.60991600	-1.35710100
C	-3.71076400	0.78872500	-1.94594200
C	-2.71211000	0.55956800	-0.75132700
H	-2.10702000	-0.35289700	1.91377200
H	-6.94855900	-0.35024800	0.67554000
H	-5.72312200	-0.06371100	-1.98573400
H	-3.56481300	1.79654100	-2.33596800
H	-5.65910700	1.56804600	-1.33166500
H	-2.16699500	1.46515600	-0.48714200
N	-1.70673400	-0.45131200	-1.11586100
O	-3.46947400	-0.05727100	-3.05814500
C	-0.45412700	-0.64529600	-0.66135000
C	-1.99349900	-1.48121600	-1.96758400
N	-0.04972900	-1.78528600	-1.22653400
N	-0.99674400	-2.31165800	-2.05577100
C	-3.28453400	-1.41829600	-2.71433100
H	-4.11219500	-1.80720100	-2.10589000
H	-3.21856200	-1.99881400	-3.63457900
C	1.17841500	-2.50129400	-1.00380500

C	1.39771100	-3.07065900	0.25411200
C	2.08922200	-2.58840400	-2.06099700
C	2.61229400	-3.72729300	0.44650900
C	3.28616900	-3.25836600	-1.81357600
C	3.56750500	-3.82200100	-0.56676000
H	2.81353000	-4.17845200	1.41495900
H	4.01695300	-3.34197800	-2.61408000
H	-6.21516100	-1.16967300	2.91826800
C	0.38903600	-2.96880900	1.36668100
H	-0.63458200	-3.09218800	0.99999000
H	0.45727500	-1.99669100	1.86833700
H	0.57550500	-3.74055500	2.11564400
C	1.79004500	-1.98047600	-3.40422900
H	1.38878800	-0.96644000	-3.29978400
H	1.04686900	-2.57433900	-3.94548800
H	2.69703400	-1.93706300	-4.01050300
C	4.88832400	-4.49578100	-0.30911800
H	5.30219800	-4.92309900	-1.22544500
H	4.78794900	-5.29166100	0.43274700
H	5.61455200	-3.77325200	0.07949700
N	-3.72452700	-1.30360400	3.82462500
O	-2.52992100	-1.38586400	4.05217000
O	-4.59654100	-1.60561300	4.62034600
C	0.25791500	0.31999400	0.25299500
O	-0.49453900	1.03135100	0.96656500
C	1.64152600	0.35711600	0.16364400
C	2.32985400	1.36450400	0.92109200
H	1.71304700	1.72111600	1.74630000
C	3.75552200	1.13589900	1.31294800
C	4.65186900	0.47887300	0.46164600
C	4.20817700	1.57890400	2.55868600
C	5.96901900	0.26689400	0.85258700
H	4.31723800	0.12524100	-0.51062600
C	5.52672900	1.36371000	2.95317700
H	3.51473700	2.08142600	3.22960500
C	6.41009400	0.70804800	2.10022800
H	6.65391200	-0.24588200	0.18422900

H	5.86154400	1.70489000	3.92771200
H	7.43816700	0.53877400	2.40456000
H	2.16840100	-0.26128000	-0.54977300
C	1.12251100	3.11409400	-0.85007400
C	0.38643800	4.05526200	-0.12262700
C	-0.91146400	4.43978800	-0.42882700
C	-1.46229300	3.84047800	-1.55941400
C	-0.75126300	2.91261500	-2.32454400
C	0.55775100	2.52828000	-1.99265300
C	2.40562600	2.91409700	-0.15612200
C	2.40179400	3.92219900	0.86015000
H	-1.45173200	5.17191900	0.15954700
H	-2.46863100	4.11160400	-1.86470200
H	-1.21251600	2.47686400	-3.20776100
H	3.32283800	2.69850800	-0.69492600
H	3.17610000	4.14551900	1.58356500
N	1.23880000	1.59073000	-2.75818500
H	2.24353100	1.58640100	-2.63418000
H	0.98465400	1.59158600	-3.73882400
N	1.21936800	4.51018300	0.91321000
H	0.93671500	5.17551500	1.62550600

TS5^{C5}-NH

C	5.47566000	-1.24443800	-0.85272300
C	4.14201700	-1.10512200	-0.47177900
C	3.72301000	-1.37082200	0.82439600
C	4.69878000	-1.77817500	1.72303500
C	6.03744400	-1.94385600	1.37482900
C	6.42967700	-1.67435600	0.06954600
C	5.67576200	-0.88000700	-2.29759600
C	4.31457200	-0.32395500	-2.78238200
C	3.28824500	-0.62885100	-1.62532400
H	2.68390800	-1.28630200	1.12043400
H	7.46930900	-1.78816200	-0.21997800
H	6.46270100	-0.13164600	-2.43611500
H	3.98385000	-0.82681700	-3.69090700

H	5.96054700	-1.75826600	-2.88427000
H	2.55237000	-1.37314700	-1.92126100
N	2.54846200	0.59035100	-1.25092400
O	4.37725000	1.04522600	-3.14370300
C	1.34018000	0.75508300	-0.67370100
C	3.12311100	1.82656500	-1.34816600
N	1.24279800	2.06719200	-0.43905800
N	2.34300700	2.74828500	-0.86355900
C	4.43867700	1.93432200	-2.04564100
H	5.26417800	1.69405000	-1.36173900
H	4.57983000	2.94478100	-2.42979100
C	0.19427600	2.78196100	0.24399400
C	0.15355600	2.71401200	1.63909100
C	-0.73560500	3.48058000	-0.52643100
C	-0.89875600	3.37278600	2.27071100
C	-1.76697400	4.12563600	0.15594400
C	-1.86848600	4.07248900	1.54762800
H	-0.96584900	3.33391100	3.35513600
H	-2.51113800	4.67562500	-0.41444800
H	6.74930600	-2.27202300	2.12241400
C	1.16981300	1.92304000	2.41585600
H	2.18571300	2.09857600	2.04862700
H	0.96186500	0.84894300	2.33723600
H	1.13592500	2.19219300	3.47283000
C	-0.65529100	3.48499200	-2.02852100
H	-0.82472100	2.47694800	-2.42624400
H	0.32564700	3.81823200	-2.37919600
H	-1.41378600	4.14647900	-2.45027300
C	-3.01508500	4.73284000	2.26422900
H	-3.72251600	3.97875700	2.62547700
H	-3.55567100	5.41637200	1.60606600
H	-2.66479900	5.29389400	3.13474100
N	4.29633000	-2.04171100	3.10981000
O	3.15104000	-1.77329100	3.43018000
O	5.12928200	-2.50755100	3.86670600
C	0.39109700	-0.37513900	-0.34588200
O	0.89686800	-1.52329000	-0.39637900

C	-0.92699100	-0.06169100	-0.02479300
C	-1.76916000	-1.11614000	0.43993000
H	-1.22229000	-1.93501300	0.90462400
C	-3.04785200	-0.79191900	1.11281300
C	-3.80056500	0.34192900	0.77381800
C	-3.52327100	-1.63899500	2.11943400
C	-4.99133000	0.62139500	1.43346600
H	-3.45912900	1.00127000	-0.02052100
C	-4.71279300	-1.35678600	2.78592400
H	-2.94685100	-2.52211200	2.38189700
C	-5.44947400	-0.22640100	2.44302400
H	-5.56641900	1.50049000	1.15941400
H	-5.06204000	-2.01912800	3.57175200
H	-6.37719600	-0.00384900	2.96111700
H	-1.30434800	0.94542800	-0.11279200
C	-4.38410600	-1.47265800	-1.85523800
C	-4.95663500	-2.52781900	-1.12115900
C	-4.19964900	-3.55578100	-0.48529900
C	-2.84730300	-3.44247900	-0.54321200
C	-2.19826500	-2.29037000	-1.13113500
C	-2.97359900	-1.38603400	-1.93164600
C	-5.45827600	-0.66444800	-2.35343900
C	-6.61454000	-1.24165300	-1.90772200
H	-4.69313900	-4.38474800	0.00983200
H	-2.21314300	-4.18827100	-0.07340800
H	-1.14506200	-2.39803100	-1.38638100
H	-5.39044300	0.23237200	-2.95231100
H	-7.64423600	-0.95059100	-2.05211700
N	-2.36355700	-0.42245800	-2.63217400
H	-2.89392600	0.25082300	-3.16608100
H	-1.36057800	-0.42647100	-2.73736900
N	-6.30237700	-2.36403700	-1.17175600
H	-6.97726500	-2.97507500	-0.73245700

TS5^{C6}-NH

C	-5.14538500	0.67045200	-0.20427300
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C	-3.76537700	0.57567500	-0.02957400
C	-3.16838100	0.80775500	1.20214400
C	-4.01669200	1.12362100	2.25407400
C	-5.39946800	1.22831100	2.11763400
C	-5.97003000	1.00123000	0.87129200
C	-5.53763100	0.39230400	-1.62917400
C	-4.24554100	-0.08686200	-2.33350600
C	-3.07123500	0.19704400	-1.31934500
H	-2.09249000	0.76986300	1.33121400
H	-7.04498000	1.07591300	0.74309600
H	-6.32010100	-0.36865600	-1.71447400
H	-4.06476600	0.46853900	-3.25355800
H	-5.92018700	1.29926600	-2.10728500
H	-2.40679600	0.98485400	-1.66900000
N	-2.24776200	-1.00935300	-1.13223600
O	-4.32460300	-1.43840600	-2.75184400
C	-0.95558500	-1.15621900	-0.77342700
C	-2.79513500	-2.26027100	-1.20925100
N	-0.78559300	-2.47580100	-0.63110400
N	-1.92118300	-3.17516700	-0.91301400
C	-4.19836900	-2.37840700	-1.70216100
H	-4.91591800	-2.19521900	-0.89029400
H	-4.37012400	-3.37469900	-2.11032200
C	0.37872300	-3.19500100	-0.17908700
C	1.14298300	-3.87028200	-1.13122700
C	0.68151300	-3.17511500	1.18585600
C	2.28306800	-4.53304600	-0.67604200
C	1.83056500	-3.85171000	1.58610500
C	2.64393600	-4.52717400	0.67192900
H	2.90331400	-5.06268600	-1.39446400
H	2.09987800	-3.84981300	2.63960000
H	-6.00523200	1.47990200	2.97966200
C	0.76472300	-3.85569800	-2.58711400
H	0.72448000	-2.83104300	-2.97337700
H	-0.22040300	-4.30499500	-2.74520100
H	1.49524800	-4.41284600	-3.17582600
C	-0.17512800	-2.42901000	2.17143100

H	-1.23904900	-2.62923400	2.01073100
H	-0.01515500	-1.34777400	2.08447900
H	0.07688500	-2.72037600	3.19247000
C	3.89213500	-5.22295600	1.14423500
H	4.38621100	-5.75244600	0.32681600
H	3.66254700	-5.94537300	1.93291400
H	4.60007000	-4.49962600	1.56109800
N	-3.42250100	1.35502700	3.57678800
O	-2.22304700	1.17823600	3.69983200
O	-4.16070400	1.70543300	4.48050700
C	0.00032900	-0.01418300	-0.53325400
O	-0.54272900	1.11447800	-0.34684400
C	1.34832200	-0.30185300	-0.53934100
C	2.30801700	0.71570900	-0.13131100
H	1.86873600	1.44421400	0.55373700
C	3.59715500	0.15272700	0.40277000
C	4.29664500	-0.84319400	-0.28545300
C	4.10879600	0.62806000	1.61268900
C	5.47809300	-1.36432700	0.23445600
H	3.91708000	-1.21639000	-1.23409900
C	5.28738300	0.10304200	2.13688800
H	3.57728700	1.41258200	2.14505300
C	5.97473800	-0.89486800	1.44977000
H	6.01027300	-2.13970300	-0.30832000
H	5.66854400	0.47552300	3.08263500
H	6.89482600	-1.30267300	1.85645200
H	1.70701600	-1.28975800	-0.79021400
C	2.31135000	4.51251200	-0.82896100
C	1.30788500	3.71108800	-1.45125100
C	1.50856800	2.40950100	-1.82697000
C	2.77074400	1.80151800	-1.47536500
C	3.83849500	2.67516800	-0.98551600
C	3.62816800	3.97506400	-0.62141100
C	1.73557100	5.75898000	-0.53984800
C	0.42008100	5.69867600	-0.98712500
H	0.72686700	1.82353700	-2.29424700
H	3.11169400	1.04204300	-2.18008400

H	4.81864400	2.23235800	-0.83594400
H	2.19722800	6.60633500	-0.05512900
H	-0.35213700	6.45466000	-0.94233200
N	4.58199900	4.78200900	-0.02002700
H	4.54110600	5.75815800	-0.28703900
H	5.52663800	4.42174700	-0.07399800
N	0.16958000	4.49007800	-1.52917300
H	-0.72451300	4.17877700	-1.88434000

TS5^{C7}-NH

C	-5.01508300	0.03690200	-0.11505500
C	-3.65053300	0.09731500	0.16681100
C	-3.17479000	0.09788100	1.47054400
C	-4.12603900	0.01453100	2.47829100
C	-5.49655600	-0.04741800	2.23461000
C	-5.94628800	-0.03224100	0.92031800
C	-5.27006200	0.06077500	-1.59679300
C	-3.87907300	-0.07475000	-2.26025500
C	-2.83028800	0.13848800	-1.10347900
H	-2.11687700	0.17734200	1.69397500
H	-7.00915900	-0.08157800	0.70765100
H	-5.92869100	-0.74801400	-1.92871500
H	-3.72921900	0.68469500	-3.02792400
H	-5.74391200	1.00242300	-1.89064900
H	-2.28256600	1.07554000	-1.20671900
N	-1.83779800	-0.94888900	-1.11125500
O	-3.72287600	-1.30447200	-2.94860200
C	-0.55678900	-0.98107700	-0.69810600
C	-2.17831900	-2.22125200	-1.47883100
N	-0.18486500	-2.25894600	-0.81108100
N	-1.18301800	-3.04142200	-1.30945300
C	-3.51845800	-2.42245200	-2.10506300
H	-4.30046900	-2.51654600	-1.33955100
H	-3.51563100	-3.32193500	-2.72069800
C	1.06038400	-2.86433400	-0.41490800
C	1.93784600	-3.27105800	-1.42356500

C	1.33187300	-2.99343300	0.94873700
C	3.15688500	-3.81267300	-1.02202900
C	2.56816100	-3.53761200	1.29454800
C	3.49087100	-3.94273300	0.32899600
H	3.86286900	-4.13861900	-1.78201100
H	2.81380800	-3.64767700	2.34770300
H	-6.18650300	-0.10869800	3.06742800
C	1.58420300	-3.10099600	-2.87618000
H	1.31362900	-2.06220300	-3.09814000
H	0.72921500	-3.72576800	-3.15147900
H	2.42929600	-3.37530900	-3.50950700
C	0.36022700	-2.53412000	2.00208900
H	-0.67567500	-2.75489200	1.72629000
H	0.44586600	-1.45281200	2.16407700
H	0.57103100	-3.02735500	2.95267100
C	4.83504900	-4.48227000	0.73781700
H	4.77902100	-4.99517900	1.70080900
H	5.55692100	-3.66464200	0.84073100
H	5.22682300	-5.18030100	-0.00572100
N	-3.66017400	-0.01238600	3.87056600
O	-2.45760700	-0.03750400	4.06761500
O	-4.50035400	-0.01394800	4.75279000
C	0.20206700	0.22841100	-0.19287000
O	-0.51497000	1.14929800	0.25033100
C	1.59805100	0.18112500	-0.26750000
C	2.34847400	1.23824000	0.30368700
H	1.77725500	1.86809500	0.98494500
C	3.75427600	0.98233100	0.71818900
C	4.60758600	0.16992100	-0.03876000
C	4.23837600	1.55389500	1.89984100
C	5.91026500	-0.07205500	0.38315500
H	4.25477500	-0.27005300	-0.96837400
C	5.53993000	1.30486500	2.32658400
H	3.58410700	2.19209900	2.48872000
C	6.37958500	0.49117800	1.56938200
H	6.56172400	-0.70068700	-0.21617700
H	5.89844400	1.74600100	3.25141000

H	7.39595100	0.29905100	1.89845300
H	2.09442000	-0.66609500	-0.72112100
C	0.37937100	3.87990800	-1.21731600
C	1.27070600	2.87519100	-1.62890600
C	2.58099500	2.69418500	-1.08550500
C	3.02579400	3.78992000	-0.27607100
C	2.18407600	4.78039900	0.15426700
C	0.82420400	4.84674200	-0.28529300
C	-0.85202000	3.67165800	-1.92380200
C	-0.66052000	2.58091200	-2.72412600
H	3.31930700	2.14605900	-1.66276000
H	4.05413800	3.78357900	0.07268900
H	2.54043300	5.54997500	0.83192200
H	-1.75240200	4.26726500	-1.87033400
H	-1.31564500	2.11879400	-3.44822900
N	0.01608500	5.81268200	0.16656200
H	-0.95403800	5.85228500	-0.10732400
H	0.34624600	6.49316400	0.83479500
N	0.62156600	2.10171700	-2.53173200
H	1.03277300	1.31991700	-3.02188200