

## Electronic Supplementary Information

# Diazadiborinine as Ambiphilic Catalyst for Metal-Free Hydrogenation: a Computational Study on the Structural Design and Reaction Mechanism

Youxiang Shao,<sup>a,b</sup> Ming Huang,<sup>c</sup> Fenglong Gu,<sup>b</sup> Cunyuan Zhao,<sup>a</sup> Ling-Bo Qu,<sup>d</sup> and Zhuofeng Ke<sup>\*,a</sup>

<sup>a</sup> School of Materials Science and Engineering, PCFM Lab, Sun Yat-sen University, Guangzhou 510275, P. R. China.

<sup>b</sup> MOE Key Laboratory of Theoretical Chemistry of the Environment, School of Chemistry and Environment, South China Normal University, Guangzhou 510006, P. R. China

<sup>c</sup> School of Clinical Pharmacy, Guangdong Pharmaceutical University, Guangzhou 510006, P. R. China.

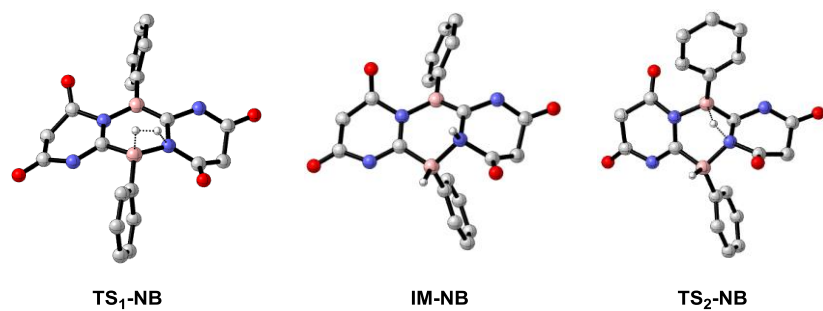
<sup>d</sup> College of Chemistry and Molecular Engineering, Zhengzhou University, Zhengzhou 450001, P. R. China.

### Corresponding Author

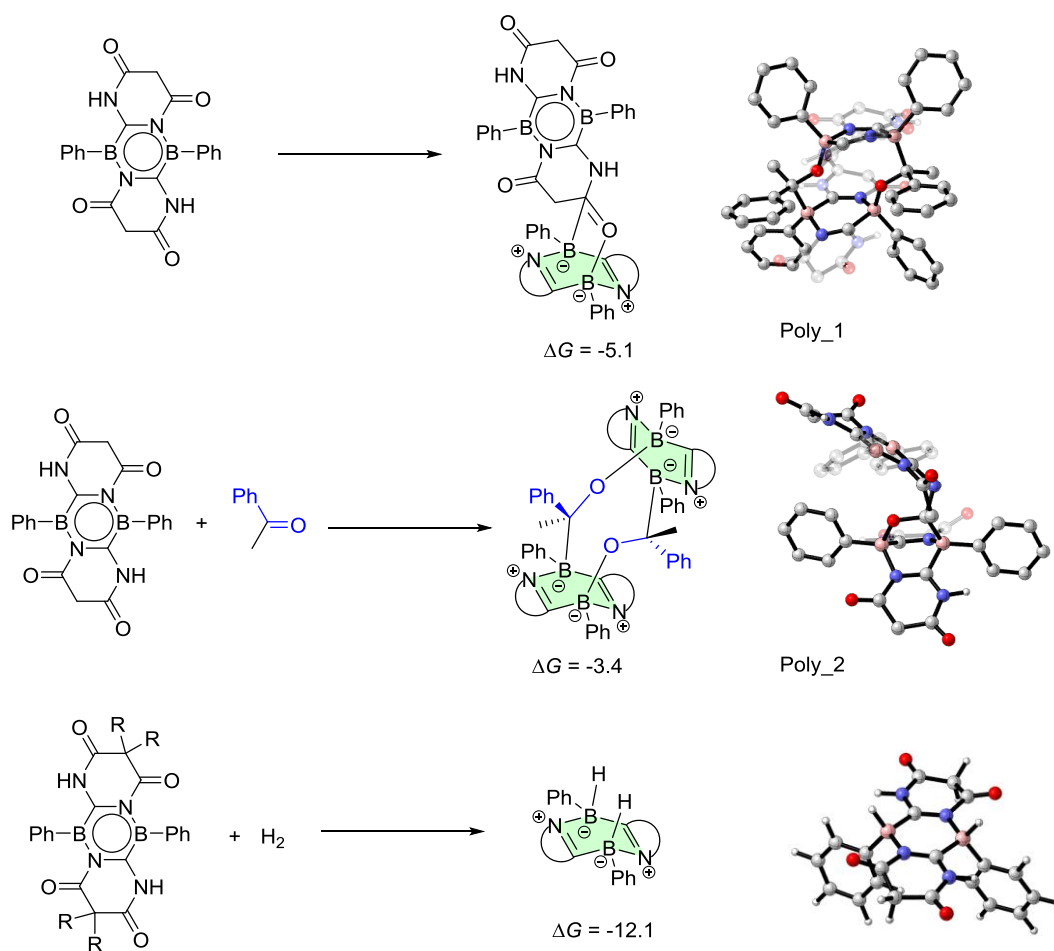
\* E-mail for Z. F. Ke.: kezhf3@mail.sysu.edu.cn

## Table of Content

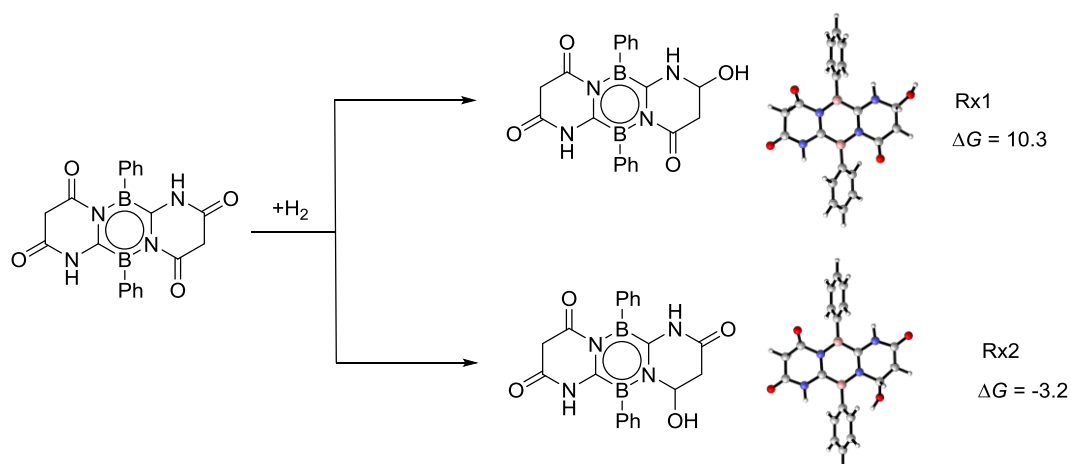
1. Alternative stepwise mechanism of compound <b>B</b> catalyzed H <sub>2</sub> activation.....	2
2. The thermodynamics of the polymerization of compound <b>B</b> .....	2
3. The thermodynamics of the reduction of carbonyl groups in the presence of H <sub>2</sub> .....	3
4. The [4 + 2] cycloaddition reaction of compound <b>B</b> with benzalmethylamine and acetophenone.....	3
5. The calculated NPA charge of <b>B</b> -H <sub>2</sub> and [DBA-H <sub>2</sub> ] <sup>2-</sup> .....	4
6. The calculated NPA charge of <b>IM</b> <sub>2</sub> <b>N</b> and <b>IM</b> <sub>3</sub> <b>N</b> .....	4
7. Optimized structure of transition state corresponding for the direct abstract of H <sub>2</sub> starting from <b>IM</b> <sub>2</sub> <b>N</b> .....	4
8. The calculated NPA charge of <b>IM</b> <sub>1</sub> <b>O</b> and <b>IM</b> <sub>2</sub> <b>O</b> .....	4
9. The optimized Cartesian coordinates (xyz) .....	5



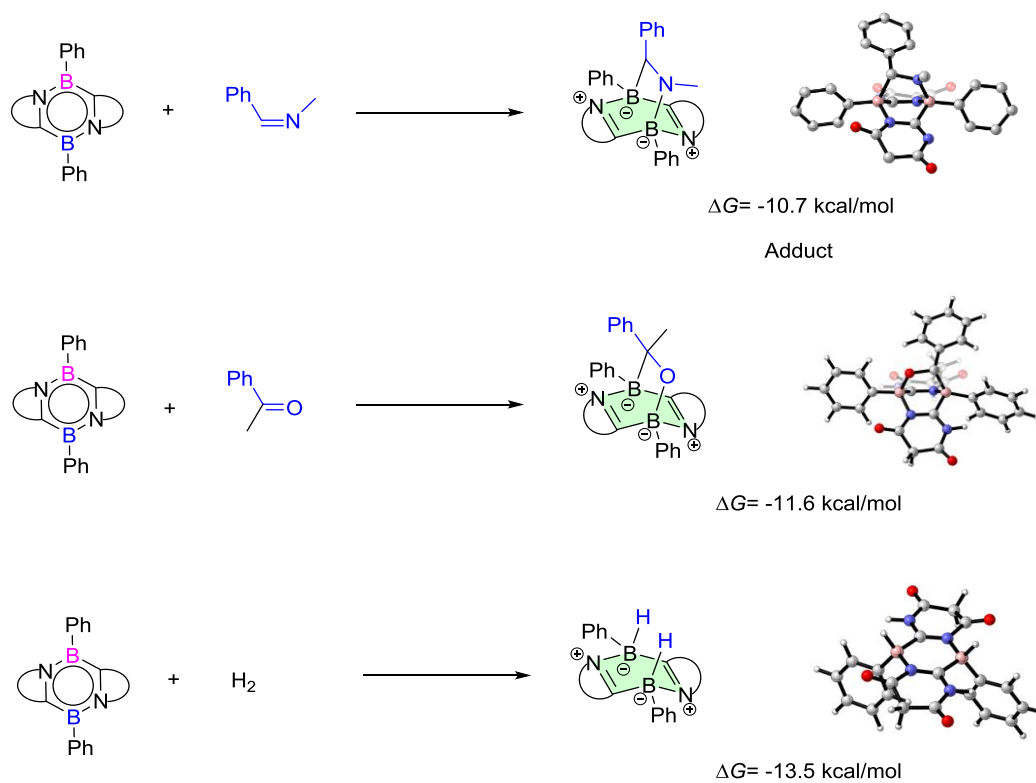
**Figure S1.** Alternative stepwise mechanism of compound **B** catalyzed  $H_2$  activation.



**Figure S2.** The thermodynamics of the polymerization of compound **B** calculated at B3LYP-D3/6-311+(d,p)//B3LYP-D3/6-31(d) level of theory.



**Figure S3.** The thermodynamics of the reduction of carbonyl groups in the presence of  $\text{H}_2$  calculated at B3LYP-D3/6-311+(d,p)//B3LYP-D3/6-31(d) level of theory.



**Figure S4.** The [4 + 2] cycloaddition reaction of compound **B** with benzaldehyde and acetophenone.

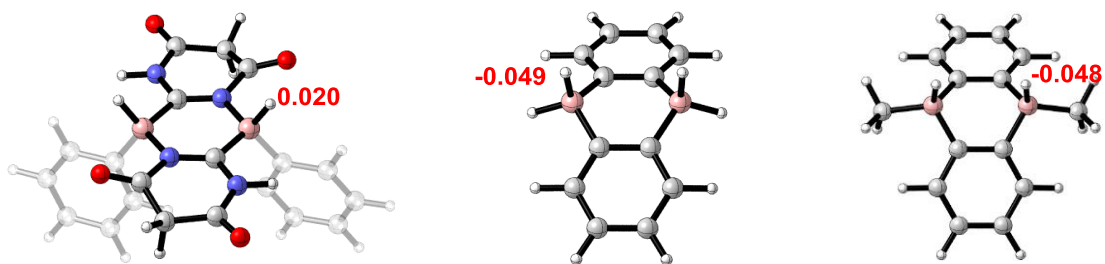


Figure S5. The calculated NPA charge of B-H<sub>2</sub> and [DBA-H<sub>2</sub>]<sup>2-</sup>.

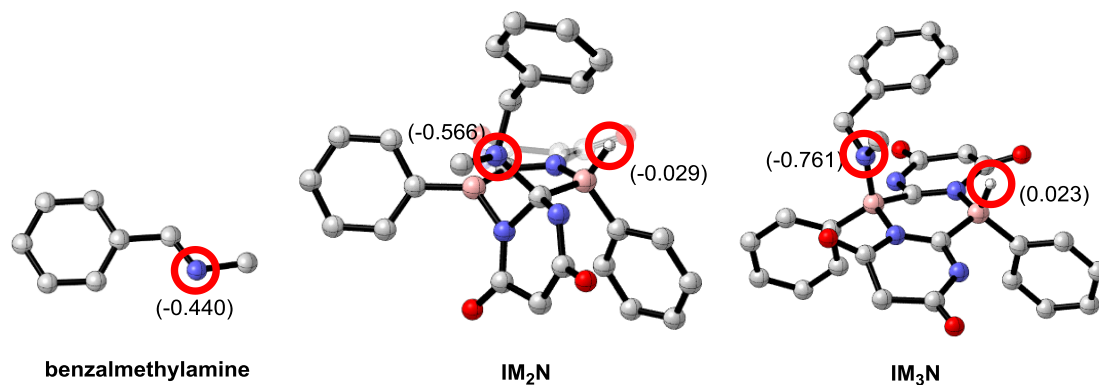


Figure S6. The calculated NPA charge of IM<sub>2</sub>N and IM<sub>3</sub>N.

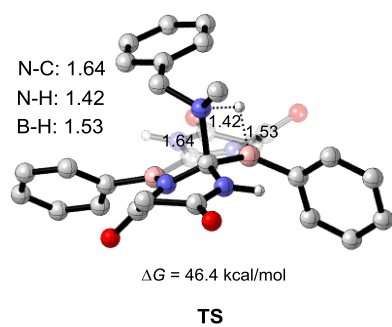


Figure S7. The optimized structure of transition state corresponding for the direct abstract of H<sup>2</sup> starting from IM<sub>2</sub>N.

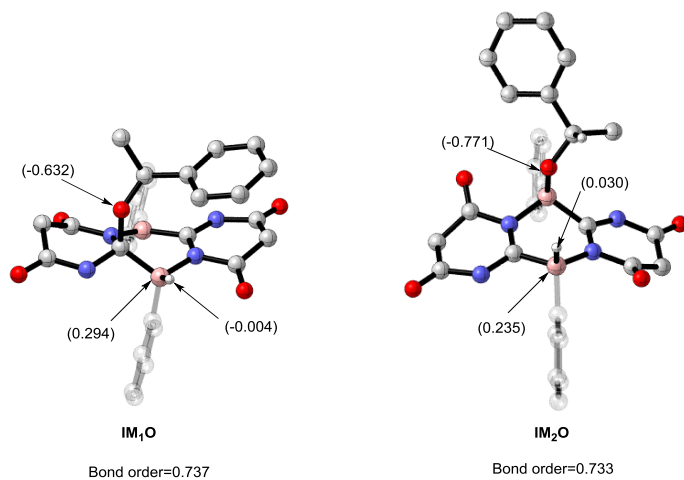


Figure S8. The calculated NPA charge of IM<sub>1</sub>O and IM<sub>2</sub>O.

## Optimized Cartesian coordinates (xyz)

<b>A</b>				C	-5.90188100	0.46737900	0.06894100
B	-1.51291400	0.04839000	0.00610600	H	-3.33759200	-0.61394600	2.01172200
C	-0.00863200	-3.35675000	-0.05457900	H	-5.79277300	-0.39353400	2.03866800
H	-0.08627100	-4.43130600	-0.08001200	H	-5.68046100	1.30949200	-1.90063600
B	1.51291400	-0.04839400	0.00609600	H	-3.22805900	1.07847400	-1.93020700
C	0.00863000	3.35674700	-0.05454200	H	-6.98186300	0.56621300	0.08090400
H	0.08626800	4.43130400	-0.07996200				
N	-0.67280700	1.23409200	-0.00859000	<b>TS<sub>0</sub>-A</b>			
C	0.72663800	1.22050000	-0.01363400	B	-1.42991600	0.11578000	-0.10990000
N	1.12290400	2.55404400	-0.06065200	C	-0.18121400	-3.35019100	0.58871700
C	-1.09384300	2.56975600	-0.01880800	H	-0.32806100	-4.40447600	0.75278300
C	2.49413000	3.02200600	-0.12038200	C	-2.99166200	0.28529000	-0.28654800
H	3.00582600	2.88152500	0.83533700	C	-3.80109600	0.81292800	0.73579100
H	3.04674500	2.47123900	-0.88322200	H	-3.34174500	1.13705200	1.66527500
H	2.49264800	4.08238400	-0.37411800	C	-5.18553200	0.91341100	0.59812500
H	-2.13612700	2.83206300	-0.00528700	H	-5.78272500	1.32072500	1.40750700
C	-2.49413400	-3.02200600	-0.12034400	C	-5.80356000	0.48260500	-0.57643900
H	-3.00580100	-2.88153800	0.83539200	H	-6.87990700	0.55708700	-0.68739600
H	-3.04677000	-2.47122500	-0.88315900	C	-5.02381500	-0.04142600	-1.60742300
H	-2.49266100	-4.08238000	-0.37409700	H	-5.49402500	-0.37380700	-2.52717800
H	2.13612500	-2.83206900	-0.00527100	C	-3.63930900	-0.13279600	-1.46092800
C	-0.72663800	-1.22050400	-0.01363700	H	-3.04326100	-0.53527800	-2.27384600
N	0.67280700	-1.23409500	-0.00860400	B	1.42992300	-0.11578400	-0.10990200
N	-1.12290600	-2.55404600	-0.06065200	C	0.18120500	3.35018100	0.58871900
C	1.09384100	-2.56976100	-0.01880600	H	0.32804700	4.40446800	0.75278000
C	3.08136500	-0.20059500	0.03389300	C	2.99167300	-0.28527900	-0.28654900
C	3.84391500	0.20037800	1.14488100	C	3.63932000	0.13283200	-1.46091900
C	3.78143200	-0.75476300	-1.05353100	H	3.04327400	0.53533900	-2.27382500
C	5.23296500	0.07449800	1.16557200	C	5.02382700	0.04146600	-1.60741100
H	3.33757800	0.61395900	2.01171800	H	5.49404100	0.37387000	-2.52715500
C	5.16930000	-0.88607400	-1.04223000	C	5.80356900	-0.48258900	-0.57643600
H	3.22807400	-1.07848200	-1.93021200	H	6.87991600	-0.55706800	-0.68739100
C	5.90188300	-0.46737400	0.06895700	C	5.18553700	-0.91342900	0.59811400
H	5.79276100	0.39354800	2.03868200	H	5.78272700	-1.32076700	1.40748600
H	5.68047900	-1.30949600	-1.90062300	C	3.80110000	-0.81294900	0.73577800
H	6.98186900	-0.56620700	0.08092800	H	3.34174100	-1.13710800	1.66524700
C	-3.08136500	0.20059500	0.03389900	N	-0.60422800	1.29282800	0.30686900
C	-3.84392200	-0.20037100	1.14488300	C	0.76367400	1.20338800	0.30538400
C	-3.78142300	0.75476100	-1.05353300	N	1.24518900	2.47230500	0.50317500
C	-5.23297200	-0.07448900	1.16556400	C	-0.96236200	2.62847600	0.46530100
C	-5.16929000	0.88607400	-1.04224100	C	2.65061700	2.84934700	0.54882600



C	-3.04167400	-0.13586200	0.02787900	C	-5.75599300	0.26712500	-0.70302200
C	-3.84758200	0.44071900	1.02373400	H	-5.82596500	0.44298700	1.44179800
C	-3.68881000	-0.70537700	-1.08134500	H	-5.36133900	0.08904900	-2.81091300
C	-5.23821700	0.44052500	0.92248000	H	-6.83387600	0.26109900	-0.82020000
H	-3.38294100	0.87497000	1.90420700	C	2.94561700	-0.32069300	-0.42126100
C	-5.07708300	-0.70835600	-1.18967000	C	3.43662800	-0.49955400	-1.72392100
H	-3.09811900	-1.15154900	-1.87655000	C	3.88793500	-0.19210400	0.61443600
C	-5.85685100	-0.13451200	-0.18584400	C	4.80617500	-0.55851600	-1.98408600
H	-5.83732700	0.88360400	1.71031300	H	2.73698000	-0.58993400	-2.54891100
H	-5.55158400	-1.15452700	-2.05686300	C	5.25670100	-0.24061100	0.36150500
H	-6.93790100	-0.13551900	-0.26766500	H	3.54485500	-0.07978900	1.63783300
B	1.47662800	0.08251100	0.11288900	C	5.71998600	-0.42579100	-0.94121400
B	-1.47663200	-0.08266100	0.11291800	H	5.15786700	-0.70151600	-3.00006300
N	-0.63580200	-1.27585900	0.14470200	H	5.96155300	-0.14324600	1.17994000
N	1.44280100	-2.43126300	-0.00050000	H	6.78513800	-0.46624100	-1.14017300
N	0.63580600	1.27571400	0.14472900	B	-1.38611300	0.19911500	-0.21403400
N	-1.44276100	2.43114100	-0.00046700	B	1.39602900	-0.17220100	-0.16085500
C	-0.73809800	1.22778100	0.07314400	N	0.52843300	-1.32364400	0.29315200
C	1.25807200	2.58783400	0.30506200	N	-1.65372700	-2.23739600	0.41254600
O	1.62833200	-4.67816200	-0.31612500	N	-0.52929200	1.37967600	0.19736700
O	-2.22034100	-2.73638000	0.99948200	N	1.66153300	2.28710100	0.34194600
O	-1.62825600	4.67800700	-0.31632400	C	0.82084200	1.20648800	0.18846300
O	2.22015600	2.73621500	0.99988700	C	-1.07271600	2.70796100	0.27262500
H	0.75051100	3.53720100	-1.52276700	O	-2.07138900	-4.44043500	0.79614700
H	-0.75034900	-3.53738100	-1.52287500	O	2.16283300	-2.67502200	1.19197300
<b>TS<sub>0</sub>-B</b>				O	2.09823800	4.48586600	0.72914200
C	0.20922400	-3.78529600	0.37456400	O	-2.16524900	2.98124600	-0.13900100
C	1.08108700	-2.58743100	0.67984400	H	-0.30131700	3.60210500	2.02888300
C	-0.81541800	-1.16450000	0.19932900	H	0.53456100	-4.64076800	0.96256600
C	-1.27688300	-3.55933000	0.56139100	H	-0.45057600	-0.08390900	-1.53137000
H	2.65441100	2.10476300	0.23387100	H	0.50896000	0.02927600	-1.51539200
C	1.29645300	3.58325100	0.65307100	<b>IM<sub>0</sub>-B</b>			
C	-0.17980800	3.72912000	0.94477800	C	-0.58418900	-3.83051500	-0.77105600
H	0.36098300	-4.02835000	-0.68588400	C	0.52924900	-2.86658100	-1.12303100
H	-2.64827100	-2.03719600	0.44776700	C	-1.02385200	-1.03572100	-0.95973100
H	-0.51697600	4.73101300	0.68830600	C	-1.98723200	-3.30959400	-0.94227400
C	-2.94910100	0.29005800	-0.40126400	H	2.99661800	1.52037200	-0.95519600
C	-3.80321100	0.37640700	0.71166500	C	1.98714100	3.30962800	-0.94226200
C	-3.54224800	0.17696500	-1.66671600	C	0.58408000	3.83062600	-0.77145400
C	-5.18937200	0.36900100	0.56678400	H	-0.45576600	-4.76203200	-1.32010400
H	-3.37926800	0.46349600	1.70845400	H	-2.99673200	-1.52034400	-0.95555100
C	-4.92788800	0.17026600	-1.82000500	H	0.45576800	4.76188900	-1.32096800
H	-2.90947100	0.10230300	-2.54502700	C	-2.36565600	0.78573000	0.36218800

C	-1.76735200	0.93091400	1.62401300	C	5.09573100	-0.98332700	1.14889500
C	-3.76456700	0.85184000	0.30090000	H	5.59678300	-1.29146900	2.06064900
C	-2.52826900	1.12865100	2.77546300	C	5.83196100	-0.79108300	-0.02008000
H	-0.68496400	0.89867300	1.71298400	H	6.90477700	-0.94998500	-0.02274900
C	-4.53661500	1.03821200	1.44826100	C	5.17734700	-0.39301400	-1.18468400
H	-4.25640400	0.78724500	-0.66523800	H	5.74084800	-0.24385200	-2.09982400
C	-3.91966100	1.17601300	2.69063500	C	3.79763700	-0.18530400	-1.17405700
H	-2.03861300	1.24260800	3.73698700	H	3.30443200	0.12231100	-2.09115700
H	-5.61736300	1.09044000	1.37090000	B	-1.47172500	0.12491200	-0.00153000
H	-4.51632500	1.32717200	3.58330600	H	-0.17355400	-4.47303600	-0.26728000
C	2.36569400	-0.78574700	0.36207700	C	-3.03375100	0.36629200	0.00924300
C	3.76459800	-0.85185300	0.30062500	C	-3.71673100	0.77436100	-1.14852200
C	1.76753600	-0.93098100	1.62396700	H	-3.16081100	0.91881300	-2.07037100
C	4.53678000	-1.03827000	1.44789000	C	-5.09522400	0.98323900	-1.15029000
H	4.25632300	-0.78722200	-0.66556700	H	-5.59591600	1.29105800	-2.06235000
C	2.52858700	-1.12876500	2.77532000	C	-5.83183500	0.79188000	0.01858800
H	0.68515900	-0.89874000	1.71306500	H	-6.90459800	0.95114500	0.02088400
C	3.91997000	-1.17612200	2.69032900	C	-5.17766700	0.39427900	1.18359900
H	5.61751900	-1.09049200	1.37040200	H	-5.74146700	0.24584600	2.09867400
H	2.03904400	-1.24275900	3.73689700	C	-3.79802000	0.18611400	1.17348800
H	4.51673700	-1.32731400	3.58292600	H	-3.30518100	-0.12113200	2.09091400
B	-1.47770700	0.50701500	-0.95857200	N	0.57887700	-1.25884300	-0.05952100
B	1.47759600	-0.50697800	-0.95856500	C	-0.78414000	-1.20412300	-0.06709600
N	0.22826200	-1.47230800	-1.00025500	C	1.05826400	-2.66429600	-0.10568700
N	-2.06238600	-1.91646300	-0.95670800	H	1.94054600	-2.73724300	-0.73993400
N	-0.22837500	1.47234800	-1.00034300	H	-1.94053500	2.73644800	0.74100600
N	2.06227400	1.91649800	-0.95657900	C	0.78413700	1.20384500	0.06697600
C	1.02373800	1.03576200	-0.95969600	N	-0.57891600	1.25849500	0.05954700
C	-0.52938300	2.86660800	-1.12314200	C	1.36591400	2.61428100	0.11238200
O	-2.97319200	-3.99780300	-1.02544300	C	-1.36592300	-2.61467300	-0.11160400
O	1.62462100	-3.23995800	-1.44027100	C	-1.05838200	2.66405500	0.10651800
O	2.97315500	3.99780300	-1.02508800	C	0.15357500	3.43766900	0.61666400
O	-1.62483000	3.23996000	-1.44015600	C	-0.15366900	-3.43825500	-0.61555500
H	0.46249800	4.06728900	0.29425100	H	-1.35105300	2.96775400	-0.90281900
H	-0.46276500	-4.06661000	0.29479700	H	0.14957500	3.44875900	1.71088500
H	-2.12608500	0.64297600	-1.96870700	H	1.35074100	-2.96756800	0.90386100
H	2.12586200	-0.64289700	-1.96878300	H	-0.14968400	-3.44963100	-1.70977800
<b>C</b>				C	2.57038200	2.75548900	1.05273300
B	1.47170100	-0.12518000	0.00144500	H	3.43245200	2.19780700	0.68468000
H	0.17365400	4.47256500	0.26872100	H	2.85619800	3.80898500	1.13926000
C	3.03372600	-0.36645000	-0.00971000	H	2.33005900	2.38199900	2.05173000
C	3.71717200	-0.77492300	1.14762400	C	1.76758900	3.05637600	-1.31347800
H	3.16157300	-0.92003300	2.06956500	H	2.56500500	2.41799000	-1.69875400
				H	0.92257200	2.99627800	-2.00531100



H	2.13031000	4.08967600	-1.30541200	C	-1.43394700	-2.54297300	0.51230500
C	-1.76741800	-3.05567200	1.31464500	C	1.43395500	2.54292000	0.51239200
H	-0.92231400	-2.99505400	2.00631700	C	1.00495000	-2.65352200	0.52800400
H	-2.56478000	-2.41694300	1.69945400	C	-0.24130300	-3.52237300	0.32992100
H	-2.13016200	-4.08897500	1.30740100	C	0.24129300	3.52234800	0.33024200
C	-2.57059600	-2.75630100	-1.05159600	H	1.84475600	-2.92309800	-0.11172900
H	-2.85661700	-3.80979800	-1.13743800	H	-0.28376600	-4.36732600	1.02017500
H	-3.43248000	-2.19823600	-0.68367800	H	-1.36270800	2.65759100	1.56247900
H	-2.33046500	-2.38345400	-2.05088500	H	0.25214000	3.91981500	-0.68853200

**TS<sub>0</sub>-C**

B	-1.38259900	0.14788800	-0.27785900
H	-0.25213200	-3.91956200	-0.68896300
C	-2.93947200	0.40608000	-0.44131500
C	-3.76198600	0.64701400	0.67263300
H	-3.32053500	0.67428100	1.66507200
C	-5.13592900	0.84590500	0.54232100
H	-5.74492200	1.02552600	1.42232900
C	-5.72803900	0.80956800	-0.72012400
H	-6.79672300	0.96049500	-0.82715500
C	-4.93404500	0.57908300	-1.84270800
H	-5.38525200	0.55180700	-2.82913000
C	-3.56006700	0.38359100	-1.69964800
H	-2.95350900	0.20171700	-2.58113500
B	1.38258500	-0.14792800	-0.27788400
H	0.28374500	4.36711600	1.02072200
C	2.93945300	-0.40609500	-0.44136700
C	3.56009300	-0.38340900	-1.69967200
H	2.95356100	-0.20144900	-2.58115900
C	4.93408500	-0.57882800	-1.84270400
H	5.38533000	-0.55140500	-2.82910400
C	5.72804400	-0.80942500	-0.72011800
H	6.79673800	-0.96029000	-0.82712600
C	5.13588600	-0.84595100	0.54230000
H	5.74485600	-1.02564900	1.42230900
C	3.76193100	-0.64713300	0.67258500
H	3.32044500	-0.67452000	1.66500700
N	-0.52802200	1.29601700	0.18910300
C	0.79157400	1.20744900	0.16355800
C	-1.00498300	2.65345900	0.52808500
H	-1.84469100	2.92311700	-0.11174800
H	1.36251300	-2.65777200	1.56245600
C	-0.79157700	-1.20746600	0.16356300
N	0.52801700	-1.29604200	0.18910900

**IM<sub>0</sub>-C**

H	-2.33035300	-3.45772100	2.27564300
H	-1.06311400	-2.27857700	2.65856500
C	-2.61643300	-2.90794100	-0.39435600
H	-3.45700400	-2.22933400	-0.24585700
H	-2.33064900	-2.86295900	-1.44835000
H	-2.95116700	-3.92632900	-0.17222400
C	1.89751900	2.49533800	1.98500500
H	1.06334300	2.27833400	2.65866100
H	2.65749900	1.72308500	2.12232200
H	2.33059800	3.45745300	2.27571600
C	2.61634900	2.90798800	-0.39435400
H	2.95100300	3.92641000	-0.17225400
H	3.45699200	2.22946000	-0.24589800
H	2.33049900	2.86297200	-1.44832900
H	-0.52552000	-0.02306100	-1.57160400
H	0.52547200	0.02319600	-1.57153200
B	1.48820700	-0.50103400	-1.04625500
H	1.12548300	3.45043900	-2.62725500
C	2.34265300	-0.88374700	0.27732900
C	1.71737700	-1.01705600	1.52773000
H	0.64016100	-0.89709200	1.59904000
C	2.43906900	-1.30295300	2.68553800
H	1.92522000	-1.39741000	3.63681200
C	3.82344500	-1.46516800	2.62078400
H	4.39162700	-1.68378400	3.51836400
C	4.46755600	-1.35308100	1.38934700
H	5.54218000	-1.49064000	1.32577300
C	3.73100900	-1.07297200	0.23707300
H	4.24527100	-1.00222300	-0.71651200
B	-1.48780000	0.50100100	-1.04607400
H	-1.26506200	-4.34427700	-1.10846300

C	-2.34274800	0.88366500	0.27715000	H	-2.14396400	0.69816400	-2.05083900
C	-3.73105600	1.07321800	0.23623800				
H	-4.24485300	1.00269100	-0.71761200	D			
C	-4.46810100	1.35340500	1.38816600	B	1.51916100	-0.07853100	0.01511300
H	-5.54266200	1.49122100	1.32407400	H	0.04968800	4.32001200	0.36339100
C	-3.82456200	1.46527300	2.61992700	C	3.08204600	-0.23122100	-0.01019100
H	-4.39313200	1.68395800	3.51724500	C	3.76669500	-1.03046000	0.92693200
C	-2.44026200	1.30275000	2.68534200	H	3.20027500	-1.54683800	1.69674300
H	-1.92684700	1.39704400	3.63686600	C	5.15390200	-1.15923600	0.91059000
C	-1.71806800	1.01676400	1.52786300	H	5.64939300	-1.77315700	1.65593500
H	-0.64091800	0.89654500	1.59970500	C	5.90837700	-0.49226000	-0.05624000
N	0.21106100	-1.40847700	-1.11803800	H	6.98831500	-0.59073100	-0.07267900
C	-1.02682900	-1.03495900	-1.05899800	C	5.25758700	0.29779600	-1.00357600
C	0.37304800	-2.87972300	-1.17721600	H	5.83267000	0.81307700	-1.76623400
H	1.14534700	-3.12466800	-1.90770700	C	3.86929500	0.42041500	-0.97899300
H	-0.71644400	3.22779200	-0.19844400	H	3.37858400	1.03020500	-1.73079200
C	1.02726000	1.03492900	-1.05895600	B	-1.51914900	0.07863900	-0.01517000
N	-0.21063700	1.40847500	-1.11751600	H	-0.04964900	-4.31990100	-0.36362200
C	1.95633000	2.24601700	-1.01296700	C	-3.08203300	0.23123000	0.01022200
C	-1.95586000	-2.24605300	-1.01299200	C	-3.76687000	1.03043200	-0.92679100
C	-0.37265700	2.87970800	-1.17630000	H	-3.20059600	1.54688800	-1.69665700
C	1.02830000	3.37093200	-1.54056000	C	-5.15408800	1.15907800	-0.91027400
C	-1.02804000	-3.37079600	-1.54117400	H	-5.64972700	1.77297900	-1.65553500
H	-1.14514400	3.12478500	-1.90655300	C	-5.90838600	0.49200000	0.05662300
H	1.26548300	4.34424300	-1.10756200	H	-6.98833100	0.59036900	0.07319200
H	0.71704800	-3.22800300	-0.19950600	C	-5.25740500	-0.29802000	1.00386200
H	-1.12556000	-3.44995000	-2.62786900	H	-5.83234900	-0.81336000	1.76658600
C	2.33707100	2.50570200	0.46482700	C	-3.86910900	-0.42050400	0.97910800
H	2.90517800	1.67274700	0.87907600	H	-3.37823800	-1.03021500	1.73086400
H	2.94859400	3.41069200	0.52663400	N	0.67556000	-1.26236700	-0.03277800
H	1.44922700	2.65211200	1.08645100	C	-0.76589100	-1.22093100	-0.06863600
C	3.22114100	2.07585300	-1.86019300	C	1.06200700	-2.56820300	-0.13344400
H	3.85922300	1.28731200	-1.45867500	C	-2.54556000	-3.14553800	-0.35425400
H	2.97358800	1.81971100	-2.89336000	H	-3.04172800	-3.26671600	0.61521800
H	3.79261000	3.00903000	-1.86443900	H	-3.18435100	-2.49677800	-0.95556800
C	-2.33614700	-2.50598700	0.46487000	H	-2.50203500	-4.12711400	-0.83630100
H	-1.44812900	-2.65242900	1.08624500	H	2.06891400	-2.92882900	-0.22055400
H	-2.90416800	-1.67309400	0.87937200	C	2.54554400	3.14567800	0.35389100
H	-2.94761300	-3.41101000	0.52672700	H	3.18486500	2.49625900	0.95390200
C	-3.22098900	-2.07571200	-1.85975500	H	3.04093600	3.26814700	-0.61583400
H	-3.79247700	-3.00887700	-1.86393400	H	2.50229700	4.12665300	0.83719800
H	-3.85889300	-1.28722300	-1.45786700	H	-2.06891900	2.92886200	0.22049400
H	-2.97378500	-1.81942800	-2.89296700	C	0.76591100	1.22102600	0.06860000
H	2.14476600	-0.69824000	-2.05072800	N	-0.67556300	1.26246300	0.03263100

C	-1.06200500	2.56832100	0.13311700	H	-2.78460500	-3.78703200	1.34179900
N	0.05746300	3.31761200	0.25308400	H	1.93344500	-3.01050700	0.48761500
N	-0.05747300	-3.31750100	-0.25331100	C	-0.80881400	-1.20124500	0.27596500
C	1.18386100	2.55419600	0.22437300	N	0.60923000	-1.31107000	0.26557900
C	-1.18387400	-2.55410100	-0.22439500	C	0.94060000	-2.60374300	0.45058400
<b>TS<sub>0</sub>-D</b>				N	-0.20470100	-3.30918600	0.58398600
B	-1.45176100	0.13729300	-0.10124300	N	0.20482800	3.30916500	0.58392300
H	-0.23961700	-4.29878000	0.77267100	C	-1.29980900	-2.48377800	0.49628700
C	-3.00998000	0.30918300	-0.27873400	C	1.29990100	2.48373300	0.49599800
C	-3.81113900	0.95007900	0.68435200	H	0.45463200	-0.00249200	-1.58768700
H	-3.34776400	1.35471600	1.57997900	H	-0.45488100	0.00251200	-1.58769900
C	-5.19532400	1.05083600	0.54222400	<b>IM<sub>0</sub>-D</b>			
H	-5.78437100	1.54518800	1.30822400	B	1.57141800	-0.08477200	-0.98482700
C	-5.82408500	0.50577300	-0.57676300	H	0.04370600	4.24880900	0.25847200
H	-6.89989400	0.58168900	-0.69187400	C	3.00106800	-0.24778500	-0.24948700
C	-5.05447100	-0.13783400	-1.54660700	C	3.11166700	-0.21784700	1.15236000
H	-5.53303500	-0.56278200	-2.42304400	H	2.21278200	-0.08006400	1.74807700
C	-3.67198100	-0.22952400	-1.39661100	C	4.33957600	-0.34527400	1.79867300
H	-3.08347100	-0.72549100	-2.16201800	H	4.39124600	-0.31413700	2.88258500
B	1.45166200	-0.13731700	-0.10163100	C	5.50766500	-0.50733300	1.05007600
H	0.23980000	4.29876800	0.77255200	H	6.46706500	-0.60303100	1.54730800
C	3.00988800	-0.30921100	-0.27896400	C	5.42851300	-0.54447500	-0.34066100
C	3.67196000	0.22869500	-1.39717300	H	6.33021000	-0.67114100	-0.93141900
H	3.08350600	0.72401800	-2.16304000	C	4.18904800	-0.41978900	-0.97441600
C	5.05449400	0.13707500	-1.54689000	H	4.13927200	-0.44868100	-2.05868600
H	5.53313500	0.56141700	-2.42357900	B	-1.57143900	0.08469800	-0.98491300
C	5.82404600	-0.50566700	-0.57643200	H	-0.04381400	-4.24891400	0.25835900
H	6.89988300	-0.58151600	-0.69132000	C	-3.00105400	0.24774600	-0.24949500
C	5.19519700	-1.04994600	0.54289100	C	-4.18903000	0.42008000	-0.97435300
H	5.78419700	-1.54362400	1.30936100	H	-4.13928700	0.44913200	-2.05862000
C	3.81097800	-0.94926500	0.68473200	C	-5.42844900	0.54488400	-0.34053100
H	3.34750700	-1.35330100	1.58057800	H	-6.33014700	0.67180800	-0.93123300
N	-0.60922200	1.31106100	0.26571000	C	-5.50755600	0.50752300	1.05020200
C	0.80883100	1.20120700	0.27580300	H	-6.46692000	0.60331300	1.54748600
C	-0.94051600	2.60374400	0.45077900	C	-4.33947000	0.34511600	1.79873000
C	2.69666900	2.99635200	0.58860500	H	-4.39110700	0.31380100	2.88263800
H	2.78498400	3.78673900	1.34143600	C	-3.11160700	0.21758100	1.15235000
H	3.37014700	2.18546800	0.86355200	H	-2.21272200	0.07952500	1.74800600
H	3.05079400	3.39882200	-0.36790600	N	0.61944800	-1.29724800	-0.56531300
H	-1.93332900	3.01056900	0.48792700	C	-0.78011700	-1.25638900	-0.57320800
C	-2.69654300	-2.99643200	0.58916400	C	1.02000200	-2.51167600	-0.22919600
H	-3.36993900	-2.18562900	0.86455400	C	-2.57283500	-3.10368800	-0.07564800
H	-3.05098200	-3.39862400	-0.36734800	H	-2.74046500	-3.48328100	0.93823000

H	-3.32551500	-2.34298300	-0.27262100	H	-3.96352100	-0.57124700	-0.70747800
H	-2.73052300	-3.93026300	-0.77723900	C	-4.45886700	1.62233800	2.43267500
H	2.04300700	-2.82983000	-0.12570900	H	-2.36415800	2.06248000	2.27621300
C	2.57275500	3.10364200	-0.07540100	C	-5.54287900	0.92719700	1.89450800
H	3.32547000	2.34293900	-0.27224300	H	-6.19412200	-0.40406700	0.33411900
H	2.73048600	3.93015800	-0.77705400	H	-4.59959800	2.25348200	3.30380800
H	2.74028600	3.48333700	0.93845500	H	-6.52568400	1.01495200	2.34406200
H	-2.04307600	2.82976900	-0.12597700	B	1.46964500	0.44941900	0.50122200
C	0.78010100	1.25632500	-0.57315900	B	-1.50285200	0.53048000	0.13689900
N	-0.61947000	1.29719500	-0.56545300	N	-0.65080000	1.77898400	-0.03488700
C	-1.02005900	2.51161900	-0.22936700	N	1.44599300	2.91164500	0.10529500
N	0.06569600	3.28042800	-0.01959300	N	0.61214500	-0.77945000	0.88203200
N	-0.06577700	-3.28049400	-0.01957200	N	-1.50291000	-1.71514800	1.26814600
C	1.21023300	2.51523700	-0.22489400	C	-0.72098100	-0.68129500	0.86859700
C	-1.21028900	-2.51531700	-0.22505300	C	1.21958100	-2.05665400	1.13365100
H	-1.68720700	0.13844600	-2.19290800	O	1.68004200	5.09871700	-0.45135600
H	1.68710900	-0.13857400	-2.19282900	O	-2.31344800	2.68023500	-1.30786600
<b>TS<sub>1</sub>O</b>				O	-1.84604000	-3.87501900	1.89782000
C	-0.33844700	3.98806400	-1.12841900	O	2.30661100	-2.33521300	0.71042600
C	-1.18921900	2.77007100	-0.82959700	H	0.55133000	-2.71716600	3.02704200
C	0.75740800	1.68038400	0.16215200	H	-0.91380500	4.88148500	-0.87737800
C	1.01538300	4.07336700	-0.46239500	H	0.88738400	0.73179700	-1.50551700
H	-2.50853200	-1.57174500	1.18624700	H	-1.59477900	-0.02041600	-1.01417600
C	-1.07584700	-2.96472400	1.72025700	C	-0.62894200	-3.89357700	-1.74642100
C	0.40634700	-3.01287700	1.97873300	C	-1.04912900	-2.58951300	-1.96659000
H	-0.18561400	4.02453500	-2.21284900	C	-0.10938600	-1.58200600	-2.23901700
H	2.37729800	2.93682500	0.50136700	C	1.25416600	-1.90526500	-2.29263100
H	0.78324200	-4.02610400	1.86018100	C	1.66710000	-3.21918900	-2.09775300
C	3.00982200	0.45014000	0.82157700	C	0.73038600	-4.21181200	-1.82331700
C	3.49566700	0.12201100	2.10023300	H	-1.35586200	-4.66043900	-1.50708300
C	3.95825100	0.85788800	-0.13167800	H	-2.09959200	-2.33869600	-1.88450200
C	4.85141500	0.18274700	2.40899800	H	1.98668000	-1.13419400	-2.49396100
H	2.79731800	-0.18109900	2.87602900	H	2.72227600	-3.45796000	-2.13308000
C	5.31875100	0.92706900	0.16799200	H	1.05648700	-5.23155600	-1.65472800
H	3.62469700	1.12805600	-1.12934400	C	-0.52728800	-0.20000600	-2.54508800
C	5.77182300	0.58510200	1.44041000	O	0.29267000	0.77773400	-2.38373600
H	5.19212100	-0.07586800	3.40606700	C	-1.66909600	0.08427800	-3.46729000
H	6.02383000	1.24660400	-0.59198000	H	-1.26944700	0.07204900	-4.48934200
H	6.82865200	0.63553900	1.67758000	H	-2.44444400	-0.67650400	-3.39955300
C	-2.98266300	0.71024100	0.71920900	H	-2.07872000	1.06953700	-3.24808300
C	-4.08743300	0.02603800	0.19246400	<b>TS<sub>2</sub>O</b>			
C	-3.19733800	1.50963100	1.85288000	C	-2.82531300	2.13578500	2.04974300
C	-5.35476100	0.12808300	0.76907900	C	-1.48672100	2.25829800	1.36569700

C	-1.43027000	-0.14896200	1.07686100	H	-1.20136800	-2.42671200	0.85933100
C	-3.17676100	0.75874100	2.56307800	H	1.11416700	0.82955700	1.04644200
H	2.08298200	0.90838700	-1.87991800	C	4.31810300	-1.67392000	0.97068400
C	2.48962800	-1.08289000	-2.26061000	C	3.41740600	-0.64443500	1.23304400
C	2.04379000	-2.44410600	-1.80902600	C	2.15774900	-0.91790600	1.77969100
H	-2.88775300	2.86359300	2.85600200	C	1.80370100	-2.24467800	2.03497600
H	-2.77158300	-1.20083200	2.17725400	C	2.70194300	-3.27804500	1.77167100
H	2.72404700	-2.73463400	-0.99578000	C	3.96339800	-2.99670900	1.24595600
C	-2.47948400	-1.50877700	-0.89152000	H	5.29070200	-1.44705800	0.54889900
C	-2.60227700	-0.59359300	-1.94868100	H	3.70056500	0.37873200	1.00889100
C	-3.50426400	-2.45428300	-0.74323000	H	0.81996300	-2.44812500	2.43772100
C	-3.69416600	-0.61214900	-2.81584200	H	2.41487800	-4.30340100	1.97546100
H	-1.83004000	0.15506100	-2.10978100	H	4.66401700	-3.79999200	1.04761300
C	-4.60386800	-2.48177200	-1.60020200	C	1.17698100	0.19980600	2.12058800
H	-3.42907800	-3.19323700	0.04833600	C	1.75308400	1.28058500	3.05048100
C	-4.70338600	-1.55834600	-2.64041400	H	1.05002800	2.11080400	3.11540700
H	-3.75813100	0.10631600	-3.62659500	H	1.88042300	0.83984500	4.04219600
H	-5.37934400	-3.22795800	-1.46254500	H	2.71988300	1.65519400	2.70936600
H	-5.55499400	-1.57961000	-3.31151900	O	-0.04742700	-0.17346600	2.45236500
C	0.70581800	2.51932100	-0.80038000				
C	1.99558700	3.02004500	-0.56902800	<b>IM<sub>1</sub>O</b>			
C	-0.10582800	3.19910200	-1.72376800	C	-2.34064400	-0.85879200	3.04741800
C	2.45600800	4.16263300	-1.22254700	C	-2.22506800	0.25973100	2.03700200
H	2.64062200	2.52875400	0.15260700	C	-0.57288100	-1.28044700	0.94837400
C	0.35005500	4.33876200	-2.38080400	C	-2.32102000	-2.24155200	2.41367300
H	-1.10950900	2.83716100	-1.92501300	H	0.75414900	2.79356900	-1.05341900
C	1.63362900	4.82436600	-2.13166100	C	2.27110700	1.83837900	-2.08581600
H	3.45218900	4.53810300	-1.01693800	C	2.80107800	0.45360000	-2.33136000
H	-0.29598800	4.84972500	-3.08607200	H	-1.47822200	-0.80100200	3.71891200
H	1.98833600	5.71307000	-2.64098700	H	-1.43934900	-3.19669100	0.85370200
B	-1.24214200	-1.46143700	0.14788300	H	3.64761600	0.31445100	-1.64478200
B	0.17630500	1.18148300	-0.16324200	C	-1.26399600	-1.92245700	-1.60036700
N	-1.07521600	1.11246500	0.60570600	C	-1.98543900	-0.90011500	-2.23377300
N	-2.51963700	-0.25908300	1.90482800	C	-1.66845500	-3.23874700	-1.87615600
N	0.11935600	-1.34008900	-0.65172800	C	-3.07238000	-1.16259800	-3.06769000
N	1.75893500	-0.03538700	-1.68474400	H	-1.70000800	0.14125700	-2.09790100
C	0.66792100	-0.16382700	-0.88766000	C	-2.75482000	-3.51895200	-2.70305700
C	0.64747600	-2.53700400	-1.23535500	H	-1.10944300	-4.06371800	-1.44379600
O	-4.00780200	0.55399300	3.41667800	C	-3.46614500	-2.47887700	-3.30013500
O	-0.82679000	3.26222900	1.42206100	H	-3.60632300	-0.34377800	-3.53879400
O	3.40759100	-0.86188100	-3.00920100	H	-3.04190400	-4.54852400	-2.88875300
O	0.02757400	-3.56298400	-1.20936900	H	-4.30933900	-2.69176200	-3.94778600
H	2.16694800	-3.17146400	-2.60970900	C	-1.35232700	2.55537900	0.13299000
H	-3.59163900	2.39377300	1.30696400	C	-0.64853700	3.62583300	0.70974300

C	-2.53376400	2.84043500	-0.56987100	C	0.42284100	-2.19530200	2.61844400
C	-1.11872400	4.93541900	0.60434100	C	0.00860000	-0.73674200	2.57707100
H	0.25964300	3.43917500	1.27709700	C	-0.51690500	-1.07601700	0.15873800
C	-2.99408500	4.14731700	-0.69045300	C	-0.15930100	-3.10102200	1.55553300
H	-3.10673900	2.03063100	-1.00815100	H	0.21981900	3.42183400	-0.09689600
C	-2.28936500	5.19838000	-0.10195400	C	-1.33631100	3.78001900	-1.42205500
H	-0.57139000	5.74496100	1.07386800	C	-2.54718000	3.06659400	-1.96703100
H	-3.91037600	4.34688600	-1.23448400	H	1.51272600	-2.19864900	2.48893000
H	-2.65421300	6.21523100	-0.19061300	H	-1.06319900	-3.02720200	-0.25414700
B	-0.04999300	-1.65578500	-0.56661300	H	-2.81991000	3.47064900	-2.94021600
B	-0.79317900	1.09844000	0.18513900	C	-3.16923800	-0.99619900	-0.21386400
N	-1.24740800	0.04932600	1.00781900	C	-3.64082800	-0.36735400	0.95104300
N	-1.50061000	-2.30762600	1.32843200	C	-3.99339500	-1.97143300	-0.79372300
N	0.81490200	-0.43527000	-1.08904400	C	-4.87210400	-0.69839900	1.51493900
N	1.13708700	1.87398600	-1.25952600	H	-3.02665000	0.38386400	1.43888300
C	0.46844100	0.79428000	-0.77659800	C	-5.22453900	-2.31569700	-0.23509900
C	1.85074600	-0.68901500	-2.05672600	H	-3.66993700	-2.45917300	-1.70816300
O	-2.99161200	-3.16820500	2.82149700	C	-5.66815300	-1.67895400	0.92283500
O	-2.90082500	1.25557300	2.08804300	H	-5.20770400	-0.19925700	2.41810900
O	2.75571300	2.85485200	-2.51351400	H	-5.83998100	-3.07521000	-0.70571800
O	1.95899300	-1.76204300	-2.57536100	H	-6.62503700	-1.94300200	1.35973700
H	3.19371100	0.37477300	-3.34417500	C	1.41940800	1.81709100	1.27104700
H	-3.25411700	-0.72667000	3.62135900	C	2.54205000	2.06701000	0.45939100
H	0.66258500	-2.61406300	-0.46699400	C	1.35608900	2.45936100	2.52037300
H	0.98877200	0.68996300	1.86900800	C	3.56988100	2.90580000	0.88287800
C	4.81061800	0.40295300	0.61880600	H	2.62700300	1.57842200	-0.50375800
C	3.57014300	0.58265100	1.22790100	C	2.37885200	3.30975100	2.93916400
C	2.70301800	-0.49951300	1.41972100	H	0.51465000	2.27278800	3.17367900
C	3.08836300	-1.76405100	0.97447700	C	3.48783400	3.53287400	2.12564000
C	4.31908400	-1.94288600	0.34344700	H	4.43246300	3.06598500	0.24586900
C	5.18751600	-0.86519300	0.17097400	H	2.31132800	3.79041600	3.90865200
H	5.47643100	1.24863500	0.48663600	H	4.28459800	4.18896300	2.45776300
H	3.27965900	1.57190500	1.57038900	B	-1.73398900	-0.64671300	-0.84195800
H	2.41052700	-2.59594700	1.10988400	B	0.25054900	0.93681800	0.71206000
H	4.59908800	-2.92712100	-0.01389500	N	-0.39206600	-0.23125500	1.34199300
H	6.14790900	-1.00965300	-0.31058800	N	-0.52225900	-2.46360400	0.38935900
C	1.40520400	-0.27924000	2.18179300	N	-1.60536300	0.93646200	-1.05924100
C	1.67398000	-0.20442400	3.68943200	N	-0.55465300	2.97316100	-0.57950600
H	0.75593400	0.04830300	4.22421200	C	-0.70610900	1.63748700	-0.39767800
H	2.03107200	-1.17376900	4.04323400	C	-2.44145800	1.55465800	-2.04125800
H	2.43209200	0.54915400	3.91268700	O	-0.30538600	-4.29388100	1.71227500
O	0.43778400	-1.30734900	2.01182800	O	0.06331400	-0.03448700	3.56348000
				O	-1.05177300	4.93068600	-1.62778500
				O	-3.04428800	0.90321200	-2.84649500

TS<sub>3</sub>O

H	-3.37589000	3.28491400	-1.27895600	C	1.49769000	0.33732100	1.70528700
H	0.21184000	-2.61393100	3.60079800	C	2.88737200	0.49791700	1.76851500
H	-1.55338300	-1.18210800	-1.90817500	C	0.79169100	0.41354000	2.91936700
H	0.68409200	-1.88293700	-1.97065200	C	3.54281700	0.72064700	2.97999000
C	4.61766600	-2.80899100	-2.44559800	H	3.47712000	0.42116400	0.86523500
C	3.31599400	-2.32718200	-2.55121400	C	1.43415800	0.62854600	4.13697100
C	2.74907800	-1.56753600	-1.52170600	H	-0.29054700	0.29748700	2.91496700
C	3.50814800	-1.30604100	-0.37999800	C	2.81970000	0.78565700	4.16914900
C	4.81419000	-1.78574200	-0.27450000	H	4.62145200	0.83440000	2.99426600
C	5.37374100	-2.53656000	-1.30507800	H	0.85932300	0.67644000	5.05581500
H	5.03937400	-3.40200800	-3.24934200	H	3.32856800	0.95616900	5.11135800
H	2.73253600	-2.55314200	-3.43857800	B	-2.06216300	-0.20310500	-1.03862300
H	3.07642600	-0.73093000	0.42763500	B	0.66965300	0.08853100	0.33571000
H	5.39151000	-1.57326100	0.61853600	N	-0.20509900	-1.26163600	0.47817600
H	6.38688700	-2.91249800	-1.22004100	N	-2.04009800	-2.55142000	-0.17450900
C	1.33020500	-1.04707800	-1.68521400	N	-1.51834900	1.21058300	-0.58189700
C	1.21971000	0.04565900	-2.74987300	N	-0.09188200	2.53227100	0.70052200
H	0.17518900	0.30056900	-2.92904100	C	-0.43995800	1.33151200	0.17685800
H	1.76646500	0.93939500	-2.43972900	C	-2.19655300	2.37078500	-1.07561500
H	1.65303200	-0.30026600	-3.68994800	O	-2.30889800	-4.75270100	0.33382400
O	0.84647600	-0.57533700	-0.41187300	O	1.62029300	-2.48223200	1.17357100
<b>IM<sub>2</sub>O</b>				O	-0.29057400	4.78631900	0.93000700
C	-0.48783700	-3.56894100	1.38024300	O	-2.86011700	2.32818200	-2.07350200
C	0.43282100	-2.42661100	1.00767200	H	-2.84353400	3.57827100	0.52122200
C	-1.36736800	-1.36950700	-0.16035900	H	-0.88112300	-3.34708200	2.38173000
C	-1.68016200	-3.73490700	0.47480500	H	-1.74053300	-0.44133900	-2.17869200
H	0.75890700	2.55146700	1.25699400	H	1.77064800	0.63663000	-2.75083100
C	-0.74494200	3.75384900	0.50748300	C	5.75547400	-0.22935100	-2.88995000
C	-2.04969200	3.62302500	-0.23715700	C	4.52798400	0.41302900	-2.75345600
H	0.07604100	-4.49734000	1.44436400	C	3.56040100	-0.06636000	-1.86115800
H	-2.91991900	-2.56571800	-0.68307800	C	3.84096500	-1.21949800	-1.12628600
H	-2.23095700	4.50817600	-0.84444100	C	5.07300300	-1.86183400	-1.25903100
C	-3.66171100	-0.26272100	-0.82327200	C	6.03579500	-1.36987100	-2.13647500
C	-4.23244100	0.02331000	0.42875700	H	6.49140900	0.15784500	-3.58620900
C	-4.53175400	-0.63630800	-1.85600000	H	4.32175900	1.29014800	-3.35877600
C	-5.60738600	-0.05132200	0.64225600	H	3.09544100	-1.61075700	-0.44862500
H	-3.58775100	0.30854300	1.25786700	H	5.27448700	-2.75225200	-0.67339200
C	-5.91021200	-0.72356900	-1.65192200	H	6.99166000	-1.87121400	-2.23986700
H	-4.12287300	-0.84144300	-2.83988500	C	2.21379500	0.64919000	-1.74550300
C	-6.45199500	-0.42913200	-0.40240900	C	2.36973200	2.12400600	-1.34889400
H	-6.02113600	0.17710700	1.61892500	H	1.41959200	2.65175900	-1.44568300
H	-6.56126800	-1.01130200	-2.47042400	H	2.73609400	2.23089400	-0.32711000
H	-7.52259400	-0.49192400	-0.24234700	H	3.08244700	2.61730600	-2.01087600
				O	1.31923300	-0.09626200	-0.93679800

**TS<sub>4</sub>O**

C	-0.31293900	4.26751700	-1.03474500
C	0.76711700	3.20985800	-0.85340500
C	-1.06904000	1.66550000	-0.33520500
C	-1.58110900	4.07640500	-0.22923500
H	2.56338100	-1.22740500	-1.11057800
C	1.35100800	-2.54365900	-2.13409400
C	-0.07996000	-2.65182700	-2.58131100
H	0.11593500	5.24393800	-0.81859100
H	-2.79461600	2.57586700	0.39917500
H	-0.37354200	-3.69568700	-2.66843000
C	-3.13488100	0.03006000	-0.15512600
C	-4.13132800	-0.11505000	-1.13555400
C	-3.55774700	0.05695400	1.18422500
C	-5.47376100	-0.24571700	-0.79616600
H	-3.85053900	-0.13411700	-2.18255700
C	-4.90279000	-0.07467700	1.53581000
H	-2.82663200	0.19505900	1.97510700
C	-5.86591400	-0.22982600	0.54377700
H	-6.21857900	-0.35695800	-1.57669200
H	-5.19364100	-0.05134500	2.58047400
H	-6.91257200	-0.33059100	0.80819700
C	2.75578000	0.99227800	0.10189900
C	3.34909700	1.37209700	1.31455600
C	3.60799700	0.86104100	-1.00822900
C	4.72349500	1.57278200	1.42808300
H	2.72188500	1.55679200	2.17884000
C	4.98381900	1.05265500	-0.90525200
H	3.19037800	0.66919700	-1.99198100
C	5.54993000	1.39857800	0.32008200
H	5.14786200	1.87594700	2.37920700
H	5.61009000	0.95269800	-1.78494000
H	6.61992300	1.55176100	0.40488200
B	-1.62671000	0.31464000	-0.51084900
B	1.17824500	0.77998000	0.00254100
N	0.31595900	1.93914800	-0.54041100
N	-1.85858700	2.76970200	0.06643900
N	-0.63226900	-0.71866400	-1.08602000
N	1.59859800	-1.38554100	-1.39204200
C	0.68533500	-0.52465700	-0.89936100
C	-1.09578400	-1.91282700	-1.73376500
O	-2.31652500	4.99477400	0.08724300

O	1.93969000	3.48989100	-1.01035800
O	2.22788800	-3.32653200	-2.39659600
O	-2.23220700	-2.28559900	-1.65133200
H	-0.13122600	-2.21097600	-3.58645200
H	-0.60364000	4.26820500	-2.09321700
H	-0.66008800	0.73949000	0.91353600
H	1.84718000	-0.30065300	2.64606200
C	1.75570700	-3.90080800	1.06555900
C	1.83192800	-2.61742800	1.60319900
C	0.67408500	-1.86801100	1.83500100
C	-0.56930700	-2.43362100	1.53399100
C	-0.64962700	-3.71310100	0.98976300
C	0.51302500	-4.44845300	0.75208100
H	2.66208400	-4.46334500	0.87530400
H	2.80092600	-2.18309000	1.82758400
H	-1.48186900	-1.87046700	1.68941400
H	-1.61934600	-4.12781500	0.74079500
H	0.45036000	-5.44256900	0.32426600
C	0.80178800	-0.45923100	2.37806700
C	-0.07165600	-0.17332200	3.59175500
H	0.08142800	0.85409400	3.92677600
H	-1.13026000	-0.30882300	3.36205600
H	0.18716600	-0.85612600	4.40368500
O	0.49974900	0.56624800	1.38672700

**TS<sub>5</sub>O**

C	-1.04138200	-2.81848600	1.70015200
C	0.34967700	-2.26364700	1.44875800
C	-0.80185700	-0.40853500	0.28148400
C	-2.14654500	-1.79622200	1.83111600
H	3.51024300	0.21035600	-1.56175800
C	3.07281400	2.12511400	-2.22053400
C	2.03500100	3.19378500	-1.98784200
H	-1.28463600	-3.45180700	0.83827000
H	-2.61570300	0.06818400	1.17956000
H	1.98475300	3.86944800	-2.83942200
C	-0.35063300	1.95496100	1.47377000
C	0.89015500	1.90728700	2.12797800
C	-1.37575600	2.67258300	2.10907600
C	1.10034100	2.52804300	3.35864500
H	1.72007600	1.36683000	1.68054100
C	-1.18210500	3.29363600	3.34274100
H	-2.34348000	2.75181200	1.62284800
C	0.05911400	3.22256300	3.97330100



H	2.07106800	2.46717200	3.83973700	H	-2.06293300	-2.48643200	-3.10667200
H	-1.99672100	3.83758900	3.80914300	H	-2.40819000	-1.06874600	-4.11044600
H	0.21540200	3.70652900	4.93108200	O	-1.07648500	-1.16694600	-1.04890900
C	2.99453300	-1.50004600	-0.02656500	H	0.24609800	-1.41508300	-1.47585800
C	3.62105700	-2.29928800	-0.99265100	H	1.15055900	-1.52139500	-1.58818200
C	3.73826900	-1.14745600	1.11356400				
C	4.93593200	-2.74135200	-0.82713800				
H	3.07434700	-2.60085600	-1.88097000	<b>TS<sub>6</sub>O</b>			
C	5.04918400	-1.57858700	1.27985700	C	-1.09266800	3.42851200	-0.86278100
H	3.27327800	-0.55243800	1.89214500	C	-1.21989600	2.04398300	-0.26424100
C	5.65382200	-2.37855000	0.30784900	C	1.02458400	1.55363000	-0.96443000
H	5.39252300	-3.37024700	-1.58326100	C	0.31292300	3.91559200	-1.08866000
H	5.59854200	-1.30163700	2.17276200	H	-0.18312900	-2.99727100	-0.22860300
H	6.67444100	-2.71930900	0.44016100	C	1.44057600	-3.66886400	-1.26199600
B	-0.63610400	1.20305100	0.07621900	C	2.54363200	-3.11602400	-2.12717400
B	1.56447700	-0.85294200	-0.22148800	H	-1.57825000	3.38930800	-1.84726200
N	0.42497500	-1.08160400	0.69238400	H	2.18757700	3.13846300	-1.42844100
N	-1.88812900	-0.63343100	1.16156900	H	2.16077500	-3.08123700	-3.15676600
N	0.60890800	1.46060700	-0.88929100	C	3.32853700	1.01372300	0.10060500
N	2.78392000	0.92358500	-1.56113000	C	2.85087700	1.23116900	1.40341400
C	1.63314600	0.62896600	-0.90200700	C	4.71510900	1.10316000	-0.10049200
C	0.65248400	2.68505400	-1.63751300	C	3.71322900	1.51100000	2.46337900
O	-3.16187400	-1.98499800	2.47039300	H	1.78703800	1.17317200	1.61140600
O	1.33003600	-2.84286600	1.85913900	C	5.58472300	1.38115400	0.95319400
O	4.07968700	2.26341700	-2.86523200	H	5.11187100	0.92365400	-1.09232300
O	-0.34916700	3.27342500	-1.93374000	C	5.08675400	1.58597600	2.24009100
H	2.37597900	3.77729700	-1.12090500	H	3.31228400	1.66868600	3.45916200
H	-1.02002000	-3.45239400	2.58390600	H	6.65293300	1.43498400	0.77056800
H	-1.62525000	1.62655700	-0.44510600	H	5.76279300	1.80282900	3.06013900
H	-1.61878000	0.42751600	-2.26608200	C	-0.47910200	-0.78692900	1.33497500
C	-5.42488300	0.68073800	-1.15638500	C	-1.60289200	-0.56250400	2.14858600
C	-4.10540000	0.64006900	-1.60830100	C	0.66337700	-1.31240600	1.96519200
C	-3.38302500	-0.55323300	-1.57027600	C	-1.59573000	-0.86920400	3.50729000
C	-3.99466800	-1.70609900	-1.06943100	H	-2.49043900	-0.12546200	1.71869100
C	-5.30498500	-1.66527800	-0.60579700	C	0.68308400	-1.61203900	3.32656700
C	-6.02483300	-0.47041300	-0.65080800	H	1.57072900	-1.47985600	1.39782800
H	-5.97590300	1.61399200	-1.18626800	C	-0.45197500	-1.39851700	4.10379300
H	-3.62917700	1.54376000	-1.97330700	H	-2.48401000	-0.68521700	4.10246600
H	-3.42992800	-2.62985600	-1.01232000	H	1.58670800	-2.00969800	3.77497900
H	-5.75871000	-2.55852400	-0.19297700	H	-0.44411800	-1.63520400	5.16209800
H	-7.04386000	-0.43671300	-0.28274800	B	2.34582100	0.66409000	-1.14838200
C	-1.95244200	-0.59199200	-2.06185800	B	-0.43148000	-0.42932200	-0.23117000
C	-1.77452000	-1.45282800	-3.30853900	N	-0.16499600	1.12256000	-0.53583300
H	-0.73615700	-1.43722100	-3.65133900	N	1.23390300	2.87578800	-1.20044400
				N	1.99226700	-0.85763800	-1.26439000

N	0.58551800	-2.68980900	-0.80702700	C	-3.35959900	-1.88589400	-0.80275900
C	0.72181400	-1.31550500	-1.03821700	C	-4.44966500	0.07388100	-2.45170200
C	2.97993600	-1.70257300	-1.77543300	H	-2.64983600	1.17543000	-2.07477600
O	0.63479700	5.07029800	-1.21252200	C	-4.62004100	-2.07098200	-1.36658000
O	-2.18806500	1.72469900	0.37036100	H	-2.93514000	-2.66538200	-0.18130100
O	1.28487100	-4.84120500	-0.99560900	C	-5.16879100	-1.09130300	-2.19466100
O	4.11024200	-1.32242600	-1.98377500	H	-4.86835100	0.84262400	-3.09220300
H	3.40402700	-3.78103300	-2.11615400	H	-5.17407700	-2.98134400	-1.16433900
H	-1.65104600	4.14043800	-0.25747600	H	-6.14964800	-1.23525100	-2.63420700
H	2.84089400	1.03261000	-2.18997600	C	1.43635600	2.42163100	-0.84075800
H	-3.11775800	-1.70602800	-2.08196500	C	2.44124700	3.38064800	-0.64865000
C	-5.74548100	0.22295600	0.94446000	C	0.48888600	2.66997500	-1.84819800
C	-4.74297800	-0.68084700	0.59100700	C	2.49702100	4.53925300	-1.42450800
C	-4.02651100	-0.51556300	-0.59398400	H	3.17493300	3.22184200	0.13438100
C	-4.34869900	0.55790000	-1.43145100	C	0.53626100	3.82312700	-2.62974600
C	-5.34660800	1.46020400	-1.08395100	H	-0.30791400	1.95160500	-2.02415500
C	-6.04692800	1.29676400	0.11197700	C	1.54533500	4.76303400	-2.41881400
H	-6.28902100	0.08530200	1.87233200	H	3.27992000	5.27001400	-1.25014000
H	-4.52283600	-1.50830100	1.25349000	H	-0.20911500	3.99021100	-3.40050700
H	-3.80082200	0.68835900	-2.35946100	H	1.58769900	5.66278300	-3.02291400
H	-5.58185300	2.28839300	-1.74307600	B	-1.21628500	-0.42104400	-0.35702800
H	-6.82512800	1.99902000	0.38828600	B	1.35706000	1.09740500	0.09053700
C	-2.92515200	-1.46022700	-1.03293700	N	0.12458000	1.16734600	1.06712500
C	-2.81183800	-2.77031700	-0.26573800	N	-2.23933800	1.22932600	1.20046800
H	-3.78314500	-3.26983500	-0.26337400	N	0.08843200	-0.85819000	-1.06595800
H	-2.10952400	-3.43978000	-0.76554200	N	2.36868800	-0.55600800	-1.48760900
H	-2.49635900	-2.62027400	0.76624600	C	1.22226800	-0.17341500	-0.87256500
O	-1.65026200	-0.73179400	-1.12355200	C	0.12800500	-2.10766500	-1.75688100
H	-0.92358600	-1.00360300	-2.08251400	O	-3.39245400	2.33049600	2.81186000
H	-0.00400700	-1.15433900	-2.43061400	O	1.35357500	2.28455900	2.63622200
				O	3.61885000	-1.96000700	-2.76913600
				O	-0.66194000	-2.98107600	-1.51811100
				H	0.88755100	-1.69887700	-3.68727200
				H	-0.95729800	3.43432100	3.07824700
				H	-1.11189400	-1.22624900	1.02590300
				H	2.37859800	0.93756800	0.70304800
				C	3.81229200	-1.58374400	1.95791700
				C	2.60510700	-1.20643000	2.53872500
				C	1.41070800	-1.83976200	2.16195600
				C	1.45230700	-2.87205500	1.20472500
				C	2.65973400	-3.24361900	0.63041300
				C	3.84420200	-2.59919400	1.00314800
				H	4.72661200	-1.07664100	2.24318100
				H	2.57639200	-0.38952700	3.25117000
<b>TS,N</b>							
C	-0.99510600	2.34743600	2.96483100				
C	0.26623800	1.92621900	2.22633200				
C	-1.08745300	0.72036000	0.60985800				
C	-2.32367900	1.98555200	2.34533700				
H	3.20937200	-0.06298900	-1.20757100				
C	2.53253700	-1.61652500	-2.37610100				
C	1.22178900	-2.23922500	-2.79104500				
H	-0.96206700	1.94734100	3.98151300				
H	-3.12244400	0.95182100	0.78766700				
H	1.36416200	-3.28391000	-3.05795900				
C	-2.61405100	-0.71961200	-1.04159700				
C	-3.19090200	0.25452100	-1.87691700				

H	0.53326000	-3.37407500	0.92861600	B	-1.28517500	-0.58898700	-0.11364400
H	2.68728200	-4.04448500	-0.10029200	B	0.87731200	1.44966700	-0.32087000
H	4.78385700	-2.89003400	0.54788300	N	-0.08034900	1.33271200	0.92868800
C	0.15012300	-1.42825300	2.75654900	N	-2.36881600	0.99969900	1.50551400
N	-0.99327900	-1.70370100	2.19545800	N	0.02654500	-0.92772200	-0.82738600
C	-2.23132500	-1.42819800	2.92321300	N	2.13147100	-0.30776700	-1.64208600
H	0.18326100	-0.86190400	3.69071800	C	0.98681600	-0.00131000	-0.98154900
H	-3.04100500	-1.28711100	2.20844100	C	0.36539500	-2.29028200	-1.09105600
H	-2.47113800	-2.29246400	3.54668400	O	-3.42173200	2.15528900	3.15192900
H	-2.16349900	-0.53887300	3.56044000	O	1.14718900	2.83609400	2.14695200
				O	3.50183200	-1.70314700	-2.81100800
				O	-0.02871600	-3.17986900	-0.37684900
<b>IM<sub>1</sub>N</b>				H	0.71377000	-2.33283700	-3.17805800
C	-1.03408800	2.39231100	2.97241000	H	-1.12648000	3.45979000	3.18082000
C	0.11066500	2.20923500	1.98396200	H	0.08785400	-2.26667300	1.57615100
C	-1.24793000	0.60034400	0.76453900	H	1.99194400	1.73291600	0.02592900
C	-2.39119800	1.86220700	2.56597100	C	4.54222100	0.00350400	1.19797300
H	2.86141200	0.39584700	-1.61626300	C	3.31361900	0.12175600	1.83504400
C	2.43750300	-1.50567700	-2.28205200	C	2.40311000	-0.95597500	1.82991700
C	1.29093200	-2.49910500	-2.25890500	C	2.77919000	-2.15944800	1.18922900
H	-0.75220900	1.93246500	3.92695900	C	4.01262100	-2.26632000	0.56335500
H	-3.26650900	0.61986600	1.23382200	C	4.89928400	-1.18550100	0.55871000
H	1.67514400	-3.51630800	-2.26962400	H	5.22279400	0.84716300	1.19443500
C	-2.55000900	-1.40359700	-0.53898300	H	3.02347100	1.06050000	2.29343400
C	-2.70286400	-1.81117700	-1.88063400	H	2.11924600	-3.01899300	1.20594800
C	-3.60265200	-1.73442200	0.33697400	H	4.29111800	-3.19510400	0.07910400
C	-3.82645000	-2.50277200	-2.32113200	H	5.85676800	-1.27292400	0.05960700
H	-1.93319300	-1.56013200	-2.60554100	C	1.13687200	-0.79020200	2.49201200
C	-4.73276000	-2.42637200	-0.09472700	N	0.06960000	-1.54415500	2.29017500
H	-3.53872900	-1.46831300	1.38645800	C	-1.07248500	-1.58020600	3.19829800
C	-4.85103500	-2.81556000	-1.42734800	H	1.02874700	0.00706200	3.21637100
H	-3.90939800	-2.79189900	-3.36341900	H	-0.81926400	-2.12997700	4.10982500
H	-5.51977800	-2.66524200	0.61240900	H	-1.38024000	-0.56870500	3.46164900
H	-5.72884700	-3.35390800	-1.76595400	H	-1.89887500	-2.07343500	2.69297600
C	0.33457700	2.51480800	-1.41288100				
C	0.94392800	3.77402200	-1.52757200				
C	-0.75952100	2.24890900	-2.25429300	<b>TS<sub>2</sub>N</b>			
C	0.47998700	4.72820200	-2.43351900	C	-0.29328000	4.10134800	0.34101500
H	1.78454800	4.01003300	-0.88358200	C	0.67638500	2.94249800	0.41635400
C	-1.22889100	3.19490900	-3.16492900	C	-1.15105100	1.40938700	-0.10833500
H	-1.27073300	1.29260800	-2.18859000	C	-1.74234200	3.73623900	0.56423300
C	-0.60800100	4.44036700	-3.25685200	H	2.54438900	-1.49885700	-0.89283400
H	0.96540400	5.69671800	-2.49572500	C	1.29797700	-3.00929300	-1.48358300
H	-2.07884900	2.96357200	-3.79867200	C	-0.16530700	-3.21199000	-1.80796700
H	-0.97056700	5.18032800	-3.96220000	H	0.00794100	4.87228600	1.04908600

H	-3.02212800	2.20103000	0.28172900	C	-0.12053100	-3.28326800	2.02402000
H	-0.43657300	-4.26037200	-1.71065400	C	1.00944500	-4.09642200	2.09598400
C	-3.20920500	-0.17377800	-0.72920500	H	3.14053700	-4.15266000	2.41413500
C	-3.72117200	-0.46783600	-2.00508300	H	3.34072000	-1.71940700	2.76205800
C	-4.13576100	-0.07732300	0.32289600	H	-0.89619600	-1.29343300	2.08511700
C	-5.08290000	-0.66406600	-2.22019400	H	-1.08953500	-3.71121000	1.79891700
H	-3.04075300	-0.53783800	-2.84945000	H	0.92252600	-5.16443600	1.93543200
C	-5.50230100	-0.26494500	0.11676200	C	1.42781700	0.11007600	2.64806200
H	-3.78145500	0.12869700	1.32939300	N	0.45499200	0.98244500	2.91012300
C	-5.98096600	-0.56142700	-1.15764300	C	0.69211600	2.28754100	3.52043700
H	-5.44674000	-0.88913200	-3.21715900	H	2.42043700	0.44517400	2.92879600
H	-6.19110200	-0.18613500	0.95104400	H	-0.18523200	2.91477700	3.36547200
H	-7.04234400	-0.70940100	-1.32264300	H	0.87215500	2.18519500	4.59481300
C	2.52961700	1.05490900	-1.14412500	H	1.54508800	2.76921000	3.03940300
C	3.85834500	0.79808400	-0.78299200				
C	2.30077300	1.63227400	-2.40279900				
C	4.91909100	1.10212500	-1.63742200	<b>TS<sub>3</sub>N</b>			
H	4.07104100	0.38117900	0.19779600	C	-3.42982000	1.44730600	1.14028700
C	3.35306700	1.95042800	-3.25933200	C	-1.99113100	1.91766500	1.08282900
H	1.28121700	1.84413300	-2.71353100	C	-1.21329700	-0.42949000	1.14593200
C	4.66848400	1.68102500	-2.88007900	C	-3.66798700	0.00057900	1.50290500
H	5.93955100	0.90033200	-1.32911800	H	2.44869000	1.52349600	-1.14957800
H	3.14948300	2.40472800	-4.22344400	C	3.04331900	-0.27299800	-1.97919900
H	5.48963900	1.92499900	-3.54490200	C	2.46976300	-1.62713300	-2.29026500
B	-1.67421900	0.09391300	-0.51518200	H	-3.99445700	2.09006900	1.81478200
B	1.28225200	0.63223500	-0.22254600	H	-2.72783500	-1.77372800	1.59900400
N	0.21085500	1.69266400	0.02029100	H	3.24941800	-2.38561300	-2.23304400
N	-2.03841300	2.43974600	0.26096700	C	-1.92420100	-1.49934000	-1.16692600
N	-0.65989600	-0.98553000	-0.79490600	C	-2.10573500	-0.41176900	-2.03651700
N	1.56438300	-1.73964600	-1.00155200	C	-2.80972200	-2.57756800	-1.30726800
C	0.66406000	-0.74794700	-0.71563100	C	-3.12878300	-0.38752500	-2.98434700
C	-1.08985300	-2.35935200	-0.97653300	H	-1.43796800	0.44259000	-1.97456800
O	-2.57920500	4.53262800	0.96418600	C	-3.83819800	-2.56704300	-2.24902700
O	1.83225500	3.11145800	0.77858700	H	-2.68444400	-3.44695800	-0.66903500
O	2.16274200	-3.83569300	-1.66044600	C	-4.00431600	-1.46769000	-3.09007900
O	-2.09771200	-2.77305800	-0.47910500	H	-3.24367600	0.47054500	-3.63898000
H	-0.29600100	-2.91476500	-2.85731900	H	-4.50893000	-3.41607200	-2.32840500
H	-0.21011200	4.53890300	-0.66292000	H	-4.80361900	-1.45448200	-3.82288200
H	-0.49937600	0.72804800	2.69987300	C	0.73229400	2.77075600	-0.14332600
H	1.75913300	0.33364500	0.93563900	C	1.70862500	3.53845900	0.50512300
C	2.25740300	-3.52689300	2.36351500	C	0.14893200	3.31178000	-1.30212300
C	2.36935200	-2.15802700	2.55796000	C	2.07913400	4.79925700	0.03301300
C	1.23686000	-1.32592700	2.48280700	H	2.17733100	3.15323700	1.40578300
C	-0.00855400	-1.90674900	2.19915800	C	0.50897600	4.56844000	-1.77881400
				H	-0.61180100	2.74615500	-1.83222100

C	1.47870500	5.31815300	-1.11085900	H	2.75887500	-2.10339300	1.02065500
H	2.83160100	5.37545700	0.56055100	C	1.68908000	-2.91899000	2.59932200
H	0.03452800	4.96588800	-2.66958400	C	0.27115500	-2.95565000	3.10953800
H	1.76135100	6.29749900	-1.48040100	H	-1.80702200	-0.48917000	-3.97846400
B	-0.78145500	-1.50980800	-0.02319700	H	-1.98898900	2.10230300	-0.79251400
B	0.36234700	1.29139900	0.32444800	H	0.25739100	-3.14362900	4.18157500
N	-1.04911900	0.94298700	0.73407000	C	-2.61524300	-1.04430500	0.41088500
N	-2.54644600	-0.77979000	1.54192000	C	-2.45968200	-2.36923700	-0.02617000
N	0.58846200	-1.07649000	-0.71380400	C	-3.90235700	-0.49305200	0.32530800
N	2.16345400	0.55601300	-1.28112200	C	-3.52819200	-3.10715100	-0.53519500
C	1.02222500	0.17304600	-0.65065800	H	-1.47743600	-2.83280600	-0.00427000
C	1.27594100	-2.07364500	-1.46688700	C	-4.97716600	-1.21477700	-0.19044300
O	-4.77575400	-0.44057500	1.74179800	H	-4.06516600	0.52606700	0.66250800
O	-1.71038600	3.08629300	1.24468200	C	-4.79283900	-2.52727700	-0.62540700
O	4.13621200	0.11002600	-2.31677100	H	-3.37083700	-4.12510800	-0.87564800
O	0.91195700	-3.21806700	-1.47138000	H	-5.95727900	-0.75467600	-0.25530900
H	2.13410000	-1.59852700	-3.33481100	H	-5.62585000	-3.09167200	-1.02959800
H	-3.85051400	1.58843500	0.13766900	C	2.72744500	-0.63024600	-0.96016100
H	-0.66349500	-2.59580000	0.46852500	C	3.81114800	-0.16071600	-0.19224600
H	1.10028900	0.98790900	1.38091400	C	3.02077600	-1.25312900	-2.18382300
C	4.11355500	-1.78566200	1.05234400	C	5.12904000	-0.29103600	-0.62761600
C	3.18345700	-0.86068000	1.51022400	H	3.63098100	0.31824900	0.76706700
C	1.91250500	-1.28122700	1.92982300	C	4.33869100	-1.38870200	-2.62156800
C	1.60609100	-2.64563000	1.93063600	H	2.20772400	-1.64376300	-2.78378300
C	2.54288500	-3.57110700	1.47920200	C	5.39475700	-0.90710700	-1.84981600
C	3.79139200	-3.14532400	1.03219200	H	5.94304800	0.08284500	-0.01624100
H	5.08392600	-1.44858600	0.70709600	H	4.53978500	-1.87587100	-3.56943100
H	3.42693800	0.19631100	1.51448500	H	6.41743800	-1.01533800	-2.19357400
H	0.63636800	-2.97132200	2.27839300	B	-1.37663600	-0.13464500	0.87625800
H	2.28886700	-4.62392900	1.46427700	B	1.24925200	-0.43682300	-0.42306600
H	4.51449600	-3.86808100	0.67204800	N	-0.03319100	-0.55636100	-1.25426000
C	0.96276900	-0.29629400	2.48975100	N	-1.53489500	1.32921700	-1.26198400
N	-0.35933200	-0.42486800	2.54246800	N	-0.25539400	-1.07162600	1.55871900
H	1.39799600	0.33583700	3.26382500	N	1.85359600	-2.08220400	1.48339600
C	-0.98534100	0.38174000	3.61153400	C	0.92464300	-1.23485800	0.98153600
H	-0.84764100	1.45504600	3.44571400	C	-0.57846500	-1.74283200	2.77764300
H	-2.04666100	0.15444100	3.66069600	O	-3.05200900	1.55518400	-2.92896900
H	-0.53690300	0.10350300	4.56513400	O	0.04342400	-2.00874900	-3.00633700
				O	2.60900800	-3.55079900	3.04946500
				O	-1.48992600	-1.38290900	3.46878500
				H	-0.21505300	-3.81167700	2.62105400
				H	-2.63326900	-1.17227800	-2.58796400
				H	-1.69818200	0.71324300	1.66388600
				H	0.49878700	1.26873800	1.89500100
<b>IM<sub>2</sub>N</b>							
C	-1.82028300	-0.50235400	-2.88893900				
C	-0.51187600	-1.10478900	-2.39466800				
C	-0.67565900	0.49961300	-0.47599800				
C	-2.19604600	0.88228400	-2.38872900				



C	2.97086000	3.00714400	-1.10941300	H	-1.01452200	-3.21381200	2.30429600
C	1.49010800	2.71628700	-1.19343000	H	3.17051800	3.32938600	-0.07823300
C	1.92540900	0.39746100	-0.77686900	H	1.38585600	-1.52999100	-1.75554000
C	3.85780700	1.81606100	-1.37109000	H	-3.07687000	1.45487600	-0.29170100
H	-2.05890700	0.53298200	1.65678500	C	-3.18821500	-2.83684100	-1.64069900
C	-2.17644900	-1.51117700	1.84182500	C	-2.63972200	-1.55363100	-1.67721500
C	-1.45529600	-2.75977100	1.40915100	C	-3.36525000	-0.45211400	-1.21616800
H	3.23209000	3.83033100	-1.77133100	C	-4.65498000	-0.66483800	-0.71732900
H	3.81777900	-0.23254700	-1.14172000	C	-5.20515700	-1.94299000	-0.67557600
H	-2.18397900	-3.47252500	1.02240200	C	-4.47220400	-3.03674800	-1.13899600
C	2.68445100	-1.94400100	0.16553900	H	-2.60086800	-3.67796500	-1.99240000
C	2.96595200	-1.66395800	1.51325900	H	-1.63271700	-1.41669500	-2.04883700
C	3.48466700	-2.89960400	-0.47451400	H	-5.22612700	0.17705700	-0.33710800
C	3.99418500	-2.31013400	2.19644300	H	-6.19928900	-2.08876400	-0.26816300
H	2.36644900	-0.92579300	2.04191000	H	-4.89696400	-4.03353800	-1.10272700
C	4.52297200	-3.54785400	0.19728600	C	-2.78849300	0.96638400	-1.22723700
H	3.27461900	-3.15532100	-1.50795500	N	-1.35468400	1.06938100	-1.40428900
C	4.77961300	-3.25541500	1.53528100	H	-3.30105200	1.53812700	-2.01460900
H	4.18755300	-2.07683600	3.23827400	C	-0.88762600	0.99803200	-2.78368200
H	5.12382000	-4.28801600	-0.32029000	H	-0.66029800	1.99500500	-3.18516000
H	5.58263700	-3.76046800	2.06064000	H	0.01007000	0.38048600	-2.88087200
C	-0.75353800	2.45477300	0.81705500	H	-1.64805000	0.54114800	-3.42080900
C	-1.55736100	3.55005200	0.47204400				
C	-0.18686800	2.45473900	2.10207500	<b>TS<sub>5</sub>N</b>			
C	-1.79642400	4.59045000	1.36808300	C	-0.99111800	4.15221700	-0.91585300
H	-1.97751400	3.59524900	-0.52606100	C	0.13559300	3.28510500	-0.38123800
C	-0.41234700	3.49239200	3.00705100	C	-1.44525100	1.45193000	-0.27265700
H	0.44812700	1.62502400	2.40688100	C	-2.36684900	3.73826100	-0.44925400
C	-1.22514200	4.56398400	2.64053800	H	2.54391800	-0.78535000	-1.19843900
H	-2.42172200	5.42640000	1.07308800	C	1.45164100	-2.22519300	-2.18668300
H	0.03943100	3.46411500	3.99294100	C	0.01057800	-2.60721200	-2.41968300
H	-1.41036300	5.37220800	3.33949100	H	-0.80342700	5.18925000	-0.64728900
B	1.51082600	-1.15327400	-0.60857100	H	-3.40088900	2.02564100	-0.04433300
B	-0.42101900	1.25696400	-0.22724600	H	-0.07630000	-3.68174400	-2.56506200
N	1.08375000	1.42687200	-0.72631500	C	-3.22318300	-0.51192500	0.12048900
N	3.22898400	0.59578600	-1.11268400	C	-4.17098700	-0.40188900	-0.91140100
N	0.14916600	-1.28470100	0.16798300	C	-3.66931000	-1.03432900	1.34454600
N	-1.60154400	-0.32754700	1.37261100	C	-5.49416600	-0.80607700	-0.73776200
C	-0.54092600	-0.20623600	0.53731700	H	-3.86594800	-0.00059100	-1.87405700
C	-0.33838400	-2.59840500	0.39781100	C	-4.98836700	-1.44464000	1.52896700
O	5.00639500	1.87486900	-1.72954700	H	-2.96770000	-1.12276300	2.16882000
O	0.69045800	3.51380400	-1.60052200	C	-5.90627600	-1.33247500	0.48530600
O	-3.15187900	-1.49362400	2.55030700	H	-6.20195900	-0.71147500	-1.55440600
O	0.14148800	-3.54647000	-0.16854900	H	-5.30226800	-1.84814900	2.48585100

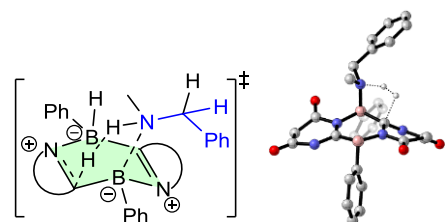
H	-6.93408000	-1.64862300	0.62525200	H	-0.82253100	2.16728100	2.25037100
C	2.46989700	1.31081400	0.07257300	H	0.11933200	1.48428700	3.56993600
C	3.35858200	1.41837100	1.15013300				
C	2.99072000	1.58486400	-1.20485800	<b>IM<sub>4</sub>N</b>			
C	4.69499300	1.77434100	0.96984200	C	-1.11942000	4.02722700	-0.91668700
H	3.00672000	1.24582700	2.15961800	C	0.05277200	3.25010400	-0.34407900
C	4.32358400	1.93713600	-1.40020900	C	-1.50627500	1.38765000	-0.20030600
H	2.33127300	1.54787600	-2.06799900	C	-2.41838400	3.68381300	-0.21016700
C	5.18579700	2.02972700	-0.30832700	H	2.54013000	-0.80802300	-1.07398200
H	5.35200800	1.85728000	1.82918800	C	1.48918300	-2.19335500	-2.15527000
H	4.68750200	2.14772900	-2.40001900	C	0.05339900	-2.54168000	-2.47752600
H	6.22430000	2.30603500	-0.45215300	H	-0.92464400	5.09355200	-0.84314100
B	-1.73552300	-0.00747300	-0.06394300	H	-3.38761000	2.02457400	0.43618300
B	0.93822600	0.85800700	0.23805400	H	-0.03280700	-3.59373400	-2.73842400
N	-0.13096000	1.90985700	-0.31748900	C	-3.30775000	-0.57465600	-0.11417100
N	-2.46565000	2.39032500	-0.18874900	C	-4.38533300	-0.04440000	-0.84658600
N	-0.65220900	-0.89715100	-0.73786300	C	-3.62173700	-1.52187600	0.87785300
N	1.59708300	-1.12125500	-1.35074100	C	-5.70343300	-0.43468600	-0.60367800
C	0.61085100	-0.47762500	-0.68115600	H	-4.18691600	0.68527000	-1.62538600
C	-0.96476000	-2.15305700	-1.35498500	C	-4.93144900	-1.91628500	1.12981100
O	-3.31433200	4.49281500	-0.36165400	H	-2.82073200	-1.97086300	1.45645700
O	1.19106300	3.77728400	-0.04740200	C	-5.98159300	-1.37170700	0.38791000
O	2.39954700	-2.77115500	-2.69542300	H	-6.50975400	-0.00714500	-1.18994000
O	-1.94456200	-2.78087000	-1.06602400	H	-5.13743900	-2.64934100	1.90269500
H	-0.29434100	-2.12130400	-3.35674300	H	-7.00379200	-1.67750400	0.58158300
H	-0.98661200	4.08122900	-2.01116000	C	2.43378800	1.35207700	-0.01240500
H	-0.91293600	0.24986600	1.19289800	C	3.42512600	1.45672400	0.97131100
H	1.77791000	-0.19312500	3.14477400	C	2.82815400	1.65263300	-1.33055100
C	3.10329900	-3.20638200	0.86669300	C	4.73330100	1.83678000	0.66802900
C	2.70902000	-2.04583600	1.52947500	H	3.19039800	1.27070300	2.01075900
C	1.36245000	-1.81950600	1.83433500	C	4.12807500	2.03126600	-1.64805900
C	0.42039900	-2.79247100	1.48770200	H	2.09026900	1.60736100	-2.12601100
C	0.80850800	-3.94897900	0.81484700	C	5.09306500	2.12186300	-0.64529000
C	2.15237800	-4.15696200	0.50059100	H	5.46811700	1.91591500	1.46208500
H	4.14814500	-3.36223800	0.62471800	H	4.38747100	2.26240600	-2.67533900
H	3.44900000	-1.29970700	1.79434700	H	6.10798300	2.41797100	-0.88499800
H	-0.62724100	-2.63347100	1.72026700	B	-1.84806100	-0.02935700	-0.33396800
H	0.06171800	-4.68492000	0.53915800	B	0.91269000	0.88893100	0.21723600
H	2.45553600	-5.05242600	-0.02923100	N	-0.16759900	1.87951500	-0.22114800
C	0.93513300	-0.56197400	2.54979300	N	-2.48663900	2.36220300	0.12151100
N	0.42154400	0.53872200	1.69779100	N	-0.67684500	-0.91655700	-0.73923000
H	0.13910700	-0.81625400	3.26005800	N	1.59981000	-1.13643600	-1.26647800
C	0.15163400	1.74527100	2.51111200	C	0.58605000	-0.48581900	-0.62311400
H	0.91511700	2.51006000	2.35443300	C	-0.90820300	-2.20187300	-1.36531200



O	-3.30062000	4.49160400	0.03305200	H	-2.99418900	-1.95061300	1.63924700
O	1.08469200	3.80019100	-0.00205300	C	-6.02143600	-1.71460500	0.12900300
O	2.45461600	-2.74459300	-2.63093700	H	-6.41997100	-0.59301900	-1.66463800
O	-1.79564200	-2.92523500	-1.01587800	H	-5.31194000	-2.72944800	1.89042500
H	-0.23008800	-1.94337300	-3.35386100	H	-7.04187000	-2.06521300	0.23730000
H	-1.23760400	3.75272900	-1.97320600	C	2.25339700	1.58541000	-0.38954900
H	2.14304400	-0.02550200	3.01776400	C	3.12238200	2.02217200	0.61981900
C	3.12273900	-3.24830400	0.85334400	C	2.72877800	1.65336600	-1.71144600
C	2.84023200	-2.06006800	1.52297300	C	4.40454500	2.48047200	0.33442400
C	1.53531700	-1.77083900	1.93496600	H	2.78361100	2.03911100	1.64569700
C	0.52146800	-2.69957400	1.68397800	C	4.00880500	2.12166700	-2.01068200
C	0.79717300	-3.87968600	0.99861600	H	2.08580200	1.34248300	-2.53001100
C	2.10001200	-4.15495900	0.58140000	C	4.85675300	2.52796100	-0.98451400
H	4.13396700	-3.45617300	0.52465400	H	5.04892900	2.81557800	1.14011500
H	3.63172900	-1.34209600	1.70531600	H	4.33991500	2.16576800	-3.04240900
H	-0.49472500	-2.49239000	2.00372400	H	5.85494300	2.88706200	-1.20852300
H	-0.00449500	-4.57771400	0.78872500	B	-1.91241900	-0.18258100	-0.28023900
H	2.31603600	-5.06922900	0.04142400	B	0.79825800	1.00572900	-0.14513000
C	1.22767400	-0.48322900	2.65083600	N	-0.40652200	1.85849500	-0.20019400
N	0.50148800	0.55494000	1.82876900	N	-2.76105400	2.14327300	0.10393900
H	0.59483200	-0.68395700	3.52098200	N	-0.70019500	-0.98322700	-0.63234800
C	0.35379900	1.81724700	2.62439800	N	1.55704200	-1.15668100	-1.28589600
H	1.26229400	2.40763100	2.53501700	C	0.53246500	-0.43889300	-0.70526700
H	-0.48033500	2.39086500	2.23082200	C	-0.81846000	-2.39640900	-0.95853100
H	0.15793900	1.57143200	3.66932800	O	-3.77198500	4.18524200	0.11663600
H	-0.45879100	0.21102200	1.68963900	O	0.69145400	3.83536700	0.26396800
				O	2.39910700	-2.85267500	-2.54934700
				O	-1.50810500	-3.12959400	-0.31145900
<b>TS<sub>e</sub>N</b>				H	-0.41086600	-2.38625200	-3.04174500
C	-1.49655100	4.02303100	-0.68418200	H	-1.53717700	3.89228400	-1.77346500
C	-0.29223900	3.27414300	-0.16039200	H	2.49220800	0.36097200	2.88897800
C	-1.68610700	1.27083300	-0.16217900	C	3.75401200	-2.74221200	0.70315400
C	-2.79736100	3.49046000	-0.11288400	C	3.35115300	-1.59900800	1.39156400
H	2.48788700	-0.76382000	-1.20804900	C	2.07730200	-1.52454400	1.96226700
C	1.44862700	-2.31476200	-2.02461900	C	1.21162300	-2.61388600	1.82774100
C	0.02116000	-2.82227400	-2.13173100	C	1.60506300	-3.75126400	1.12566200
H	-1.39672700	5.08203500	-0.46065600	C	2.88102700	-3.81938800	0.56642700
H	-3.64110400	1.70857300	0.35323600	H	4.74067100	-2.78476500	0.25688100
H	0.01682000	-3.90534800	-2.22711800	H	4.02321400	-0.75150900	1.47283800
C	-3.35613200	-0.80090600	-0.14781900	H	0.21954900	-2.57751600	2.26804000
C	-4.35789000	-0.43772400	-1.06654300	H	0.91575900	-4.58089500	1.01833600
C	-3.73873400	-1.63624100	0.91675700	H	3.18654200	-4.69818000	0.01159400
C	-5.67223900	-0.88866100	-0.93665700	C	1.63798100	-0.29373400	2.71434900
H	-4.10321600	0.21250700	-1.89812900	N	0.60266700	0.48975600	1.99741900
C	-5.04829000	-2.08638500	1.05754900				

H	1.25256900	-0.58572100	3.70242000
C	0.15033400	1.64245300	2.79939600
H	0.94057200	2.39164400	2.84779500
H	-0.71927700	2.09606600	2.32887400
H	-0.12311800	1.34193500	3.81858500
H	-0.20587200	-0.11393500	1.85570300

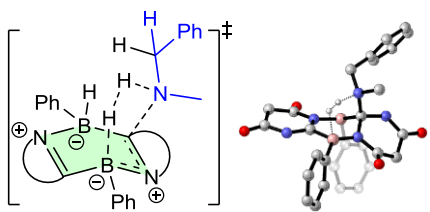
**TS<sub>7</sub>N**



C	0.32359000	3.01647600	-1.06111500
C	-0.56106100	1.92159600	-1.60631900
C	0.86912900	0.21696700	-0.39072600
C	1.73667600	2.58853300	-0.73138100
H	-3.32375400	-1.96268100	-0.13848400
C	-2.72860600	-3.10439800	1.48201800
C	-1.50164500	-3.33179700	2.32571500
H	0.34903700	3.85113000	-1.75811400
H	2.80960700	0.98453600	-0.17784000
H	-0.96777300	-4.18281100	1.88142000
C	0.15458100	1.14492600	1.99680200
C	-1.19375400	1.48715100	2.17638700
C	1.10471500	2.06793900	2.46366000
C	-1.58293800	2.69415000	2.75949300
H	-1.97725900	0.80490400	1.85884100
C	0.73337500	3.28133300	3.03870400
H	2.16016400	1.84044900	2.35722900
C	-0.61638100	3.60317300	3.18470900
H	-2.63665600	2.92399400	2.88025200
H	1.49630000	3.97769700	3.36941900
H	-0.91002400	4.54619900	3.63223700
C	-2.96967200	-0.00129400	-1.43050300
C	-3.55844700	-0.75475900	-2.45574900
C	-3.75915000	0.97458200	-0.79567200
C	-4.88112100	-0.53551900	-2.84392800
H	-2.97424400	-1.50815000	-2.97349700
C	-5.07776700	1.19515100	-1.17997500
H	-3.33037000	1.58174100	-0.00512000
C	-5.64419900	0.43884100	-2.20645100
H	-5.31041000	-1.12310300	-3.64780300

H	-5.66320500	1.96034100	-0.68244400
H	-6.67116400	0.61124600	-2.50782100
B	0.64733900	-0.16645500	1.19832100
B	-1.52238000	-0.25850100	-0.86561700
N	-0.43025500	0.68034100	-0.95112900
N	1.88789300	1.25733300	-0.49556100
N	-0.48697200	-1.30052800	1.26005700
N	-2.55155100	-2.11716900	0.50640500
C	-1.48389800	-1.28570800	0.39164400
C	-0.51065100	-2.18275400	2.38803900
O	2.66470500	3.37632500	-0.68039600
O	-1.37810900	2.12010000	-2.47702000
O	-3.76195700	-3.71474900	1.57999000
O	0.24930100	-2.04881200	3.30546800
H	-1.78564000	-3.62743600	3.33442300
H	-0.12590700	3.36085300	-0.12108400
H	1.64135800	-0.62630100	1.67556300
H	1.83363700	-2.23558500	0.21742300
C	5.56507400	-0.66599700	0.47285200
C	4.22392200	-1.04571100	0.44494000
C	3.65494500	-1.57848500	-0.71829100
C	4.47223900	-1.75092400	-1.84123500
C	5.81282500	-1.37246100	-1.81661500
C	6.36147400	-0.82081400	-0.66010700
H	5.98657300	-0.25179800	1.38175700
H	3.61413300	-0.92881200	1.33253200
H	4.05849700	-2.18886300	-2.74357200
H	6.42820700	-1.50968500	-2.69860800
H	7.40294300	-0.52110800	-0.63995100
C	2.18330300	-1.95535300	-0.77315000
H	-0.16518700	-1.53417200	-1.66103600
H	-1.00995500	-1.65910400	-1.88209700
N	1.26385200	-0.91817900	-1.30336000
H	2.06133200	-2.82788700	-1.42384800
C	1.60398500	-0.49522800	-2.67408200
H	0.79168900	0.10456100	-3.08464800
H	2.53092200	0.07917500	-2.72078000
H	1.70680100	-1.38773500	-3.29507600

**TS<sub>8</sub>N**



C	1.39862000	3.76831200	0.22345800	C	0.03268100	-1.18670200	-0.03876300
C	0.23840200	2.81670800	0.05215600	C	1.59909800	-2.78848500	-0.89035400
C	1.74818400	1.11593600	-0.70000000	O	3.46246000	4.21466100	-0.93691100
C	2.60758100	3.43168800	-0.61007000	O	-0.90581100	3.18021500	0.11179100
H	-0.99910200	-1.74843300	1.65851900	O	-0.33984400	-4.14877900	1.88561800
C	-0.00588200	-3.41310600	0.98434100	O	2.55837400	-3.08236700	-1.56471500
C	0.70242600	-3.84477100	-0.27269700	H	1.26668600	-4.75971100	-0.11024000
H	1.07466500	4.79010400	0.03676100	H	1.71143900	3.70366700	1.27453300
H	3.54757300	1.76421900	-1.36269400	H	2.23361900	-0.27633700	-2.39490600
H	-0.08651300	-4.05829600	-1.00955000	H	-2.90841000	1.75214300	-0.02520400
C	3.67771100	-0.58746900	-0.56426500	C	-6.49738800	0.12224400	-0.65148400
C	3.85287400	-0.73569500	0.82104900	C	-5.30616000	0.82733000	-0.49682200
C	4.82687600	-0.58228400	-1.36519000	C	-4.14796900	0.44403100	-1.18251800
C	5.11895200	-0.87900100	1.38487400	C	-4.21083800	-0.66796000	-2.02699200
H	2.98138900	-0.75126300	1.47178300	C	-5.40049200	-1.37941800	-2.18027100
C	6.10067900	-0.71664700	-0.80978300	C	-6.54822800	-0.98707000	-1.49458500
H	4.71925000	-0.50468900	-2.44259200	H	-7.38200800	0.43278700	-0.10661800
C	6.25017600	-0.86506300	0.56782000	H	-5.26946800	1.67964600	0.17442000
H	5.22623000	-1.00040600	2.45775300	H	-3.32915100	-0.99711200	-2.56318600
H	6.97412300	-0.71996400	-1.45324000	H	-5.42796800	-2.24306300	-2.83535200
H	7.23785200	-0.97585100	1.00154500	H	-7.47141700	-1.54297200	-1.61176700
C	-1.24443700	0.54230200	1.52896900	C	-2.88809200	1.27138000	-0.99908000
C	-2.51556100	0.02784600	1.84272400	H	-1.63400500	-0.87285300	-1.22627900
C	-0.48974400	1.04706800	2.59981900	H	-1.17617100	-1.69804800	-1.16691600
C	-3.01796600	0.04885600	3.14428200	N	-1.62256400	0.51103200	-1.14797100
H	-3.13314000	-0.40601500	1.06442200	H	-2.88919400	2.09127700	-1.72527500
C	-0.98213100	1.07651400	3.90292500	C	-0.99096400	0.78129600	-2.45431800
H	0.51689700	1.41490300	2.42438500	H	-0.61171600	1.80646700	-2.51447600
C	-2.25454500	0.58011500	4.18081600	H	-0.16400600	0.09005600	-2.62426700
H	-4.00452600	-0.35443400	3.34454400	H	-1.72191800	0.64125500	-3.25323800
H	-0.36942000	1.47756300	4.70304600				
H	-2.64045400	0.59709900	5.19367000				
B	2.19914200	-0.35252000	-1.18350700	<b>TS</b>			
B	-0.60452700	0.38434200	0.05606800	C	-0.81323300	3.85013000	0.52755400
N	0.57355200	1.44092900	-0.15424500	C	0.06865000	3.05401500	-0.41838200
N	2.67563200	2.07982100	-0.94538800	C	-1.19103200	1.10074200	0.37951700
N	1.20640900	-1.45645100	-0.68681900	C	-2.24452800	3.34988600	0.49158100
N	-0.31428900	-2.06224500	0.97943700	H	2.71671700	-1.33040300	-0.78161900
				C	1.65133700	-2.97476400	-1.29368500
				C	0.21008700	-3.36102800	-1.58962800
				H	-0.42819000	3.73057300	1.54791500
				H	-3.22591100	1.58486600	0.20161200
				H	0.08505400	-4.43780700	-1.51793100
				C	-3.09913700	-0.68842600	-0.57409700
				C	-3.33441300	-0.75301500	-1.95831500

C	-4.21049000	-0.79835300	0.27585600	H	-0.45903200	-1.87740700	2.77783400
C	-4.61959600	-0.92091600	-2.47090000	H	0.77482400	-3.98840200	2.57231900
H	-2.49870400	-0.66498700	-2.64691600	H	3.20280500	-3.97872600	2.04970400
C	-5.49961700	-0.96416500	-0.22824200	C	0.52423900	0.70034900	2.44190100
H	-4.06160800	-0.78571500	1.35136800	N	-0.87202900	0.68489600	1.93361300
C	-5.70752900	-1.02506400	-1.60540400	H	0.49471500	1.03415200	3.48421000
H	-4.77299600	-0.96709600	-3.54372800	C	-1.84948800	1.16744800	2.92198400
H	-6.33959600	-1.05518000	0.45175300	H	-1.74418900	2.24244300	3.10058100
H	-6.70869600	-1.15514100	-2.00063200	H	-2.86239700	0.96958300	2.57769800
C	2.48973300	1.24493200	-1.06884000	H	-1.68996800	0.63210900	3.85872500
C	3.18668500	2.11385900	-0.21016700				
C	3.17802800	0.78563700	-2.20553100				
C	4.49995200	2.49434100	-0.45965200				
H	2.69046500	2.51336000	0.66836800	<b>TS1-NB</b>			
C	4.49036500	1.17348500	-2.47345900	C	-0.28651400	3.60558200	0.71048700
H	2.67473800	0.12217100	-2.90078200	C	-1.12722700	2.64666300	-0.09746600
C	5.15884300	2.02440400	-1.59697700	C	0.75084600	1.19802800	-0.30551000
H	5.00969300	3.16318100	0.22529700	C	1.18680400	3.52880000	0.37383100
H	4.98898600	0.80939400	-3.36492600	H	-2.58270100	-2.36278500	-0.35479100
H	6.18165800	2.32293500	-1.79763700	C	-1.17059200	-3.62439400	0.36407200
B	-1.63292300	-0.41779800	-0.05447600	C	0.26266800	-3.57537100	0.87904500
B	1.03454000	0.74734900	-0.75563700	H	-0.65034700	4.62330300	0.58855500
N	-0.02204300	1.64952200	-0.27140200	H	2.56422400	2.12058100	-0.23801100
N	-2.30862100	1.99000200	0.34495500	H	0.67774200	-4.57922400	0.91524800
N	-0.52094300	-1.23960000	-0.53815500	C	3.02670200	-0.22560200	-0.37460800
N	1.77620200	-1.66121700	-0.95302000	C	3.44957100	-0.33628600	0.95948400
C	0.72784000	-0.73714700	-0.79364700	C	4.00367600	-0.04239600	-1.36127900
C	-0.74923200	-2.66633500	-0.66004200	C	4.79903100	-0.28286900	1.29423600
O	-3.22192700	4.06571000	0.54980200	H	2.71462900	-0.48258500	1.74608300
O	0.79090900	3.58680500	-1.22433800	C	5.35848000	0.01336900	-1.03235100
O	2.58774000	-3.74886300	-1.36760200	H	3.70821900	0.04279300	-2.40243300
O	-1.62241800	-3.22267800	-0.05249000	C	5.75836100	-0.10733900	0.29611200
H	-0.01123600	-3.03802400	-2.61544200	H	5.10503000	-0.38202200	2.32965800
H	-0.78332900	4.90328300	0.26206400	H	6.09897000	0.14548700	-1.81319500
H	-1.34748200	-0.56249800	1.44543100	H	6.81051900	-0.06739900	0.55407300
H	1.08743000	1.45049200	1.88497400	C	-3.05450200	0.24628900	-0.12267000
C	3.32841900	-1.83009200	1.99547900	C	-3.87786700	-0.01129100	-1.23052400
C	2.62457800	-0.63187700	2.08821000	C	-3.68709800	0.57997200	1.08630100
C	1.25181300	-0.62921900	2.35662300	C	-5.26745700	0.06841700	-1.14023100
C	0.60198900	-1.84879500	2.56016300				
C	1.30152500	-3.04965400	2.44508200				
C	2.66503400	-3.04496800	2.15967200				
H	4.38850100	-1.81506300	1.76926400				
H	3.14232800	0.30467500	1.91622600				

H	-3.42274000	-0.26909500	-2.18199400	C	-2.26229100	-0.73158000	0.54203800
C	-5.07416300	0.66919500	1.18455900	C	-1.53877900	-0.44670000	1.71394000
H	-3.08420200	0.76264700	1.97176300	C	-3.65550900	-0.86340800	0.65919300
C	-5.86979100	0.41275900	0.06837800	C	-2.17686200	-0.28351200	2.94203700
H	-5.87895400	-0.13469100	-2.01283400	H	-0.46300000	-0.32007300	1.66384000
H	-5.53540800	0.92794800	2.13172000	C	-4.30239600	-0.69825600	1.88404900
H	-6.94982000	0.47568300	0.14191800	H	-4.24262100	-1.08377600	-0.22614800
B	1.48072800	-0.18878300	-0.69727900	C	-3.56374600	-0.40588600	3.02927400
B	-1.49116800	0.07999500	-0.20736700	H	-1.59477000	-0.05535100	3.82832400
N	-0.56936900	1.30068600	-0.19742400	H	-5.38092700	-0.79576300	1.94336700
N	1.56895800	2.26994000	-0.09463000	H	-4.06360800	-0.27527600	3.98259900
N	0.57320000	-1.43693600	-0.27648900	C	2.38828600	0.93319500	0.19616100
N	-1.59719600	-2.42858100	-0.13218200	C	3.21161600	1.91416000	-0.37721600
C	-0.85648300	-1.22443400	-0.16531700	C	2.71799100	0.49221300	1.48896700
C	1.15223000	-2.68791400	0.04147100	C	4.30579000	2.43968600	0.30792000
O	1.97651000	4.42950200	0.50511800	H	3.01393700	2.25178900	-1.39059000
O	-2.15429800	2.93341100	-0.63154300	C	3.81048000	1.00926900	2.18160600
O	-1.85723700	-4.63086700	0.40157500	H	2.10305800	-0.26382700	1.97190300
O	2.25489100	-2.99970000	-0.34975400	C	4.60839400	1.98925500	1.59183500
H	0.23039600	-3.16452600	1.89715100	H	4.92703300	3.19413200	-0.16248600
H	-0.38635700	3.32346000	1.76741500	H	4.03781600	0.65362200	3.18094900
H	1.31896700	-0.27234800	-2.04085500	H	5.45939200	2.39538300	2.12697700
H	0.86589500	-1.06486300	-1.54244200	B	-1.57351200	-0.88015900	-0.90346300
				B	1.11783900	0.37348300	-0.53151500
<b>IM-NB</b>				N	0.98293600	-1.16344000	-0.63860800
C	1.98126800	-3.39999800	-0.19910200	N	-0.35017000	-3.07775500	-0.79915400
C	2.16219400	-1.99135700	-0.71856800	N	-1.20190100	0.56978200	-1.59437500
C	-0.21570600	-1.72701500	-0.77542200	N	-0.03102100	2.59915600	-1.01896000
C	0.65676300	-4.02531200	-0.56641700	C	0.01746600	1.17509100	-1.00293000
H	0.83958500	3.10713900	-1.09193700	C	-2.42529600	1.43458000	-1.51536200
C	-1.11793900	3.33511600	-0.64726900	O	0.44052900	-5.20648400	-0.64020000
C	-2.35106000	2.44614600	-0.41833000	O	3.19331800	-1.56796800	-1.15392200
H	2.80254600	-4.03379300	-0.52688900	O	-1.14388400	4.54570700	-0.54840000
H	-1.27893400	-3.44333300	-0.97868900	O	-3.28358700	1.29683100	-2.33666200
H	-3.25297400	3.05062500	-0.40084400	H	-2.21273100	1.92588500	0.53555000

H	2.01032100	-3.34480400	0.89784600
H	-2.29508300	-1.44096400	-1.68926400
H	-1.08456600	0.39874400	-2.59688200

**TS2-NB**

C	0.61887200	4.01756400	-0.40356400
C	1.33135300	2.69978300	-0.64458500
C	-0.59639100	1.56033000	0.25031800
C	-0.88347300	3.94084500	-0.26465100
H	1.13523100	-2.01309400	-2.35140000
C	0.02044400	-3.25791600	-1.22815700
C	-0.94064100	-3.21034100	-0.03355800
H	1.00085500	4.41348300	0.54716500
H	-2.33766400	2.58216700	0.31451000
H	-1.06573500	-4.20487700	0.38725000
C	-2.73544000	-0.08329100	0.52764900
C	-3.16063400	-0.18896400	-0.80961400
C	-3.69158500	-0.30207000	1.53193800
C	-4.48159200	-0.49903300	-1.12873700
H	-2.43464200	-0.04392600	-1.60392600
C	-5.01571600	-0.61368600	1.22029000
H	-3.38956900	-0.23652900	2.57214300
C	-5.41321300	-0.71309200	-0.11189900
H	-4.78480300	-0.57625400	-2.16740000
H	-5.73398100	-0.78302300	2.01519100
H	-6.44093300	-0.95723600	-0.35736700
C	2.79125900	-0.20072900	0.15583700
C	3.42151700	-1.39812300	-0.23337100
C	3.56847800	0.73572600	0.87034700
C	4.76381500	-1.63294300	0.05022900
H	2.85634500	-2.16435200	-0.74551400
C	4.90984500	0.50896000	1.14396400
H	3.11417500	1.65652700	1.21702600
C	5.51649800	-0.68000000	0.73381100
H	5.22171200	-2.56477600	-0.26246800

H	5.48292500	1.25241300	1.68670100
H	6.56149500	-0.86442500	0.95571800
B	-1.21699600	0.24674200	0.90823400
B	1.30749900	0.14408900	-0.19997600
N	0.71373500	1.56281700	-0.05838800
N	-1.33989100	2.67971300	0.14828200
N	-0.19793600	-0.90065800	0.43714200
N	0.60076700	-2.05593200	-1.49417900
C	0.22859900	-0.79941100	-0.91694200
C	-0.49018800	-2.25277100	1.02359700
O	-1.64148500	4.85659900	-0.44784500
O	2.35389600	2.61618000	-1.26917600
O	0.21436300	-4.27787700	-1.86534900
O	-0.37171600	-2.45392300	2.19162600
H	-1.90483800	-2.84769700	-0.41579900
H	0.88566700	4.72914800	-1.18294000
H	-1.05166200	0.42292100	2.09964200
H	0.98486900	-0.46907200	1.24870500

**Adduct**

C	0.53713200	4.28781900	0.25534900
C	-0.46851400	3.24554300	-0.19804400
C	1.18211000	1.55259000	0.16902000
C	1.98017100	3.87883300	0.09440300
H	-2.54339100	-0.92696400	1.51368800
C	-1.34279000	-2.41272800	2.30568100
C	0.12200900	-2.70841100	2.48953400
H	0.35274600	5.22795500	-0.26008300
H	3.11829000	2.15566900	0.09896500
H	0.28550300	-3.78172000	2.55733300
C	3.08938500	-0.33878600	-0.04771400
C	3.76447600	-1.03727800	-1.05807700
C	3.83915200	0.04657700	1.07524000
C	5.12286400	-1.32724900	-0.96073200
H	3.20779800	-1.38350600	-1.92164100
C	5.20021500	-0.24008800	1.18607100
H	3.34719400	0.56040300	1.89873800
C	5.84827200	-0.92563100	0.16132600
H	5.61712100	-1.87491600	-1.75611400
H	5.75027800	0.06625700	2.06941400

H	6.90606000	-1.15131000	0.23845400	<b>Poly_1</b>			
C	-2.64967400	1.13110200	0.13969700	C	3.52672300	3.19323000	-0.08236600
C	-3.55016400	1.32259300	-0.91822900	C	3.17992800	1.94756200	0.711111000
C	-3.12405800	1.43266700	1.42872100	C	1.88138000	1.15922800	-1.12927400
C	-4.85552500	1.75493200	-0.70655200	C	2.59779400	3.50176800	-1.23918500
H	-3.21639500	1.16732100	-1.93753600	H	4.12588900	-2.77451500	-0.13106200
C	-4.43028300	1.86946500	1.65745100	C	3.80043300	-3.47015600	-2.06149100
H	-2.45459500	1.34555600	2.28147400	C	3.13597000	-3.01292900	-3.33852700
C	-5.30567500	2.02300700	0.58647500	H	3.56549700	4.05130200	0.58890800
H	-5.52107500	1.89562500	-1.55142100	H	1.18549300	2.54390300	-2.42821900
H	-4.75877700	2.09210600	2.66701400	H	2.79163500	-3.87606500	-3.91151900
H	-6.32296300	2.35886300	0.75385600	C	-0.16818600	0.43064800	-2.70893300
B	1.52263700	-0.01109400	-0.13107200	C	-1.52621000	0.47520700	-2.34262300
B	-1.12156100	0.67747900	-0.06247600	C	0.18288800	0.97867400	-3.95568200
N	-0.11388300	1.90058000	0.10095100	C	-2.48929700	1.03005100	-3.18769700
N	2.15962300	2.49424300	0.11751400	H	-1.82541000	0.06249000	-1.38323800
N	0.63335600	-0.85595200	0.90642400	C	-0.77258600	1.54778400	-4.80169400
N	-1.57393400	-1.21554200	1.61554900	H	1.21898700	0.93549200	-4.28974800
C	-0.65075700	-0.48105400	0.95966000	C	-2.11484400	1.57602900	-4.41775400
C	1.03662700	-2.11852700	1.43230000	H	-3.53617200	1.02765700	-2.89043300
O	2.91019700	4.64063800	-0.00145300	H	-0.47168400	1.95879900	-5.76200700
O	-1.49096000	3.54743300	-0.75292000	H	-2.86220500	2.01349500	-5.07440600
O	-2.24871600	-3.07841300	2.73532300	C	3.67104400	-1.00456100	1.53142500
O	2.03948500	-2.67683400	1.08271400	C	3.33830500	-1.35328200	2.85219800
H	0.41480900	-2.26407300	3.45054500	C	5.04299000	-0.96436200	1.20926700
H	0.37237400	4.45468300	1.32828900	C	4.31977600	-1.66334500	3.79429900
C	-3.05034700	-3.09138900	-1.82728600	H	2.29659200	-1.34231500	3.15682600
C	-2.54290300	-1.79445500	-1.79326000	C	6.03358100	-1.27095100	2.14461800
C	-1.17225600	-1.55516700	-1.61791300	H	5.34899600	-0.67002800	0.20456400
C	-0.32743900	-2.66687800	-1.50208900	C	5.67081000	-1.62946600	3.44329500
C	-0.83435800	-3.96647300	-1.52825000	H	4.02888900	-1.92606100	4.80815200
C	-2.20034000	-4.18747100	-1.68426800	H	7.08228500	-1.22695400	1.86150000
H	-4.11584600	-3.24388500	-1.96111300	H	6.43447300	-1.87331500	4.17704500
H	-3.22832300	-0.96532600	-1.89533900	B	0.89519100	-0.06826700	-1.62447100
H	0.73723200	-2.50688500	-1.39983500	B	2.57221800	-0.65600700	0.41837600
H	-0.15331200	-4.80524600	-1.43064300	N	2.63076900	0.87997200	-0.06214200
H	-2.59706300	-5.19616800	-1.70100100	N	1.84086600	2.39499000	-1.66124100
C	-0.62115200	-0.13661200	-1.49279600	N	2.01063400	-1.20993700	-2.02141600
N	0.84451800	-0.11118600	-1.51513900	N	3.60334200	-2.58583200	-0.98570600
H	-1.01009700	0.46843800	-2.31903300	C	2.77893800	-1.51621300	-0.97020900
C	1.38504400	0.67303900	-2.61797600	C	1.99236800	-2.01565500	-3.19112500
H	2.47116300	0.73506800	-2.55046100	O	2.51540600	4.57003500	-1.79620600
H	1.12959400	0.20713000	-3.57529400	O	3.34812400	1.85060100	1.90092600
H	0.99115000	1.70558800	-2.64337000	O	4.48164000	-4.46043100	-1.94221600

O	1.14666800	-1.89615400	-4.04309500	O	-1.23676800	-3.32257200	2.36232800
H	3.91339800	-2.52416700	-3.94499000	O	-6.81700500	1.20941900	-0.32481600
H	4.53299800	3.04956600	-0.50385200	O	-3.57345500	3.48136300	1.81195900
C	0.54172100	-2.34702800	1.07766200	H	-4.23854100	2.45554300	-0.97468000
C	-0.81444400	-2.36461600	1.76562700	H	0.46196300	-2.95978100	0.17216600
C	-0.91017600	0.03820400	1.79038800				
C	0.97034900	-0.91992400	0.72796700	<b>Poly_2</b>			
H	-5.50099400	-0.70999500	0.57070300	C	3.31935600	-1.57398100	-3.16800300
C	-5.66100000	1.25043800	0.05942300	C	3.61907200	-0.71389600	-1.95312600
C	-4.78281400	2.49316100	-0.01847100	C	1.55514900	-1.47636500	-0.96066900
H	1.24655000	-2.83686600	1.75477800	C	1.86222700	-1.86601800	-3.37868100
H	0.94166200	0.79936200	1.92882700	H	3.18677700	0.93698300	2.76541400
H	-5.40031400	3.39065800	0.00325900	C	1.97053100	-0.02387000	4.10960700
C	-0.76403200	2.69416700	1.54821100	C	1.19762400	-1.30748400	4.18772100
C	0.10552900	3.08043200	2.58438000	H	3.75599100	-1.10380500	-4.04885100
C	-0.76914700	3.48583300	0.38150900	H	0.23802100	-2.36268600	-2.22740300
C	0.91805800	4.21231500	2.47487500	H	0.39256400	-1.24626900	4.92360700
H	0.14249400	2.49050000	3.49779200	C	0.76011300	-3.53949400	0.25584400
C	0.02795100	4.62279600	0.26732700	C	1.85393800	-4.11422700	0.92783900
H	-1.40273300	3.19708400	-0.45537000	C	0.00573400	-4.40102000	-0.56143700
C	0.87699300	4.99071700	1.31732100	C	2.15946400	-5.47196200	0.82727400
H	1.57968200	4.48289300	3.29329900	H	2.48590700	-3.48922900	1.55566700
H	0.00981400	5.21282600	-0.64463300	C	0.29893600	-5.76101800	-0.67180600
H	1.50099200	5.87612300	1.22574700	H	-0.83823800	-4.01136500	-1.12337800
C	-3.76863900	-2.55259400	0.90971200	C	1.37822900	-6.30561700	0.02610500
C	-4.10792900	-3.52260800	1.87198300	H	3.00876700	-5.87753200	1.37200900
C	-4.22373300	-2.76386200	-0.40881300	H	-0.31742900	-6.39410200	-1.30540800
C	-4.85951900	-4.64773800	1.53420500	H	1.61023600	-7.36412300	-0.05723800
H	-3.76423200	-3.39819200	2.89311800	C	4.49287100	0.11947500	0.82633100
C	-4.97049100	-3.89191300	-0.75515600	C	5.43962800	1.15288200	0.76006100
H	-3.97919500	-2.03442400	-1.17911700	C	4.95088300	-1.11302500	1.33498900
C	-5.29202000	-4.83754200	0.21938100	C	6.75434200	0.98120000	1.19838300
H	-5.10722500	-5.38008600	2.29853300	H	5.17010300	2.10024600	0.31014900
H	-5.29829200	-4.03079800	-1.78232700	C	6.26230000	-1.30365600	1.76870800
H	-5.87632800	-5.71598200	-0.04270800	H	4.26539300	-1.95994500	1.37523200
B	-1.59979000	1.36860900	1.61571600	C	7.17206300	-0.24646900	1.71229500
B	-2.99605000	-1.21996900	1.23320400	H	7.45692900	1.80772100	1.12453300
N	-1.59987300	-1.14189400	1.66117800	H	6.57320700	-2.27363200	2.14983600
N	0.48163700	-0.10209000	1.86064100	H	8.19497000	-0.38129800	2.05407000
N	-3.00731600	1.30327500	1.24577100	B	0.52894900	-1.92337900	0.26940900
N	-5.00002700	0.17215800	0.59147900	B	2.92519300	0.19322600	0.37038900
C	-3.66005200	0.10988000	0.99720800	N	2.70060800	-0.80148000	-0.85042400
C	-3.76459700	2.53386500	1.09381700	N	1.17140600	-1.96294800	-2.16723500
O	0.22715100	-0.55525100	-0.44890900	N	1.15816100	-1.31862800	1.65670100



N	2.47504300	0.21494900	2.83111800	H	-3.00823100	5.87841900	1.36895400
C	2.09971000	-0.37023900	1.66167900	H	0.31709800	6.39327100	-1.30987500
C	0.63408900	-1.82721700	2.87590100	H	-1.61017600	7.36409700	-0.06172600
O	1.31648700	-2.06335600	-4.44200100	C	-4.49317700	-0.11855600	0.82562300
O	4.61016000	-0.02953500	-1.91390300	C	-5.43980300	-1.15215100	0.76106500
O	2.20008800	0.71959800	5.03809200	C	-4.95132800	1.11479800	1.33216200
O	-0.20340900	-2.69848400	2.89620600	C	-6.75459000	-0.97983400	1.19901800
H	1.89316500	-2.07764300	4.55319700	H	-5.17020900	-2.10026800	0.31278400
H	3.82129000	-2.54176400	-3.01507100	C	-6.26276300	1.30602900	1.76547500
C	2.15725400	1.67590300	-0.01709500	H	-4.26589600	1.96183100	1.37090900
C	2.50181600	2.10656500	-1.44342500	C	-7.17244200	0.24864600	1.71081600
C	1.84347800	1.51253600	-2.53567900	H	-7.45707800	-1.80655900	1.12651300
C	3.48297000	3.06449600	-1.73450300	H	-6.57381100	2.27661700	2.14492800
C	2.13839000	1.85523400	-3.85572200	H	-8.19537200	0.38399000	2.05231300
H	1.08490100	0.76606900	-2.34246100	B	-0.52895500	1.92353500	0.26804700
C	3.79728400	3.40014600	-3.05317600	B	-2.92538500	-0.19278600	0.37016500
H	4.00807500	3.56880400	-0.93167700	N	-2.70052200	0.80083300	-0.85136900
C	3.12897400	2.80093300	-4.12163100	N	-1.17109400	1.96145500	-2.16867200
H	1.58107000	1.39005100	-4.66386200	N	-1.15827600	1.31970100	1.65575000
H	4.56547700	4.14528100	-3.24308900	N	-2.47626700	-0.21232400	2.83103000
H	3.36947300	3.07455800	-5.14494000	C	-2.10027200	0.37170500	1.66123200
C	2.48959500	2.78165600	0.99582300	C	-0.63427000	1.82884600	2.87469200
H	3.56639200	2.89944700	1.11911400	O	-1.31531900	2.05958900	-4.44360100
H	2.07579100	3.74636700	0.69796200	O	-4.60997000	0.02815200	-1.91453000
H	2.05783500	2.55971000	1.96570400	O	-2.20121400	-0.71613400	5.03820300
O	0.74757500	1.30559600	0.00353100	O	0.20369800	2.69969200	2.89476700
C	-3.31856000	1.57101200	-3.16994500	H	-1.89403900	2.08101900	4.55113600
C	-3.61871000	0.71222000	-1.95427500	H	-3.82088100	2.53881100	-3.01839100
C	-1.55514300	1.47577300	-0.96183300	C	-2.15723900	-1.67585800	-0.01582100
C	-1.86141800	1.86323200	-3.38028100	C	-2.50160000	-2.10770600	-1.44184800
H	-3.18840300	-0.93400100	2.76565600	C	-1.84306500	-1.51455300	-2.53445900
C	-1.97156400	0.02688900	4.10938500	C	-3.48268900	-3.06588100	-1.73229800
C	-1.19844100	1.31037800	4.18675900	C	-2.13770400	-1.85834400	-3.85427500
H	-3.75462500	1.09974300	-4.05049600	H	-1.08456300	-0.76790100	-2.34165200
H	-0.23761800	2.36097900	-2.22889100	C	-3.79672600	-3.40263900	-3.05076000
H	-0.39373900	1.24971000	4.92306800	H	-4.00795100	-3.56951900	-0.92915900
C	-0.75994800	3.53965700	0.25352800	C	-3.12821200	-2.80430300	-4.11957500
C	-1.85354100	4.11483200	0.92553000	H	-1.58026400	-1.39381500	-4.66270700
C	-0.00582800	4.40067400	-0.56452700	H	-4.56485400	-4.14795500	-3.24022300
C	-2.15910700	5.47250800	0.82419300	H	-3.36847900	-3.07881100	-5.14270300
H	-2.48531300	3.49026600	1.55398600	C	-2.48983800	-2.78074600	0.99799900
C	-0.29906800	5.76059400	-0.67567500	H	-3.56666100	-2.89935900	1.12021900
H	0.83796600	4.01066100	-1.12649100	H	-2.07482200	-3.74537200	0.70169400
C	-1.37814200	6.30564500	0.02223200	H	-2.05954000	-2.55713300	1.96813100

O -0.74767400 -1.30567500 0.00499800

**Rx1**

C -0.40198700 3.68582800 0.38447300

C -1.19688500 2.58641400 -0.27980200

C 0.75877100 1.17172400 -0.08692800

C 1.03575900 3.66616000 -0.10881300

H -2.54668200 -2.35682000 -0.15038800

C -1.08120300 -3.69126200 0.25735200

C 0.41529900 -3.72062400 0.53948800

H -0.87416900 4.64341700 0.17823500

H 2.52078100 2.16147100 -0.03299600

H 0.81592900 -4.70615800 0.31567700

C 3.01409200 -0.27106900 -0.04830300

C 3.66405000 -0.77152100 1.09171600

C 3.81978000 0.21947200 -1.09007900

C 5.05378600 -0.79465400 1.18476800

H 3.07430100 -1.15160000 1.92073200

C 5.21137100 0.19748600 -1.00513200

H 3.35188300 0.59733100 -1.99468900

C 5.83279200 -0.31000600 0.13473900

H 5.52970200 -1.19029900 2.07543600

H 5.80979300 0.56571200 -1.83151300

H 6.91466600 -0.33043800 0.20336000

C -3.05970500 0.17947000 -0.03609600

C -3.87929900 -0.31904100 -1.06210200

C -3.69601500 0.70426400 1.10099200

C -5.27011400 -0.28705100 -0.96366100

H -3.42294800 -0.72180900 -1.96164000

C -5.08421400 0.74158100 1.20647200

H -3.09561500 1.08807400 1.92108600

C -5.87719200 0.24505600 0.17203400

H -5.87831900 -0.67329100 -1.77443900

H -5.54876300 1.15263100 2.09639800

H -6.95821300 0.27079900 0.25230800

B 1.44716300 -0.19033000 -0.12310400

B -1.49380200 0.07445200 -0.12097600

N -0.60982900 1.26433600 -0.15876300

N 1.52100600 2.30511700 0.00545700

N 0.57735200 -1.34068300 -0.14831900

N -1.54324200 -2.44373400 -0.04260400

C -0.80902200 -1.24222200 -0.08471300

C 1.16069200 -2.67137800 -0.23967400

O 1.80079200 4.53686500 0.69820300

O -2.22257200 2.76816000 -0.87107700

O -1.78579500 -4.68264400 0.30644600

O 2.14264200 -2.88059600 -0.89530700

H 0.54748000 -3.51656500 1.60976100

H -0.38415900 3.51114600 1.46562400

H 2.53411700 4.89440200 0.18787800

H 1.08132000 4.00007600 -1.15734800

**Rx2**

C 0.26652000 -3.70520000 0.70542900

C 1.22298300 -2.66107300 0.14776000

C -0.76141500 -1.19335500 -0.05725400

C -1.13137100 -3.63840100 0.15542300

H 2.48456500 2.33446600 -0.21578300

C 1.03499100 3.68227100 0.21994200

C -0.44309000 3.70822500 0.57810900

H 0.67848100 -4.69947900 0.54350600

H -2.51411900 -2.22689600 -0.33609700

H -0.86039000 4.68966300 0.36851000

C -3.04482000 0.20910500 -0.10635800

C -3.74721700 0.62173500 1.03731400

C -3.79686500 -0.21337200 -1.21483200

C -5.13957700 0.62392100 1.07117000

H -3.19818600 0.94644800 1.91643100

C -5.19087200 -0.21304300 -1.18768800

H -3.28772200 -0.52456000 -2.12246400

C -5.86625300 0.20613800 -0.04320800

H -5.65835800 0.94862800 1.96655600

H -5.74822400 -0.53474100 -2.06054900

H -6.95015200 0.20664600 -0.01900100

C 3.01340100 -0.16210300 -0.10314600

C 3.60717800 -0.70585900 -1.25933300

C 3.87659900 0.38475000 0.86572100

C 4.99090800 -0.71608100 -1.43421300

H 2.97527000 -1.11747500 -2.04090800

C 5.26003500 0.38219700 0.69404200

H 3.45599400 0.80647000 1.77291100

C 5.82162500 -0.17082700 -0.45646000

H 5.41875100 -1.14042900 -2.33578400

H 5.89948500 0.80782800 1.45935600

H 6.89726200 -0.17474700 -0.59075800

B -1.47647000 0.14884900 -0.11327400

B 1.44084100 -0.09758700 0.04227400

N 0.58758400 -1.28589900 0.06371700

N	-1.52923400	-2.35281900	-0.13103200
N	-0.62516300	1.31976700	-0.07372300
N	1.48942300	2.42045400	-0.05005200
C	0.75459200	1.22453400	0.01298700
C	-1.21316300	2.64855000	-0.16624700
O	-1.87277500	-4.59281800	0.03078200
O	2.31888900	-2.68700100	1.01091200
O	1.73860700	4.67260000	0.18627400
O	-2.20982600	2.85374300	-0.79825000
H	-0.52313600	3.50511800	1.65374500
H	0.19927200	-3.54585000	1.78771700
H	3.05147800	-2.18392800	0.63229700
H	1.51530300	-2.90884400	-0.87975000